Consorzio Interuniversitario per lo Sviluppo dei Sistemi a Grande Interfase

Report 2025

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Summary

Research Projects

1A: Hard Matter (Nanomaterials and Solid Interfaces)

1B: Soft Matter (Nanomaterials and Liquid Interfaces)

1C: Theory and Modelling

2A: Art Restoration and Environmental Remediation

CSGI Research Activity

Outline

CSGI's mission is to promote and coordinate scientific activities in the field of large interface systems, in agreement with national and international research programs for the benefit of companies and private/public research institutions.

The CSGI (Center for Colloid and Surface Science) was established in Florence in December 1993. It was officially recognized by the Italian government in 1994 and is under the supervision and control of the Ministry of University and Scientific Research (MUR). CSGI began its scientific activity in 1995, dedicated to basic research and to the development of new high-tech processes. CSGI, also, contributes to the activities of small and medium-sized enterprises that cannot afford the financial burden of independent research activities.

The mission and strategic functions of CSGI have always been focused, since its foundation, on basic and applied scientific research, with particular attention to the dissemination of the results achieved and to the technology transfer, both nationally and internationally. In this context, among the activities of the CSGI, training plays a role of primary importance.

CSGI research is mainly centered on the field of chemistry and physical chemistry of dispersed systems with a high surface area such as hard and soft nanomaterials, colloids of various kinds, functionalized surfaces, and thin films. In these areas, CSGI organizes, coordinates, and implements specific actions aimed at promoting both basic and applied research, promoting the technology transfer of the results achieved to business and industry. The CSGI consortium gathers research units belonging to several Italian universities (http://www.csgiscience.eu) working in the field of physical chemistry of colloids, nanomaterials, and functionalized surfaces. The excellence of the CSGI network is validated by the assessment of the Italian research system (VQR2 relating to the period 2015-19 and earlier), which testifies that CSGI is among the best Italian consortia per scientific production level, always positioning in the very high ranking for scientific quality and for the third mission activities. Preliminary results of VQR3 (2020-2024) consolidated CSGI to the first position among all the Italian consortia in the field of chemistry. In particular, to achieve these results, the financial support that the Ministry of University and Research (MUR) provides annually represents a driving force of primary importance allowing for the attraction of further fundings, both from the industrial world and through the participation in competitive national and/or European tenders. In practice, this financial support has the fundamental function of "multiplier" for attracting funds on a competitive basis. In fact, the average budget available on an annual basis, for about 95%, refers to collaborations with organizations as industry and, above all, with international organizations and the European Union.

Scientific research

CSGI gathers the most important Italian research groups in the field of chemistry and physical chemistry of Soft Matter, nanomaterials, surfaces and thin films. CSGI's

laboratories represent a fundamental reference for both Italian and foreign scientists operating in the aforementioned research fields. CSGI has been and still is pioneer of the application of nanotechnologies in the field of conservation of the world's cultural and artistic heritage.

- CSGI's activity is focused on promoting technology transfer with numerous production companies, both Italian, European, and non-EU. Third mission activity of CSGI has had a significant development over the years through the involvement of numerous companies, with particular reference to multinationals active on the global market in strategic sectors such as: ENI, Procter & Gamble, Biomeuriex, Shiseido, IDI pharmaceutical companies, Dompé, Rottapharm, Ecocem and Solvay.

- CSGI supports conservation of cultural heritage through "Solutions for Conservation", products for the conservation of the world's artistic heritage. In particular, the Nanorestore formulations have obtained the Solar Impulse Efficient Solution Label from the SOLAR IMPULSE FOUNDATION in Lausanne as materials that respond 100% to the EU Green Deal. The certificate was obtained after a rigorous evaluation process, which identifies efficient and economically profitable solutions that respond to environmental challenges on a global level.

- CSGI coordinates the European Union CLUSTER ECHOES - Enabling Cultural Heritage-Oriented European Strategies. It is a European cluster created on the initiative of the European Commission, which involves the main stakeholders in the field of cultural heritage conservation (universities, research centres, small and medium-sized enterprises, museums, and restorers). With more than 350 members, ECHOES is an important platform available to the scientific community with the aim of sharing, on behalf of the EU, results obtained within the funded projects and proposing to the European Commission strategies and policies for the conservation and enhancement of cultural heritage. ECHOES also contributes to the definition of research guidelines regarding innovative materials applied to the conservation of objects of historical-artistic and architectural interest.

- CSGI has been selected by the European Commission to participate in the Common Exploitation Booster Support Services initiative to support the dissemination activities of the results obtained in the best projects funded by the European research program Horizon 2020. The services offered included meetings and collaborative workshops with external consultants with the aim of developing an effective entrepreneurial strategy for the exploitation of the results obtained within the Nanorestart project (Nanomaterials for the Restoration of Works of Art) coordinated by CSGI. At the end of the process, CSGI was selected to share its successful experience at the conference organized in May 2022 (Info Session on the Horizon Results Booster – NANORESTART best practices – online, 25 May 2022) in order to sponsor these services at European level.

- The Nanorestore products (Advanced solutions for the conservation of Cultural Heritage) developed within the H2020 Nanorestart project have been recognized by the European Commission as Key Exploitable Results ‑ and, therefore, published

in the Horizon Results Platform, the European platform that connects the main Europe-wide innovations with potential investors.

- CSGI has been recognized as a Key Innovator at European level by the European Commission's Innovation Radar Committee regarding 11 innovations generated within projects funded by the H2020 Program (Nanorestart, Apache, EvFoundry, Bow).

- CSGI is a member, together with the National Research Council, of BRCHGA – Belt and Road Cultural Heritage Alliance – an alliance sponsored by the People's Republic of China which supports scientific research and protection of cultural heritage of countries and regions located along the New Silk Road (Belt and Road).

Several start-ups have been generated by CSGI researchers: LifeCARES (Life Cycle Assessment, Renewable Energy and Sustainability), which was born as a spin-off of the University of Siena; a mixed CSGI-INSTM work team is active at the Florence operative units, called WeGoNANO (Working Group on carbon-based and Glycan-based NANOstructured materials), coordinated by CSGI, devoted to the development of biocompatible nanomaterials based on carbon and carbohydrates that can be functionalized on-demand according to the requests of public institutions and/or private companies.

Since February 2018, CSGI is a member of the National Energy Technology Cluster (CTNE) with the aim of developing strategic plans aimed at aligning and integrating national scenarios and actions with European (SET-Plan, Energy Union) and global (COP 21, Mission Innovation) ones in the energy sector. CSGI thus contributes to strengthening Italy's role in the future EU SET-Plan and contributes to the development of the Integrated National Plan for Energy and Climate (PNIEC).

CSGI obtained funding from the EU in different actions within the Marie Curie H2020 program. Many European projects are currently ongoing. As an example: GREENART, "GREen ENdeavor in Art ResToration" (HORIZON-CL2-2021-HERITAGE-01- 01, CSGI coordinator), IMPACTIVE, "Innovative Mechanochemical Processes to synthesize green ACTIVE pharmaceutical ingredients" (HORIZON-HLTH-2021-IND-07, CSGI partner), AURORA “Artwork Unique RecognitiOn and tRacking through chemicAl encoded data, miniaturized devices and blockchain alliance” (HORIZON-CL2-2022-HERITAGE-01, CSGI partner), OTTERS - Social Transformation for Water Stewardship through Scaling Up Citizen Science (Grant Agreement 101094041, Call Horizon-Miss-2021-Ocean-05, CSGI partner) and SURFTOGREEN “Bio-based sustainable SURFactants TO foster GREEN industry” (HORIZON-JU-CBE-2023-IA-05, CSGI coordinator).

Educational Activity, Dissemination and Technology Transfer

The training activity, dissemination and technological transfer are a significant part of both intellectual and economic resources of CSGI and take concrete form in: the provision of research grants, post-doc positions, research doctorates and research

grants; the organization of workshops, schools, conferences; the training finalized and aimed at the needs of production activities.

- During the period 2023-2025, CSGI members supervised over 415 bachelor/master theses, about 60 doctoral theses and 50 post docs (co-founded by CSGI).

- CSGI actively collaborates with the associated universities by making the research infrastructure available both for the training and for scientific research.

- CSGI actively promoted the constitution of the hybrid Italian multidisciplinary Research Infrastructure for Complex Materials and Interfaces ISIS@MACH ITALIA (IM@IT), hub of ISIS neutron and muon source (UK). IM@IT responds to the growing need of the Italian academia and production system, of SMEs. Unlike large corporations, SMEs usually have limited resources and skills to access and exploit the most advanced tools, which are nonetheless essential for understanding, developing and improving their "productive fabric".

Structure and Organization of CSGI

Management Offices
President, Council, Director, Audit Council, Technical-Scientific Board.

Director of CSGI
Prof. Emiliano Fratini, Department of Chemistry, University of Florence.

President of CSGI
Prof. Piero Baglioni, Department of Chemistry, University of Florence.

Audit
3 members: 1 member, the president, nominated by the MEF (Ministry of Economy and Finance); 2 members nominated by MUR (Ministry of University and Research).

Website
http://www.csgiscience.eu/

Foundation
December 21st, 1993

Official recognition by the Italian Government
November 15th, 1994 (G.U. Nr. 267)

Academic and Associated Members

Academic

- University of Florence (headquarters)
- Scuola Normale Superiore in Pisa
- University of Bari "Aldo Moro"
- University of Bergamo
- University of Catania
- University of Cagliari
- University of Molise (Campobasso)
- University of Naples "Federico II"
- University of Pavia
- University of Siena
- University of Perugia

Associated

- Brera Accademia di Belle Arti
- CGA Palermo
- CNR-ISMN Bologna
- Department of Sciences Malpighi, Messina
- Opificio delle Pietre Dure
- Polytechnic Institute of Milan
- STEBICEF Palermo
- University of Bologna
- University of Brescia
- University of Milan, Bicocca
- University of Palermo
- University of Rome, La Sapienza
- University of Rome, Tor Vergata
- University of Rome - TRE
- University of Venice

Personnel

CSGI gathers about 400 researchers including Full Professors, Associate Professors, University Researchers.
Moreover, CSGI employs 18 researchers and 5 administration employees on its own. Several PhD and post-doc students are financially supported through CSGI fellowships. CSGI hosts researchers hired by industrial companies for training and specific research activities, in the framework of various European projects.

CSGI Patents

1) Bottiroli Giovanni, Croce Anna Cleta, Baglioni Piero, Monici Monica – "Macroemulsioni acqua-in-olio a lunga stabilità, loro preparazione ed uso". Italian Patent PCT/EP96/03201, deposit date 19/07/1996.

2) Baglioni Piero, Dei Luigi, Ferroni Enzo, Giorgi Rodorico – "Sospensioni stabili di idrossido di calcio". Italian Patent FI/96/A000255, deposit date 31/10/1996.

3) Matteazzi Paolo, Baglioni Piero, Basset Diego – "Process for Recycling, by Milling, Solid Industrial Waste and Materials at the end of their Service Life". European Patent Application 97203735.2, Priority IT96 FI96A000280.

4) Grassi Giuliano, Chiaramonti David, Baglioni Piero – "Apparato a combustione di etanolo o miscele etanolo per cucine, stufe e illuminazione a uso domestico". Italian Patent FI/98/A42, deposit date 24/ 02/ 1998.

5) Ambrosone Luigi, Ceglie Andrea – "Software per l'analisi grafica e numerica di dati di Risonanza Magnetica Nucleare per la determinazione della polidispersità di emulsioni". Italian Patent FI99A000044, deposit date 09/03/1999.

6) Baglioni Piero, Carretti Emiliano, Dei Luigi – "Microemulsioni ed emulsioni di olio in acqua, loro uso per la solubilizzazione di resine polimeriche e impacchi contenenti detti microemulsioni o emulsioni". Italian Patent FI99A000071, deposit date 02/ 04/1999.

7) Baglioni Piero, Fratini Emiliano, Ricceri Riccardo, Sarti Giuseppe, Chiaramonti David – "Engine fuels consisting of an emulsion comprising mineral and/or natural oils, their preparation and use in internal combustion engine". PCT International Application WO n. 99936473.0 del 02/07/1999.

8) Baglioni Piero, Bardi Ugo, Bonini Massimo – New method for the production of solid powder and films by compartimentalised solution thermal spraying (CSTS). European Patent Application EP 00-105673.8, deposit date 17/03/2000.

9) Angelico Ruggero, Ceglie Andrea, Hochoeppler Alejandro, Palazzo Gerardo, Stefan Alessandra – "Macroemulsioni acqua-in olio a lunga stabilità, loro preparazione ed uso". Patent Query N. FI2001A000016, Italian Patent N. 0001328470, deposit date 29/01/2001.

10) Baglioni Piero, Dei Luigi, Fratoni Laura, Lo Nostro Pierandrea, Moroni Michelangelo – "Processo per la preparazione di nano e microparticelle di ossidi e idrossidi di metalli del secondo gruppo e di transizione, nano e microparticelle così ottenute e loro impiego in campo ceramico, tessile e cartario". Patent Query N. FI2002A000052, deposit date 28/03/2002 – EP 03745367.7.

11) Baglioni Piero, Dei Luigi, Giorgi Rodorigo, Claudio Vinicius Schettino – "Basic Suspensions their Preparation and Use in Processes for Paper Deacidification". European Patent Application EP 02714088.8, deposit date 15/01/2002.

12) Ambrosone Luigi, Ceglie Andrea – “Materiale assorbente e suoi usi nei processi di bonifica di falde acquifere inquinate da prodotti chimici”. Patent Query FI2003A000236, deposit date 11/09/2003.

13) Ambrosone Luigi, Ceglie Andrea – “Gel stabili contenenti gelatina”. Patent Query N. FI2003A000237, deposit date 11/09/2003.

14) Baglioni Piero, Dei Luigi, Fratoni Laura, Lo Nostro Pierandrea, Moroni Michelangelo – “Preparation of nano and micro-particles of group II and transition metals oxides and hydroxides and their use in the ceramic, textile and paper industries”. PCT Int. Appl. (2003), 10 pp. CODEN: PIXXD2 WO 2003082742 A2 20031009 CAN 139:278604 AN 2003:796605.

15) Fratoni Laura, Lo Nostro Pierandrea – “Composizione detergente a base di un estere dell’acido L-ascorbico”. Patent Query N. TO2003A001032, deposit date 22/12/2003.

16) Baglioni Piero, Dei Luigi, Giorgi Rodorico, Ninham Barry W. – “Process for preparing nano- and micro-sized particles of inorganic compounds”. European Patent Application EP 04101822.7, deposit date 29/04/2004.

17) Ambrosi Moira, Baglioni Piero, Bonini Massimo, Fratini Emiliano – “Nanoparticelle monodisperse di ossidi ed idrossidi metallici e loro applicazione nei settori tessile, cartario e ceramico”. Patent Query FI 2006A000313 – RIF. 7845 PTIT, deposit date 11/12/2006.

18) Baglioni Piero, Ambrosi Moira, Dei Luigi, Faneschi Mauro, Mancioli Luciano, Santoni Sergio – “Ceramic products comprising nanoparticles of zirconium hydroxide and/or glass frits”. Patent Query 7303 PTEP/2006 EP06112439.2, deposit date 10/04/2006.

19) Ceglie Andrea, Venditti Francesco, Lopez Francesco, Palazzo Gerardo, Colafemmina Giuseppe, Angelico Ruggero, Ambrosone Luigi – “Materiale adsorbente contenente tensioattivo cationico, sua preparazione ed uso per la rimozione di metalli da soluzioni acquose”. Patent Query N. FI 2006 A000113 – RIF. 7490 PTIT, Italian Patent N. 0001368154/2009, deposit date 10/05/2006.

20) Ballistreri Alberto, Cambria Maria Grazia, Carnemolla Giovanni Marco, Guglielmino Salvatore Pietro Paolo, Impallomeni Giuseppe, Nicolo Marco Sebastiano – “Production of biodegradable plastics from Brassica carinata oil with high content of erucic acid and from very long chain fatty acids”. Italian Patent IT 1392236, deposit date 13/10/2008.

21) Ballistreri Alberto, Cambria Maria Grazia, Carnemolla Giovanni Marco, Guglielmino Salvatore Pietro Paolo, Impallomeni Giuseppe, Nicolo Marco Sebastiano – “Production of biodegradable plastics from Brassica carinata oil with high content of erucic acid and from very long chain fatty acids”. World Organization Patent WO 2010044118 Priority IT 2008-RM545.

22) Hochkoeppler Alejandro, Baglioni Piero, Stefan Alessandra – “Espressione batterica di un gene artificiale per la produzione di CRM 197 e derivati”. Patent Query FI 2009A000137 – RIF. 9741 PTIT, deposit date 25/06/2009.

23) Primiceri Giuseppe, Roda Elena, Stefan Alessandra, Panizza Lucio, Hochkoeppler Alejandro – “Enzyme composition for reducing the release of pharmaceutical active ingredients into the environment”. WO/2009/138455A1.

24) Hochkoeppler Alejandro, Roda Elena, Panizza Lucio, Stefan Alessandra – “Method for preventing and controlling biofouling on marine objects”. WO/2010/145905A.

25) Panizza Lucio, Roda Elena, Stefan Alessandra, Hochkoeppler Alejandro – “Method for preventing and controlling organisms that infest aqueous systems.” WO/2010/145988A1.

26) Smets Johan, Pintens An, Keijzer Olav Pieter Dora Tony, Bodet Jean-Francois, Lebron Ariel, Fratini Emiliano, Vannucci Chiara, Ambrosi Moira, Baglioni Piero, Guinebretiere Sandra Jaqueline, Yan Nianxi, Liu Hongwei – “Encapsulates”. Attorney’s Docket No. 11547P, 21/04/2010.

27) Fernandez Prieto Susana, Smets Johan, Aouad Yousef Georges, Wevers Jean, Baglioni Piero, Ambrosi Moira, Vannucci Chiara – “Particles”. Attorney’s Docket No. 11812P2, 15/04/2011.

28) Angelico Ruggero, Lampis Sandrina, Monduzzi Maura, Ceglie Andrea – “Metodo innovativo per la "plastificazione" di grassi vegetali”. Italian Patent FI2012A000186, deposit date 19/09/2012.

29) Paduano Luigi, D’Errico Gerardino, Montesarchio Daniela, Vitiello Giuseppe, Mangiapia Gaetano, Luchini Alessandra, Irace Carlo, Colonna Alfredo, Santamaria Rita – “Nanoparticelle ibride magnetite-oro funzionalizzate con struttura nucleo-guscio”. Italian patent, deposit date 19/10/2012.

30) Rossi Ranieri, Giustarini Daniela – “Metodo per la misura del glutatione su sangue prelevato tramite digitopuntura” Italian Patent N. 0001420029, deposit date 18/06/2013.

31) Baglioni Piero, Del Buffa Stefano, Ridi Francesca, Bonini Massimo – “Materiale per la rigenerazione dei tessuti ossei contenente minerali argillosi aventi morfologia nanotubolare e stronzio”. Italian Patent FI2013A000240, deposit date 15/10/2013.

32) Bettini Ruggero, Hochkoeppler Alejandro, Melegari Cecilia, Primiceri Giuseppe, Stefan Alessandra – “Composizioni farmaceutiche con ridotto impatto ambientale.” Italian patent IT 0001415653, deposit date 12/05/2015.

33) Rosace Giuseppe, Colleoni Claudio – “Prodotto antibatterico stabile ai cicli di manutenzione”. Italian Patent 102017000138046, deposit date 30/ 11/ 2017.

34) Torsi, Luisa; Palazzo, Gerardo; Cioffi, Nicola; Angione, Maria Daniela; Magliulo, Maria; Cotrone, Serafina; Scamarcio, Gaetano; Sabbatini, Luigia; Mallardi, Antonia "Organic field-effect transistor sensor" International Application PCT/IT2011/000364, US9575029(B2) (WO2013065073-A1; WO2013065073-A8), deposit date 10/10/2011. Published on 21/02/2017.

35) Torsi Luisa, Scamarcio Gaetano, Macchia Eleonora, Manoli Kyriaki, Palazzo Gerardo, Cioffi Nicola, Picca Rosaria Anna – "A field effect transistor sensor and a corresponding array device" PCT International Application PCT/IB2018/050491, deposit date 26/01/2018. Application status: pending.

36) Aouad Yousef Georges, Smets Johan, Zannoni Luke Andrew, Baglioni Piero, Tempesti Paolo, Bartolini Arianna – "Benefit agent containing delivery particle". Patent N. US10538631B2, publication date 21/01/2020.

37) Aouad Yousef Georges, Smets Johan, Zannoni Luke Andrew, Baglioni Piero, Tempesti Paolo, Bartolini Arianna – "Process for making a composition comprising benefit agent delivery particles". Patent N. US10556995B2, publication date 02/11/2020.

38) Hulskotter Frank, Smets Johan, Tahon M. Cedric, Fernandez Prieto Susana, Bodet Jean-Francois, Mamusa Marianna, Baglioni Piero – "Liquid compositions that include delivery particles". European Patent Office S. N. 19175821.8.

39) Fratini Emiliano, Baglioni Piero, Ferraro Giovanni (Notari M., Rausa R., G. Assanelli) – "Method for the assessment of the dispersing capacity of new or used lubricating compositionsand of additives for lubricating compositions". Application n. 17/917,758 dated 07/10/2022.

40) Zeppa Lucio, Costagliola Lucio, Luigi Ambrosone – "Capsula lenticolare artificiale per contenere il cristallino artificiale o l'iride". Italian Patent N. 102022000021123 date 13/10/2022.

41) Zuliani Alessio, Guaragnone Teresa, Baglioni Piero, Rizzarelli Paola, Rapisarda Marco, Brilli Federico, Baccelli Ivan – "Castor oil-based material for the release of biogenic volatile organic compounds for agricultural applications" - N. P.O. 22962IT-01 del 10.8.23 - PCT/EP2024/072425.

42) Anselmi Cecilia, Centini Marisanna, Costa Jessica, Pogni Rebecca, Sega Alessandro, Signori Giulia – "Cosmetic compositions with enhanced sun protection factor and preparation thereof" - European Patent Application 23425009.0, No. EP4431081A1, deposit date 13.03.2023.

43) Dallinger Alexander, Greco Francesco, Giorgi Rodorico, Camerini Rachel – "Method of scribing laser-induced graphene", EP24170488, 16 April 2024.

44) Baglioni Piero, Zuliani Alessio, Chelazzi David, Giorgi Rodorico – "VOC adsorbing component made of castor oil-based organic-inorganic composite material",

Brevetto Europeo, n. 22725467.9; Data di deposito: 26.4.2022 EP4330323, 6 March 2024.

45) Conti Luca, Giacomazzo Gina Elena, Giorgi Claudia, Valtancoli Barbara, Diddi Alessia, Casula Luca, Murgia Sergio, Schlich Michele, Sinico Chiara – "A ruthenium (ii) polypyridyl complex as a photo-sensitiser in photodynamic therapy, and a procedure for making said ruthenium (ii) polypyridyl complex", PCT number: WO 2024/105603 A1.

46) Galiotis Costas, Baglioni Piero, Anagnostopoulos George, Pastore Carbone Maria Giovanna, Poggi Giovanna, Papadimitriou Konstantinia, Paterakis George, Kotsidi Maria, Gorgolis George - "Art Protection with the Use of Graphene Materials". Brevetto internazionale (US) depositato presso il United States Patent and Trademark Office (USPTO) il 18/12/19 (US 20220081301 A1) e concesso in data 04/06/2024 (US 11,999,623 B2)

47) Galiotis Costas, Baglioni Piero, Anagnostopoulos George, Pastore Carbone Maria Giovanna, Poggi Giovanna, Papadimitriou Konstantinia, Paterakis George, Kotsidi Maria, Gorgolis George - "Art Protection with the Use of Graphene Materials". Brevetto internazionale (EU) depositato presso la European Property Organisation (EPO) il 18/12/19 (PCT/EP2019/085993 - WO 2020/141078 A1) e concesso in data 02/04/2025 (EP3906160).

CSGI Registered Trade Marks

1) Nanorestore® International Class 01,37,40 FI2008C00067527508 RIF. 19558

2) Nanorestore Paper® International Class 01, 16, 40 FI2011C0009935263 RIF. 27175

3) Nanorestore Gel® International Class 01, 03, 37 Registration n. 12696308 del 12/08/2014 RIF. 30346

4) Nanorestore Cleaning® International Class 01, 03, 37 Registration n. 013603006 del 07/05/2015 RIF. 30836

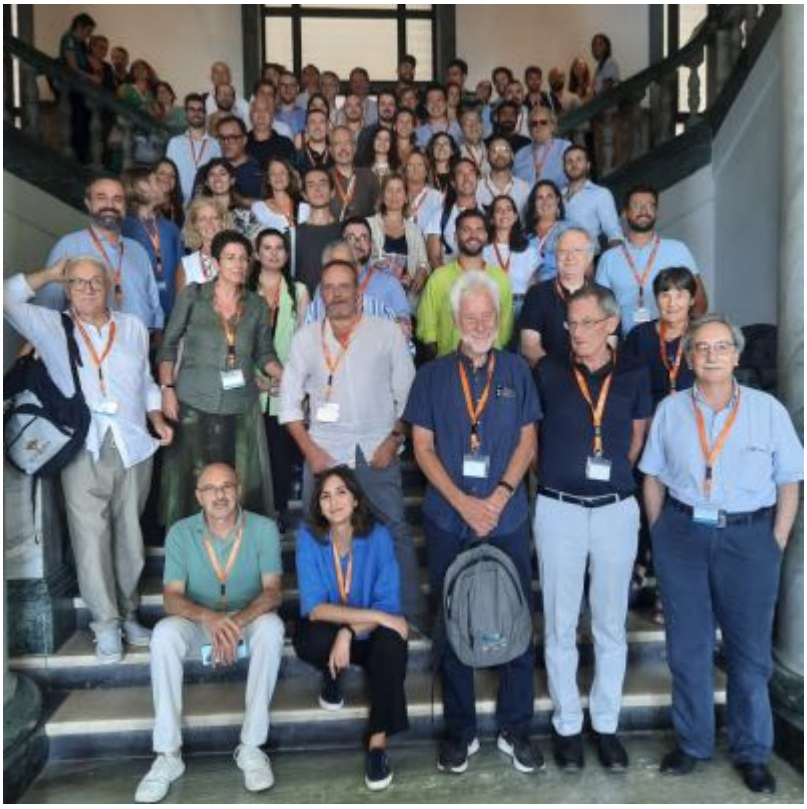
5) Nanorestore Plus® International Class 01, 37, 40 Registration n. 014414262 del 30/11/2015 RIF. 30836

6) Nanorestore Graffiti® International Class 1, 3, 37 Registration n. 018474575 del 19/05/2021 RIF. T021622EM-01

7) Nanorestore® VOCs Adsorber® class 1, 40 - Registration N. 018637349 del 11.01.22 - Registration N. UK00003742478 del 12.1.22 NS. RIF. T021773EM

Prospective CSGI Activity

CSGI is involved in several European projects (H2020), in several international and national projects, and in collaborations with industries and SME (small and medium enterprises).
CSGI is developing its own research activity to optimize the application of research projects inspired by the urging demands of small and medium size companies.
CSGI is actively working to offer a valid support to the Italian industrial system to set and develop projects and pre-industrial processes.



List of Publications

In the 2023-2025 period, CSGI researchers published more than 2650 articles in international scientific Journals indexed on WOS/Scopus databases.

The updated list of all the publications of CSGI members can be accessed using the QR code or link reported below:

The complete list of publications is on CSGI website: https://www.csgiscience.eu/publications.php

Theses (undergraduate, master and PhD)

U.O. Bari

Bachelor in Chemistry (Laurea triennale)

- Calia, D.: "Sintesi, caratterizzazione e impiego di un catalizzatore a base di calcio supportato su chitosano" (2023).
- Carella, G.: "Sviluppo di film antifungini per imballaggi alimentari" (2023).
- Cucci, E.: "Sviluppo e caratterizzazione analitica di nanomateriali per il food packaging" (2023).
- Pugliese, A.: "Preparazione di materiali nanocompositi per l'industria alimentare" (2023).
- Faranda, A.: "Elettrosintesi di nanoantimicrobici a base di ZnO e benzalconio cloruro: ottimizzazione e caratterizzazione analitica" (2024).
- Gatti, D.: "Sviluppo di LIBS Applicati a Sistemi Immunologici" (2024).
- Giannini, M.: "Development of LIBS for Application in Immunological Systems" (2024).
- Mazzilli, M.: "Nanoparticelle metalliche per applicazione in imballaggi attivi" (2024).
- Piccolo, A.: "Sintesi e caratterizzazione analitica di nanostrutture di ZnO per applicazioni fotocatalitiche" (2024).
- Roscini, G.: "Sviluppo di Polimeri a Stampo Molecolare per la Determinazione Ultrasensibile di Idrocarburi Policiclici Aromatici" (2024).
- Stucchi, C.: "Sintesi e caratterizzazione chimico-analitica di materiali antimicrobici a base di fosfato di argento" (2024).
- Basile, C.: "Polimeri a Stampo Molecolare Self-Signalling per la Determinazione Multiplexing di Idrocarburi Policiclici Aromatici" (2025).
- Di Clemente, A.: "Formulazione e Caratterizzazione di Surfattanti Bio-based" (2025).
- Fedele, G.: "Preparazione e caratterizzazione analitica di carbonati di zinco e rame" (2025).
- Pellegrini, C.D.: "Sviluppo e Caratterizzazione di Soft-Electrodes a base di Polidopamina e Alginato per Biosensori Edibili" (2025).
- Petrosillo, A.: "Spettroscopia LIBS intensificata per l'analisi elementare di fluidi biologici" (2025).
- Piccirillo, D.: "Nanovettori per il rilascio di polifenoli" (2025).
- Rescina, V.: "Laser Induced Plasma for elemental analysis and nanotechnological process." (2025).
- Sansaro, L.: "Influence of nanoparticle dimensions on Laser Induced Breakdown Spectroscopy (LIBS) signal during Lateral Flow Strip (LFS) ablation." (2025).
- Sgobio, D.: "Sviluppo di Polimeri a Stampo Molecolare per la Determinazione Ultrasensibile di Benzo(a)pirene" (2025).

Bachelor in Materials Science (Laurea triennale)

- D'Agostino, D.: "Sviluppo di antimicrobici non convenzionali per imballaggio alimentare" (2023).

- Quarato, D.: “Sviluppo di ossidi metallici misti Zn, Ca” (2023).
- Gentile, Loredana: “Effetto dei solventi sulle proprietà chimico-fisiche di sistemi polimerici a base cellulosa” (2024).
- Giovinazzo, L.: “Soft-Electrode per Applicazioni Biomedicali” (2025).

Master in Chemistry (Laurea magistrale)
- Calabrese, M.: “Mechanistic understanding of monoethanolamine (MEA) key role in degreasing” (2024).
- Chincoli, M.C.: “Struttura e Comportamento di Fase dell'autoassemblaggio di Fmoc-Difenilalanina” (2024).
- Giannone, S.: “Mechanistic Insights into Detergent-Phospholipid Vesicle Interactions: A Model for Virucidal Activity of Surfactants.” (2025).

Master in Industrial Chemistry (Laurea magistrale)
- Muggeo, A.: “Fosfato di zinco: sintesi elettrochimica, caratterizzazione analitica e applicazione in rivestimenti polimerici” (2024).
- Speranza, S.: “Formulazione di uno sgrassatore commerciale e studio del sistema solvente” (2024).
- Amoia, M.: “Preparazione e caratterizzazione analitica di compositi per il food packaging” (2025).

Master in Materials Science and Technology (Laurea magistrale)
- Brattelli, A.: “Formulazione e caratterizzazione di materiali biodegradabili: da soluzioni colloidali a pellicole di biopolimeri in solventi innovativi” (2024).

Master in Pharmaceutical Chemistry and Technology
- Luisi, R.: “Sviluppo di dispositivi bio-elettronici per la rilevazione precoce di HPV” (2024).

Master in Pharmacy (Laurea magistrale)
- D’Ingeo, S.: “Sviluppo e Caratterizzazione di una Cella Enzimatica a Biocombustibile per Biosensori Autoalimentati Realizzata Mediante Stampa Serigrafica” (2023).
- Boccuzzi, A.: “Quantificazione ultrasensibile di biomarkers infiammatori per lo studio del morbo di Alzheimer in modelli murini” (2024).
- Schirone, E.: “Shared neoantigens in cancer: analytical strategies in mass spectrometry” (2025).

PhD in Chemical and Molecular Sciences
- Hossain, S.I.: “Silver and silver chloride-based nanoantimicrobials: preparation, analytical characterization, and evaluation of their bioactivity” (2023).
- Kukushkina E.: “Development of multicomponent antimicrobial nanomaterials providing synergistic bioactivity, fighting antimicrobial resistance” (2023).
- Schirone D.: “Rationalizing the performances of green surfactants” (2023).
- Scandurra, C.: “Metodi analitici ultrasensibili per la rilevazione di biomarcatori clinicamente rilevanti” (2025).
- Veronico, L.: “Towards Biosurfactants: From Physicochemical Properties to Industrial Applications” (2025).

PhD in Engineering and Aerospace Sciences (interuniversity program UNIBA-POLIBA)

- Brattelli, A.: "Innovative and tunable Cellulose-based Materials for Environmentally friendly Aerospace Components" (ongoing).
- De Cataldo, A.: "Storage and transportation of green fuels via viscoelastic materials (GreenGelFuels)" (ongoing).
- Kanok, K.k.: "Sustainable Electrospun Cellulose-Based Hybrid Mats for Enhanced Interlaminar Toughness and Durability" (ongoing).
- Nettis, F.C.: "Production of bio-based materials for aerospace industries using bio-solvents" (ongoing).

PhD in Pharmaceutical Sciences

- Caputo, M.: "Advancing Single-Molecule Point-of-Care Diagnostics: Optimization and Clinical Translation of SiMoT Biosensors" (2025).
- Catacchio, M.: "A binary sensor with single molecule digit to discriminate biofluids enclosing zero or at least one biomarker" (ongoing).
- Mongelli, V.: "Research action for reducing the impact on agricultural and natural ecosystems of the harmful plant pathogen Xylella Fastidiosa" (ongoing).

PhD in Sustainable Technologies for the Industrial Development of Medicines and Diagnostics (TeSSMeD)

- Cimino, A.: "Studio e sviluppo di tecnologie environmentalfriendly per il miglioramento di processi di estrazione e purificazione di intermedi e principi attivi farmaceutici di interesse industriale" (ongoing).

Post-doc

- Izzi, M.: "Sviluppo di nanoantimicrobici sinergici e loro caratterizzazione chimico-analitica" (ongoing).
- Karmakar, A.: "Progettazione e caratterizzazione di nano-vettori come carrier per polimeri antiossidanti" (ongoing).
- Milica Vinic: PRIN2022-PNRR: Enhanced Laser Spectroscopy Techniques for autism diagnosis" (ongoing).
- Veronico, L: "Structures and Properties of bio-based materials resilient to morphological changes" (ongoing).

U.O. Bergamo

Bachelor in Engineering for Technologies of Health (Laurea triennale)

- Arrigoni, V.: "Problematiche relative ai biomateriali che comportano la revisione dell'artroplastica totale di ginocchio" (2023).
- Belotti, P.: "Studio dei materiali e ruolo delle membrane nelle procedure emodialitiche" (2023).
- Biraghi, A.: "Valutazione della velocità di corrosione di leghe di magnesio per dispositivi biomedici a riassorbimento graduale" (2023).
- Bonfanti, G.: "Biomateriali e metodi utilizzati dall'ingegneria tessutale per la realizzazione di innesti vascolari sintetici e biologici di grosso, medio e piccolo calibro" (2023).

- Bonometti, C.: “Distribuzione dei gas medicali in ospedale: un tassello fondamentale per la vita” (2023).
- Bresciani, M.: “Confronto tra stent coronarici riassorbibili e permanenti” (2023).
- Bruschi, D.: “Produzione additiva e tecniche di lavorazione nel settore odontoiatrico” (2023).
- Casoni, D.: “Trattamenti superficiali per l’osteointegrazione della protesi d’anca in titanio” (2023).
- Facheris, D.: “Protesi valvolari meccaniche analisi delle evoluzioni tecnologiche e sull’evoluzione dei materiali di realizzazione” (2023).
- Gattillo, P.: “Analisi dei problemi legati ai materiali delle protesi d’anca e le implicazioni sulla necessità di revisione” (2023).
- Locatelli, V.: “Leghe di magnesio per dispositivi medicali bioriassorbibili” (2023).
- Ammar, N.: “Nanomateriali utilizzati per la somministrazione di farmaci: caratteristiche e applicazioni” (2024).
- Bonfanti, G.: “Biomateriali e metodi utilizzati dall’ingegneria tissutale per la realizzazione di innesti vascolari sintetici e biologici di grosso, medio e piccolo calibro” (2024).
- Filali, Y.: “Biomateriali per la prevenzione delle complicanze nelle valvole cardiache artificiali” (2024).
- Furlan, D.: “I Biovetri, stato dell’arte e prospettive” (2024).
- Mauri, O.: “Studio della velocità di corrosione di leghe di magnesio rivestite mediante Plasma Electrolytic Oxidation per dispositivi biomedici a riassorbimento graduale” (2024).
- Scauzillo, L.: “Biomateriali per la realizzazione di protesi vascolari, Corso di laurea in Ingegneria delle Tecnologie per la Salute” (2024).
- Zamudio Olimpo, A.: “Utilizzo del nanomateriale ossido di ferro Fe3O4 per migliorare la prestazione della risonanza magnetica” (2024).
- Bani, E.: “Studio delle Interazioni Biochimiche dei Farmaci Chemioterapici Taxani e Antracicline nelle Cellule del Cancro al Seno” (2025).

Master in Engineering and Management for Health (Laurea magistrale)

- Vitali, E.: “Corrosion assessment and ion release of additive manufactured Ti6Al4V for biomedical applications” (2023).
- Fragasso, M.: “Development of Degradable Electroformed Fe-Based Alloys for Antibacterial Applications” (2024).
- Roncalli, C.: “Evaluation of ion release of different additively manufactured Ti6Al4V in simulated body fluid” (2024).
- Beatrice, F.: “Development and characterization of advanced methodologies for dispersion of brake particle emissions for toxicological assessment” (2025).
- Salvato, L.: “Electrochemical and corrosion behavior of additively manufactured Ti6Al4V alloy in simulated body fluids” (2025).

Master in Mechanical Engineering (Laurea magistrale)

- Pelucchi, M.: “Studio del comportamento di acciai inossidabili in ambiente geotermico” (2023).
- Randon, M.: “Studio del comportamento a corrosione- erosione di leghe inossidabili” (2023).

- Ferrari, S.: “Effetto delle condizioni ambientali e di sollecitazione sulla suscettibilità a Stress Corrosion Cracking di una lega di alluminio ad alta resistenza meccanica” (2024).
- Fiorona, D.: “Caratterizzazione a corrosione di una lega inossidabile AISI 316L ottenuta con tre diverse tecnologie di additive manufacturing” (2024).
- Pea, L.: “Effetto dell'ossidazione anodica sulle cinetiche di passivazione di leghe di titanio ottenute con tecnologie additive” (2025).

Master in Mechatronics and Smart Technology Engineering (Laurea magistrale)
- Locatelli, M.: "Intergranular corrosion and stress corrosion cracking susceptibility of high-strength aluminium alloys" (2023).
- Damini, C.: “Intergranular corrosion of additively manufactured 316L stainless steel: testing and qualification” (2024).

PhD in Engineering and Applied Science
- Carugo, F.: “Development and investigation of innovative materials produced by means of additive manufacturing technologies” (2023).
- Ahmad, H.: “Study of green fluids and lubricants for industry and electrochemical synthesis of hydrocarbons from renewable sources” (2025).

Post-doc (Assegno di ricerca CHIM/07)
- Grosso, S.: “COMIC – Complessi OrganoMetallici Intrinsecamente Chirali” (2024).

U.O. Bologna

Master in Industrial Chemistry (Laurea magistrale)
- Tazzari, A.: “Produzione di bevande vegetali a base di avena: vantaggi nell'uso di α-amilasi termosensibili” (2024).

Master in Chemistry (Laurea magistrale)
- Marangoni, M.: “Design e sintesi di peptidomimetici in fase solida inibitori dell’enzima lattato deidrogenasi come potenziali composti ad attività antitumorale” (2025).

U.O. Cagliari

Bachelor in Chemistry (Laurea triennale)
- Meloni, G.: “Estrazione e purificazione di proteine con proprietà antimicrobiche (Istatina 5 e 6) e loro adsorbimento su nanoparticelle di silice mesoporosa” (2023).
- Raga, C.: “Effetto dose-dipendente dell'ibuprofene sul profilo metabolomico NMR del granchio blu” (2024).
- Loi, A.: “Modelling Molecular Polarizability with Damped Oscillator Representations: A Computational and Theoretical Study.” (2025).
- Palmas, C.: “Caratterizzazione del profilo molecolare del muscolo di sogliola (Solea senegalensis) mediante spettroscopia NMR e approccio metabolomico: influenza dei sistemi di acquacoltura a ricircolo” (2025).

Master in Chemical Sciences (Laurea magistrale)

- Masala, C.: "Weak electrolytes effects on Vancomycin adsorption and release from radial silica nanoparticles" (2023).
- Tozzi, M.: "Toll like receptor 2 (TRL2) and enzymes decorated mesoporous silica nanoparticles (MSN) against Gram-positive bacteria" (2023).
- Caddeo, E.: "Buffer effects on protein corona formation on functionalized silica nanoparticles" (2024).
- Congiu, R.: "L'importanza del pre-processing degli spettri 1H NMR di campioni di plasma e urina per analisi metabolomiche" (2024).
- Ballicu, A.: "Protein corona formation on mesoporous silica nanoparticles (MSNs) studied by BSA adsorption" (2025).
- Cherchi, F.: "Interactions between porphyrins and duplex or G-quadruplex DNA in phosphate buffer" (2025).
- Meloni, G.: "Interactions between BSA at the isoelectric point and mesoporous silica nanoparticles" (2025).

PhD in Chemical Science and Technology

- Mura, M.: "Modulation of the interactions at the biointerface: Specific buffer effects" (2025).

Doctor of Philosophy (Murdoch University, Australia)

- Dagmawi B. Tadesse: "Ion Specific Effects in Equilibrium Modelling of Electrolytes" (2023).
- Nowosielska, A.M.: "Saltwater and Sulfide Mineral Flotation: Theoretical and Experimental Perspective" (2023).

U.O. Campobasso

Bachelor in Agricultural Sciences and Technologies (Laurea triennale)

- Calzone, L. "Indagine sulla birra artigianale con particolare attenzione alla regione Puglia" (2023).
- Pascale, F. "Studio sulla filiera del ciliegio (Prunus avium L.) con particolare attenzione alla regione Campania" (2023).
- Faienza, E. "Studio sui prodotti enologici del vitigno nero di Troia (2023).
- Cocchiarella, G. "Uso dell'ozono nei trattamenti post raccolta della frutta", (2024).
- Di Gregorio, G. "Indagine sulla sostenibilità del settore enologico" (2024).
- Zotti, A. "Evoluzione e innovazioni del packaging nel settore enologico" (2024).
- Mastrantuono, V. "Proprietà nutrizionali e funzionali del latte di capra e prodotti derivati" (2025).

Bachelor in Biological Sciences (Laurea triennale)

- Calvano, C. "Differenziamento delle cellule della linea cellulare PC12 in neuroni per mezzo di acido valproico incapsulato in Nano carriers di liposoma-chitosano stabilizzati core-shell" (2025).

Bachelor in Food Sciences and Technology (Laurea triennale)

- Boccalone, F.M., “Le frodi dell'olio di oliva” (2023).

Bachelor in Medical Engineering (Laurea triennale)

- Mangano, A.: “Caratterizzazione chimico fisica di biomateriali polimerici per 3D bioprinting” (2024).
- Musto, M.A.: “Caratterizzazione meccano-chimica di biopolimeri riassorbibili” (2024).
- Niro, T. “Biostampaggio e caratterizzazione del sacco capsulare del cristallino” (2024).
- Primavera, M. “Fabbricazione di patch biomedicali e prove di rilascio” (2024)
- Mercurio, C. “Analisi ottica e caratteristiche chimico-fisiche di cocktail chimico per la rigenerazione cardiaca” (2025).

Master in Food Sciences and Technology (Laurea Magistrale)

- Turilli, M.: “Miglioramento della shelf-life di banane tramite applicazione di edible coatings a base di emulsioni di alginato” (2024).

Master in Medical Engineering (Laurea magistrale)

- De Nigris, A. “Costruzione mediante bioprinting di medical device e sviluppo di modelli matematici per la previsione delle cinetiche di rilascio” (2023).

Master in Pharmacy (Laurea magistrale)

- Bortolusso, D. "Sistemi ad idrogel nel contesto dell'infarto del miocardio" (2023).
- Skorup, A. "Fibrosi epatica: cause, trattamenti con approcci convenzionali e metodologie innovative" (2024).
- Zinutti, A. "Lesioni da pressione (LdP): trattamenti convenzionali e nuove prospettive basate su stampa 3D nella rigenerazione tissutale" (2024).

PhD in Agriculture, Technology and Biotechnology

- Iacovino, S.: “Evaluation of pasting and rheological properties of flours with different extraction rate and their impact on the production of fresh-pasta” (2023).
- Iftikar, A.: “Sustainable recovery of bioactive compounds from olive oil industry by products and potential application in the food sector” (2025).

PhD in Biology and Applied Sciences

- Minò, A.: “Physicochemical analysis of nanosystems for biomedical applications” (2024).

Post-doc

- Iacovino S.: “Valutazione della shelf life di prodotti di IV gamma a seguito dell’applicazione di coating polimerici” (2023-2024).
- Cofelice, M.: “Sviluppo di nuovi sistemi per aumentare la shelf life dei prodotti alimentari di IV gamma” (2023-2025).

U.O. Catania

Bachelor in Chemistry (Laurea triennale)

- Arriva, D.: "Processi di adsorbimento di molecole biologiche su film polimerici elettroattivi" (2023).
- Attinasi, G.: "Studio del comportamento di tensioattivi fotosensibili all'interfaccia acqua/aria" (2023).
- Casabene, V.: "Studio dei processi di desorbimento di monostrati di Langmuir fotosensibili" (2023).
- Frazzetta, S.: "Stabilità di monostrati di Langmuir parzialmente solubili" (2023)
- Ganci, G.: "Processi di adsorbimento di nanocolloidi decorati da proteine alle interfacce liquide" (2023).
- Lancia, D.: "Polimeri conduttori per biointerfacce intelligenti" (2023).
- Licata, D.: "Studio delle proprietà interfacciali di nanocompositi proteina-nanoparticelle" (2023).
- Liruzzo, G.: "Processi di adsorbimento di proteine su film sottili di PPy-co-PCL" (2023).
- Albergo, S.: "Superfici intelligenti di film compositi PANI/CuHCF" (2024).
- Coco, A.: "Stabilità dinamica di nano-colloidi all'interfaccia acqua-aria" (2024).
- Di Prima, F.: "Film sottili ibridi di PEDOT:PSS/HNTS per applicazioni biologiche" (2024).
- Distefano, A.: "Preparazione e caratterizzazione di film sottili di poli-dopamina" (2024).
- Fuccio, D.: "Studio di monostrati di Gibbs di nanoparticelle decorate da albumina da siero bovino" (2024).
- Gibilisco, E.: "Studio e caratterizzazione di film nanostrutturati di politiofene" (2024).
- Calì, S.: "Preparazione e caratterizzazione di film nanocompositi di PEDOT:PSS/CNC per biointerfacce intelligenti" (2025).
- Marletta, D.: "Proprietà chimico-fisiche di film sottili di PANI elettrodepositati su oro" (2025).
- Tomarchio, A.: "Preparazione e caratterizzazione di film ibridi di PANI/CuHCF" (2025).

Master in Chemical Sciences (Laurea magistrale)

- Bartolotta, A.: "Studio dell'assemblaggio di metal-organic frameworks (MOF) su superfici di ossidi" (2023).
- Di Franco, A.: "Auto-organizzazione e stabilità di monostrati fotosensibili all'interfaccia acqua – aria" (2023).
- Fabiano, L.: "Driving neural cell fate: conductive scaffolds properties and protein interaction" (2023).
- Laudani, F.: "Studio di monostrati di nanoparticelle non all'equilibrio all'interfaccia acqua/aria" (2023).
- Valvo, S.: "Studio sulla microseparazione di fase di film di PS-b-PMMA a confinamento variabile" (2023).
- Careri, A.: "Studio di monostrati di nanoparticelle sottoposte a deformazioni interfacciali" (2024).

- Lucifora, G.: “Monostrati rispondenti a stimoli all’interfaccia liquida: proprietà e struttura” (2024).
- Strazzanti, P.: “Elettronica organica: il ruolo del PEDOT:PSS” (2024).
- Cardaci, S.: “Caratterizzazione di sistemi ibridi tramite cluster-SIMS” (2025).
- Contrafatto, M.: “Effetto della curvatura nanometrica sulla cristallizzazione di film sottili polimerici” (2025).
- Petralia, S.: “Caratterizzazione chimico-fisica tramite ToF-SIMS di dispositivi per power electronics” (2025).

Master in Chemistry - Environment, Industry and Cultural Heritage (Laurea magistrale)
- Castellino, B.: “Indagine su emulsioni fotografiche di negativi fondo fotografico Rosario Carta” (2024).

Master in Materials Science (Laurea magistrale)
- Vitale, R.: “Studio chimico-fisico degli strati di passivazione di dispositivi di potenza” (2023).

PhD in Chemical Sciences
- Malannata, E.M.: “Development of nanostructured semiconductor devices for simultaneous remediation of pollutants and hydrogen production” (2025).

PhD in Materials Science and Nanotechnology
- Campione, P.: “Study of structural and physico-chemical properties of active interfaces” (2025).

U.O. Firenze

Bachelor in Biotechnologies (Laurea triennale)
- Peluso I.: “Nanoformulazioni a base di sansa di olive e lipidi: produzione , caratterizzazione ed effetto su insetti infestanti” (2023).
- Piomboni G.: “Progettazione di nanovettori lipidici per il trasporto di acidi nucleici” (2023).
- Ioana M.: “Applicazione di nanoformulazioni biocompatibili per la modulazione del profilo lipidico di Tenebrio molitor” (2024),
- Parigi, E.: “Impatto delle nanoparticelle di ossido di ferro nell'aria su Tillandsia usneoides come pianta modello per valutare l'inquinamento in aree ad alto traffico” (2024).

Bachelor in Chemical Technology (Laurea triennale)
- Pacini S.: “Preparazione e caratterizzazione di nanosistemi ottenuti da lipidi e sansa di olive per la somministrazione di antimicrobici naturali” (2023).
- Soldani G.: “Nanoformulazioni biocompatibili per il rinforzo della dieta di insetti ad interesse nutrizionale” (2024).

Bachelor in Chemistry (Laurea triennale)

- Francavilla, C.: "Studio dell'alterazione di polimeri plastici in procedure preanalitiche e prove di fuoco (Investigating the alteration of plastic polymers in pre-analytical procedures and fire tests)" (2023).
- Barontini, C.: "Influenza della concentrazione di tensioattivo nella sintesi di particelle colloidali termoresponsive" (2024).
- Castellani, A.: "Effetti di confinamento e di agenti antimicrobici sulla motilità batterica" (2024).
- Di Rienzo, L.: "Formulazioni "green" a base di fibroina e biomolecole per il consolidamento della seta" (2025).
- Franchi, L.: "Sintesi e caratterizzazione chimico-fisica di network polimerici ad idrofilicità variabile" (2025).
- Cheloni, R.: "Nanoparticelle lipidiche per il trasporto di RNA: caratterizzazione chimicofisica e interazione con membrane biomimetiche" (ongoing).
- Enang, C.: "Preparazione e caratterizzazione di nanoparticelle cubiche a base lipidica con fosfolipidi cationici" (ongoing).
- Faralli, T.: "Progettazione e studio di formulazioni a base lipidica per applicazioni in ambito cosmetico" (ongoing).
- Gallorini, B.: "Sintesi e caratterizzazione di particelle di silice funzionali per applicazioni antimalariche) (ongoing).

Bachelor in Diagnostics and Materials for Conservation and Restoration (Laurea triennale)

- Bucciacchio, L.: "Green hybrid gels based on Jin Shofu starch: synthesis, characterization and applications" (2023).
- Marsiaj, G.: "Assessment of cold atmospheric pressure plasma for natural and synthetic varnish cleaning" (2023).
- Greco, N.: "Starch based formulation for the consolidation of paint layers and graphics on drawings and sketches" (2024).
- Marinangeli, G.: "Hydrogel cleaning performance evaluation through hyperspectral imaging on frescoes surfaces" (2024).
- Spadoni, C.: "Zinc oxide Quantum dots as marker for artworks anti-counterfeit" (2024).
- Lettieri, F.: "Chemical organogels for microsampling of paintings" (2025).

Bachelor in Science for Conservation of Cultural Heritage (Laurea triennale)

- Dini, E.: "Messa a punto e caratterizzazione di organogel siliconici da impiegarsi per la rimozione di patine di degrado da superfici pittoriche di interesse storico artistico" (2023).
- Trapuzzano, E.: "Analisi diagnostiche strumentali di pellicole cinematografiche in nitrato di cellulosa" (2023).
- Mele, F.: "Messa a punto, sviluppo e caratterizzazione chimico-fisica di organogel a base di polidimetilsilossano a porosità controllata per la pulitura di superfici pittoriche" (2025).

- Secci, I.: “Inibizione della “sindrome dell’aceto” mediante nanomateriali inorganici. Applicazioni per il trattamento di pellicole cinematografiche in triacetato di cellulosa” (2025).

Master in Biology (Laurea magistrale)

- Butelli V.: “Miglioramento del profilo lipidico di Tenebrio molitor mediante nanoformulazioni biocompatibili” (2024).

Master in Chemical Sciences (Laurea magistrale)

- Anselmi, E.: “Sviluppo di consolidanti nanostrutturati a base proteica per tessili di interesse storico-artistico” (2023).
- Belfiore, I.: “Polyvinyl alcohol-based cryogels with tunable porosity” (2023).
- Bertaglia, A.: “Preparazione e caratterizzazione chimico-fisica di materiali porosi a base di fosfati per la rimozione di inquinanti organici” (2023).
- Briganti, D.: “Preparazione e caratterizzazione di particelle a base di fosfati amorfi di calcio e magnesio per applicazioni in campo nutraceutico” (2023).
- Cappellini, C.: “Preparazione e caratterizzazione chimico-fisica di materiali compositi con proprietà di isolanti termici” (2023).
- Gabellini, C. “Pickering emulsions with functionalized ZnO nanoparticles for cosmetics applications” (2023).
- Rossi, G.: “Sviluppo di una piattaforma microfluidica per la determinazione di acidi nucleici” (2023).
- Rupolo, A.: “Synthesis and structural characterization of castor oil-based microgels” (2023).
- Canonico, B.: “Gel a base di cellulosa batterica per la pulitura di beni culturali” (2024).
- Cheli,L.: “Preparazione e caratterizzazione di particelle a base di fosfato di calcio a diverso grado di cristallinità per applicazioni nutraceutiche” (2024).
- Degli Innocenti, J.: “Caratterizzazione chimico-fisica di biochar per accumulo di energia ottenuti da pirolisi di biomasse” (2024).
- Fantappié, E.: “Semi-Interpenetrated Hydrogels for the removal of heavy metals from waste water” (2024).
- Lenzi, N.: “Effetto della quantità di solfati sulle proprietà chimico fisiche di cementi ternari a basso tenore di carbonio” (2024).
- Leonardi, V.: “Mesoporous silica for the delivery of active ingredients in agriculture” (2024).
- Macigni, A.: “Study of the photocatalytic properties and Zn^{2+} ion release of core-shell nanoparticles for cosmetic applications” (2024).
- Spissu, L.: “Effetto del rapporto acqua/solido sull’idratazione e sulla porosità di cementi ternari a basso tenore di carbonio” (2024).
- Tamantini, S.: “B. Subtilis mobility in hydrogels with different ionization degree” (2024).
- Ulivieri, N.: “Particelle amorfe a base di fosfato di calcio come veicolo per il caricamento e il rilascio di flavonoidi” (2024).
- Anello, C.M.: “Biomateriali a base di fibroina e nanocellulosa per il rinforzo di manufatti artistici in seta” (2025).

- Barielli, L.: “Preparazione e caratterizzazione di particelle a base di fosfato di calcio stabilizzate da bifosfonati” (2025).
- Cervelli, L.: “Synthesis and characterization of dendronized side chain liquid crystalline poly(2-oxazoline)s polymers for proton-conducting membranes” (2025).
- Conticelli, G.: “Effect of sugarcane wax and glycerol monostearate gelators on the structure and rheology of avocado oil edible gels” (2025).

Master in Chemical Science for Conservation of Cultural Heritage (Laurea magistrale)
- Ascolese, M.: “Estrazione e caratterizzazione di microplastiche da reflui acquosi urbani mediante Laser Direct InfraRed (LDIR)” (2023).
- D’Aleo, C.: “Pellicole cinematografiche in triacetato di cellulosa: analisi della sindrome dell’aceto e messa a punto di una procedura per la sua inibizione” (2023).
- Forcellini, C.: “Metodologie innovative per l’inibizione della sindrome dell’aceto in pellicole cinematografiche in triacetato di cellulosa” (2023).

Master in Environmental Engineering
- Barbari, I.: “Messa a punto di una procedura innovativa per l'analisi quali-quantitativa delle microplastiche nelle acque reflue: caso studio nell'impianto di Baciacavallo (Prato)” (2024).

Master in Food Science and Technologies (Laurea magistrale)
- Guglielmino, V.: “Synthesis and characterization of agar microgels as food-foams stabilizers” (2024).

Master in Molecular Biotechnology (Laurea magistrale)
- Piomboni G.: “Novel cationic lipid nanoparticle and beta-cyclo dextrins for delivering nucleic acids: physico-chemical characterization and in vitro assays” (2025).

Master in Science and Materials for Cultural Heritage Conservation (Laurea magistrale)
- Mini, C.: “The study and the effectiveness of autogeneously air-setting mortar for the consolidation of wall paintings detachments. The study case of Brancacci’s chapel” (2024)
- Yuewen, P.: “Chemical organogels for the cleaning of artworks surfaces” (2024)
- Dore, B.: “Gomme poliuretaniche a base di olio di ricino e oligoesteri per la pulitura di beni culturali” (2025).

Master in Science for Conservation of Cultural Heritage (Laurea magistrale)
- Lisi, L.: “Le pellicole cinematografiche in triacetato di cellulosa: studio e inibizione della "sindrome dell'aceto" (2024).
- Santini, G.: “Messa a punto di una metodologia analitica innovativa per l’analisi di Acido Acetico emesso da pellicole cinematografiche in triacetato di cellulosa” (2024).

PhD in Chemical Sciences

- Bassu, G.: "Transport of Brownian particles and bacteria in hydrogels with tunable porosity" (2023).
- Cabigliera, S.B.: "Inquinamento da micro e nanoplastiche: strategie di mitigazione per ridurre il loro rilascio da tessuti sintetici durante i processi di lavaggio e il loro impatto ecologico" (2024).
- Spena, R.: "Advanced methods for the development of green industrial formulations" (2024).
- Porpora, F.: "Development of a methodology for the treatment of triacetate cellulose media of historical and artistic interest with a focus on those affected by 'vinegar syndrome'" (2024).
- Conti, L.: "Smart nanomaterials for the delivery of therapeutic nucleic acids" (2025).
- De Santis, I.: "Harnessing the Synergy of Gold Nanoparticles and Lipid Membranes for Biomedical Applications" (2025).
- Soto-Bustamante, F.: "Optimizing the structure of sustainable hydrogels for nano/microfiltration, selective absorption, and anti-biofouling behavior" (2025).
- Adamo, C: "Formulazione e caratterizzazione chimico-fisica di aggregati self-assembly di biomolecole e microcapsule "green" e sostenibili" (ongoing).
- Bonavolontà, D.: "Sviluppo di una piattaforma biotecnologica per produzione trasporto e validazione dell'efficacia di composti bioattivi per il settore cosmetico nutraceutico e agroalimentare" (ongoing).
- Pacciani, V.: "Engineering Liquid Crystalline Mesophases for Biomedical Applications: Tailored Design and Characterization Strategies" (ongoing).

Post-doc

- Balestri, A. "Interaction between self-assembled functional nanocarriers and biomimetic Interfaces" (01/01/2022-31/12/2024).
- Cardellini, J. "Lipid Nanovectors for Nucleic Acid Delivery: a Composition-Structure-Function Relationship Approach" (01/10/2024-31/12-2025).

U.O. Napoli

Bachelor in Biomedical Engineering (Laurea triennale)

- Abbatiello, E.: "Nanoparticelle magnetiche come agenti di contrasto per la risonanza magnetica per immagini (MRI)" (2023).
- Agliottone, A.: "Nanoparticelle bioispirate per il trattamento fotodinamico del melanoma" (2023).
- Angelino, D.: "La spettroscopia EPR per la rivelazione dei melanomi" (2023).
- Angelino, R.: "Carbon-dots colloidali funzionalizzati per la nanomedicina" (2023).
- Cappiello, L.: "Gli acidi nucleici per la biosensoristica: i DNAzimi" (2023).
- Cesarino, S.: "Nanosistemi lipidici nei trials clinici: dalla nanomedicina per il cancro al vaccino per il covid-19" (2023).
- Coppola, R.: "Nanoparticelle ibride a base di polifenoli con proprietà antiossidanti" (2023).

- D'Aniello, S.: "Biointerfacce nanostrutturate per il rilevamento di endotossine batteriche" (2023).
- Di Talia, M.: "Nanomateriali a base grafenica per applicazioni biomediche" (2023).
- Falzarano, F.: "Nanomateriali melanin-like: sintesi e applicazioni biomediche" (2023).
- Forte, C.: "Interazione cellula-virus: meccanismi di fusione virale e sviluppo di strategie antivirali" (2023).
- Gasparo Rippa, F.: "Progettazione di nanoparticelle dopate di ZnO con avanzate proprietà radicaliche" (2023).
- Iannotti, F.: "Progettazione di liposomi per la somministrazione di farmaci" (2023).
- Marrazzo, A.: "Classificazione e metodi di rilevamento dei biomarcatori associati allo stress ossidativo" (2023).
- Morra, M.: "Nanomateriali intelligenti a base di terre rare per la rigenerazione del tessuto osseo" (2023).
- Pace, I.A.: "Progettazione di nanoparticella melaniche per applicazioni terapeutiche" (2023).
- Pascale, N.: "Le nanoparticelle plasmoniche come marcatori ottici per la diagnosi della Sindrome di Alzheimer" (2023).
- Palmieri, F.: "Progettazione di nanomateriali ecoispirati a base di polifenoli per applicazioni biomedicali" (2023).
- Petruccelli, A.: "Le melanine: pigmenti naturali per la progettazione bioispirata di nanomateriali per applicazioni biomediche" (2023).
- Renzi, A.C.: "Processi neurodegenerativi nella Sindrome di Alzheimer: il ruolo della proteina tau e del peptide beta-amiloide" (2023).
- Santoro, S: "Progettazione di nanovettori regolatori delle Specie Reattive dell'Ossigeno (ROS) per il trattamento delle infiammazioni del miocardio" (2023).
- Schettino, D.: "Progettazione e uso di nano-biomateriali per il trattamento della retinite pigmentosa" (2023).
- Trapanese, I.: "Nanomateriali bioispirati per applicazioni biomedicali" (2023).
- Tucci, A.: "Progettazione di nanomateriali per la sterilizzazione e disinfezione da agenti patogeni" (2023).
- Velotti, C.: "I nanotubi di carbonio nei dispositivi bioelettronici e biomedicali" (2023).
- D'Agnelli, E.: "Progettazione di glico-nanoparticelle per applicazioni biomediche" (2024).
- D'Amato, G.: "Nanoparticelle di ossidi di terre rare per applicazioni biomedicali" (2024).
- Fortunato, M.: "Nanoparticelle lipidiche con proprietà bioattive per la nanomedicina" (2024).
- Gabriele, M.: "Nanomateriali carboniosi ingegnerizzati per la diagnostica medica" (2024).
- Lattuca, L.: "Quantum dots di ZnS per la optobioelettronica e la biosensoristica" (2024).
- Marino, G.: "Nanosensori per la rivelazione di biomarcatori di patologie neurodegenerative" (2024).
- Marone, A.: "Nanoparticelle ingegnerizzate per applicazioni biomedicali" (2024).

- Minichiello, V.: “Le nanoparticelle metalliche per la diagnosi del cancro polmonare” (2024).
- Modano, A.: “Nanoparticelle a base di melanina: avanzamenti nella terapia fototermica e nel trattamento selettivo del cancro” (2024).
- Napolitano, D.: “Quantum dots: struttura, proprietà ottiche e applicazioni biomedicali” (2024).
- Sabatino, G.: “Quantum dots per la rivelazione ottica di biomarcatori del melanoma (2024).
- Sequino, F.: “Nanomateriali con avanzate proprietà ottiche per la diagnostica” (2024).
- Tiano, L.: “Biointerfacce nanostrutturate per l’adesione cellulare” (2024).
- Basagni, A.: “Progettazione di nanosensori per la rilevazione di biomarcatori del diabete” (2025).
- Di Lillo, S.: “Nanoparticelle di ossido di rame ingegnerizzate: dalla sintesi chimica alle applicazioni biomedicali” (2025).
- Esposito, V.: “Ingegnerizzazione di gliconanoparticelle come vaccini antitumorali” (2025).
- Maglione, M.: “Nanoparticelle di metalli nobili per il trattamento del melanoma” (2025).
- Marmo, A.: “Quantum Dots come nanosensori biomedicali per la rilevazione di Specie Reattive dell’Ossigeno” (2025).

Bachelor in Chemical Engineering (Laurea triennale)

- Credendino, P.: “Design of metal-oxide based nanomaterials for the photodegradation of endocrine disrupting compounds (EDC)” (2023).
- Manzoni, D.: “Progettazione di nanomateriali carboniosi per la rimozione di metalli da reflui” (2023).
- Messore, E. “Quantum dots colloidali di ZnO per la rivelazione ottica di contaminanti ambientali” (2023).
- Percopo, R.: “Tecnologie e processi chimici per la degradazione delle microplastiche” (2024).
- Russo, B.: “Progettazione di nanosensori chimici per la rivelazione di inquinanti” (2024).
- Baiano, M.: “Nanoformulazioni fertilizzanti per il controllo dello stress ossidativo nelle piante” (2025).
- Civero, F.: “Strategie tecnologiche ecosostenibili per il trattamento di microplastiche” (2025).
- Prisco, V.P.: “Nanosensori ingegnerizzati per la rivelazione di endotossine batteriche” (2025).

Bachelor in Chemistry (Laurea triennale)

- Arnone, G.: “Funzionalizzazione delle nanoparticelle di ossido di cerio: dalla nanoparticella singola all’aggregato ordinato” (2023).
- Bifani, A.: “Sviluppo di nanocompositi funzionali per il packaging alimentare” (2023).
- De Martino, I.: “Caratterizzazione chimico-fisica di nanocristalli d’argento in diversi solventi” (2023).

- Di Meglio, V.: “Effetto della polarità del solvente sulle proprietà chimico-fisiche dei nanocristalli d’oro” (2023).
- Liguori, A.: “Caratterizzazione chimico-fisica dell’interazione tra sistemi modello di batteri e surfattanti polmonari” (2023).
- Molinaro, S.: “Design e caratterizzazione chimico-fisica di nanovettori lipidici per lo sviluppo di potenziali farmaci antitumorali” (2024).
- Vigna, F.: “Caratterizzazione chimico-fisica di aggregati supramolecolari ibridi contenenti nanocristalli d’oro e d’argento” (2024).

Bachelor in Industrial Chemistry (Laurea triennale)

- De Angelis, C.: “L’acido levulinico come solvente per la produzione di particelle a base di lignina” (2024).
- Zarrella, C.: “Caratterizzazione EPR di antiossidanti polifenolici ottenuti da scarti enologici ed inclusi in film polimerici” (2024).

Bachelor in Materials Science and Engineering (Laurea triennale)

- Izzo, D.: “Progettazione chimica di nanocompositi ibridi ecosostenibili per applicazioni tecnologiche” (2024).

Master in Chemical Engineering (Laurea magistrale)

- Martino, R.: “Nanoparticelle ibride a base di melanina e ossidi semiconduttori come piattaforme multifunzionali biologicamente attive” (2023).
- Savio, A.: “Progettazione di un aptasensore nanostrutturato di ZnO per il riconoscimento di endotossine batteriche” (2023).
- Bella, M.: “Can we produce fluids without physical contaminations?” (2024).
- Ciampa, G.: “Degradazione di microplastiche di PHB in presenza di irraggiamento solare catalizzata a base di nanocristalli ibridi ZnO/CDs” (2024).
- De Biasi, N.: “Eco-sustainable emulsions for cosmetic formulations” (2024).
- Ferrara, A.A.: “Processi fotocatalitici in presenza di nanoparticelle ibride TiO_2/HS per applicazioni energetico-ambientali” (2024).
- Iovino, C.: “Design of fluorescent amphiphilic nanoformulations of F-ZnO quantum dots” (2024).
- Rossi, M.: “Progettazione e sintesi di quantum dots a base di ZnS: effetto del doping sulle proprietà fotoattive” (2024).
- Cupersito, A.: “Design of carbon colloidal nanosensors from biowaste for the detection of environmental pollutants” (2025).
- Rispoli, F.: “High-Performance peptide immobilization via pyroelectrodynamic jetting for advanced biosensing” (2025).
- Santangelo, A.: “Holistic Sensorial Assessment of Home Care Detergents” (2025).

Master in Chemical Sciences (Laurea magistrale)

- Romano, B.: “Interaction between phospholipid bilayers and neuropeptides: an EPR spectroscopy study” (2023).
- Tancredi, M.: “Eco-sustainable emulsions for cosmetic formulations” (2023).

Master in Materials Engineering (Laurea magistrale)

- Marfuggi, A.: “Freestanding liquid film manipulation and colloidal nanoparticles sorting” (2023).

Master in Mechanical Engineering (Laurea magistrale)

- Landria, S.: "Nanocoatings anticorrosivi a base di nanocompositi ibridi" (2023).

Master in Sciences and Technologies of Industrial Chemistry (Laurea magistrale)

- Cuofano, O.: "Preparazione di nano-vettori per l'incorporazione e il rilascio di composti fenolici con proprietà antiossidanti" (2023).
- Falzarano, F.: "Formulazioni acquose ecocompatibili di alcaloidi naturali antiparassitari" (2023).
- Longobardi, V.: "Sintesi e caratterizzazione di microgel multi-responsivi a base di PNIPAM" (2023).
- Migliaccio, C.: "Sintesi, funzionalizzazione superficiale e studio delle proprietà chimico-fisiche di carbon-dots ottenuti da biomasse" (2023).
- Adaldo, G.: "Strategie per la modulazione del rilascio di principi attivi di interesse agronomico da hydrogel di alginato" (2024).
- Capria, F.: "Nano-vettori per l'incorporazione ed il rilascio di oligomeri polifenolici con proprietà antiossidanti" (2024).
- Di Maio, M.: "Preparazione e caratterizzazione chimico-fisica di hydrogel come sistemi carrier nell'agricoltura di precisione" (2024).
- Iovino, A.: "Studio dei meccanismi di azione di agenti viscosizzanti e disperdenti in formulazioni tricologiche modello prive di siliconi" (2024).
- Lanzara, A.: "Fotodegradazione di inquinanti emergenti utilizzando semiconduttori nanostrutturati" (2024).
- Marino, F.: "Nanosistemi lipidici per la somministrazione di farmaci idrofobici" (2024).
- Sgamato, M.: "Studio chimico-fisico del processo di auto-aggregazione di ramnolipidi in soluzione acquosa per il design di formulazioni ecosostenibili" (2024).

PhD in Chemical Sciences

- Esposito, R.: "Structural and dynamic study of the molecular mechanism of superspreading: towards the rational use of new eco-friendly wetting agents" (2023).
- Gallucci, N.: "Hybrid nanostructured systems: physico-chemical properties and applications in biomedical and technological fields" (2023).

PhD in Industrial Product and Process Engineering

- Pota, G.: "Design of nanostructured material for enzyme immobilization" (2024).

U.O. Pavia

Bachelor in Biological Sciences (Laurea triennale)

- Cavestri, Z.: "Valutazione dell'attività antiglicante di un estratto di tutolo di mais" (2023).
- Stranieri, C.: "Carrier da prodotti di scarto agroalimentare per la formulazione di nutraceutici" (2023).

- Lanati, F.: “Nanoparticelle di Blu di Prussia: stabilizzazione con Transferrina a pH fisiologico” (2024).
- Li Ranzi, E.: “Studio della stabilità a pH fisiologico e in presenza di albumina di nanoparticelle di blu di Prussia a diversa stechiometria Fe3+/K4[Fe(CN)6]” (2025).
- Pelizzari, F.: “Studi di bioaccessibilità di un formulato contenente florizina” (2025).

Bachelor in Chemistry (Laurea triennale)

- Garbaccio, M.: “Zeolitic Imidazolate Frameworks (ZIFs): proprietà e applicazioni” (2023).
- Gussoni, A.: “Metal Organic Frameworks a base di Ferro per il rilascio controllato di fertilizzanti” (2023).
- Khomynets, A.: “Composti di intercalazione con struttura a strati: sintesi e applicazioni” (2023).
- Petino, M.: “Recenti progressi nelle batterie al potassio” (2023).
- Ferrari, M.: “Minerali argillosi per il rilascio di farmaci: focus sul sistema clay-insulina” (2024).
- Menditto, G.: “Materiali stampati in 4D per applicazioni biomediche” (2024).
- Aiazzone, F.S.: “Materiale catodico Na3V2(PO4)3 per SIBs: strategie per il miglioramento delle prestazioni” (2025).

Bachelor in Environmental Engineering (Laurea triennale)

- Demicheli, R.: “Verifica della funzionalità di una piattaforma per il trattamento di rifiuti liquidi” (2023).
- Bellezza, G.: “Recupero dei residui da un sistema MBR termofilo aerobico per la minimizzazione dei fanghi biologici: prove sperimentali” (2024).
- Petrone, C.: “Valutazione sul possibile effetto inibente di sostanze perfluoroalchiliche su biomasse aerobiche” (2024).
- Sacco, E.: “Impianto di trattamento rifiuti liquidi: monitoraggio e minimizzazione dei fanghi” (2024).

Master in Advanced Biotechnology (Laurea magistrale)

- Caso, F.: “Ibridi organici-inorganici a base di idrossiapatite o brushite: il caso del Tenoxicam e della Bumetanide come esempi di farmaci poco solubili” (2023).
- Cerea, B.: “Miglioramento del profilo di rilascio di Meloxicam da sistemi ibridi a base di idrossiapatite” (2023).
- Balduzzi, J.: “Fotobiomodulazione transcranica: la luce NIR come nuova frontiera per il trattamento della malattia di Alzheimer” (2024).
- Fabris, D.: “Caratterizzazione di nanocompositi magnetici utilizzati come vettori di farmaci poco solubili” (2025).
- Marcinnò, D.: “Il Social-Life Cycle Assessment nell'industria della plastica: un caso studio per la valutazione dell'impatto sociale di elastomeri termoplastici innovativi” (2025).
- Monterosso, F.: “Idrossidi a doppio strato come sistema di somministrazione di farmaci poco solubili” (2025).

Master in Bioengineering (Laurea magistrale)

- Elicio, A.: "Sintesi e caratterizzazione di cementi brushitici per la rigenerazione ossea con rilascio controllato di piroxicam" (2023).
- Cappellini, B.: "Sintesi e caratterizzazione di cementi brushitici puri e drogati con silicio per sistemi di drug delivery" (2024).
- Mauro, A.: "Sintesi e caratterizzazione di cementi brushitici puri e drogati con bario per il rilascio di piroxicam" (2024).
- Imparato, G.: "Sintesi e caratterizzazione di cementi brushitici puri e drogati con stronzio come sistema di drug delivery per il rilascio di meloxicam" (2025).
- Loi, C.: "Idrossiapatiti drogate come sistemi di drug delivery di farmaci poco solubili" (2025).

Master in Chemistry (Laurea magistrale)

- Aliotta, S.: "Preparazione e caratterizzazione di Biochar da scarti vegetali pretrattati con funghi wood decay per lo stoccaggio dell'idrogeno" (2024).
- Buscarini, A.: "Progettazione, cristallizzazione e caratterizzazione di sali e cocristalli di pimozide" (2024).
- Carta, M.: "Preparazione di carbonio attivato da biomasse pretrattate con funghi wood decay per lo stoccaggio di idrogeno" (2024).
- Conti, E.: "Sintesi e caratterizzazione di leghe ad alta entropia per lo stoccaggio di idrogeno allo stato solido" (2024).
- Pedalà, A.: "Preparazione e decorazione di materiali a base carbonio da scarti alimentari: una strada per l'economia all'idrogeno?" (2024).
- Pellegrini, A.: "Ricerca di nuovi polimorfi del principio attivo imepitoina" (2024).
- Bianchi, G.: "Da scarti agroalimentari a carbonio attivato per l'immagazzinamento di idrogeno: una strada per l'economia circolare? (2025).

Master in Environmental Engineering (Laurea magistrale)

- Pennacchio, S.: "Biochar da fanghi: una soluzione sostenibile per il trattamento degli effluenti dei depuratori" (2023).
- Rigoldi, L.: "Ottimizzazione di un reattore di digestione anaerobica, mediante l'inserimento di un pastorizzatore in serie" (2023).
- Silva, A.: "Biochar da residui organici: prove di adsorbimento per la depurazione di acque reflue" (2023).
- Calabria, L.M.R.: "Produzione di biochar 'green' da fanghi di depurazione: impiego come carbone attivo nel trattamento delle acque" (2024).
- Grecchi, G.: "Rifiuti liquidi contenenti AOX: valutazione del possibile effetto inibente e criticità relative alla metodica analitica" (2024).
- Bonomo, G.: "WATER SAFETY PLAN: la gestione del rischio del sistema idropotabile di Pavia" (2025).
- Dimitri, A.: "Valutazione del possibile effetto inibente su biomasse aerobiche di reflui contenenti sostanze per- e polifluoroalchiliche (PFAS) mediante prove respirometriche" (2025).

Master in Industrial Nanobiotechnologies for Pharmaceuticals (Laurea magistrale)

- Martin, L.J.: "Formation of a Transferrin (Tf) protein corona on Prussian Blue Nanoparticles" (2025).

Master in Pharmaceutical chemistry and technology (Laurea magistrale a ciclo unico)

- Blundo, M.P.: "Preparazione e caratterizzazione chimico-fisica di nanocompositi a base di silicio e carbonio per la somministrazione della Levodopa" (2023).
- Di Mario, S.: "Nanotubi come carrier in formulazioni innovative per il trattamento di malattie neurodegenerative: preparazione e caratterizzazione chimico-fisica (2023).
- Di Vita, G.: "Progettazione e caratterizzazione chimico-fisica di forme farmaceutiche innovative per il trattamento dell'ipercolesterolemia" (2023).
- Ferrari, G.: "Preparazione e caratterizzazione chimico-fisica di nanocarrier innovativi per il delivery della Curcumina come agente anticancro" (2023).
- Giacobone, A.: "Metodo di estrazione e analisi di nanoparticelle di argento mediante cloud point extraction utilizzando come tensioattivo il Triton X 100" (2023).
- Monzini, G.: "HNT e liposomi come carrier per l'insulina: preparazione, caratterizzazione e prove di rilascio" (2023).
- Rana, A.: "Preparazione e caratterizzazione di sistemi cutanei antibatterici per il rilascio controllato di clorexidina" (2023).
- Spanò, M.: "Valorizzazione degli scarti di asparago (Asparagus officinalis): ottimizzazione del processo estrattivo della frazione fenolica" (2023).
- Arseni, F.: "Preparazione e caratterizzazione di miscele costituite da alfa-tocoferolo acetato e acidi grassi con azione antibatterica e fotoprotettiva" (2024).
- Cazzaniga, G.: "Caratterizzazione chimico-fisica di nanotubi di halloysite funzionalizzati per la veicolazione del Resveratrolo" (2024).
- Ciocca, M.: "Caratterizzazione chimico-fisica e funzionalizzazione di nanotubi di Halloysite per la somministrazione di ciprofloxacina" (2024).
- Colucci, I.: "Analisi di frammenti e polveri di bottiglie di vetro nelle scienze forensi" (2024).
- Denaro, I.: "Microemulsioni a base di curcumina ed acidi grassi ad attività antibatterica: preparazione e caratterizzazione chimico-fisica" (2024).
- Gambuzza, M.: "Sistemi a rilascio modificato Ibuprofene-acidi grassi: preparazione e caratterizzazione chimico-fisica" (2024).
- Marei Elmitwalli Elbayoumi Bayoumi, A.: "Caratterizzazione chimico-fisica di miscele di clorexidina e acidi grassi ad attività antibatterica per la preparazione di gel di membrana mucoadesivi" (2024).
- Noris, G.: "Strategie per la gestione dell'iperglicemia: formulazione, produzione e messa in commercio di un integratore alimentare" (2024).
- Scorza, V.: "Estratto di Passiflora incarnata L.: strategie di incapsulamento e studi di bioaccessibilità" (2024).
- Vacchini, E.M.: "Nanoclay di Halloysite (HNT) per la veicolazione dell'acido gamma-aminobutirrico nel trattamento dell'epilessia: preparazione e caratterizzazione chimico-fisica delle miscele HNT-GABA" (2024).
- Zambelli, A.: "Caratterizzazione chimico-fisica di miscele costituite da Clorexidina ed acidi grassi ad attività antibatterica per la preparazione di ovuli vaginali" (2024).

Master in Pharmacy (Laurea magistrale a ciclo unico)

- Afifi, D.: "Preparazione, caratterizzazione e impiego dei liposomi per il trattamento dei tumori" (2023).

- Cesari, A.: “Impiego di nutraceutici nella sclerosi laterale amiotrofica” (2023).
- Lopane, A.: “Copertura sanitaria universale ed efficiente distribuzione dei farmaci nelle emergenze umanitarie. Il farmacista e la conservazione del farmaco” (2023).
- Marino, K.: “SIDS – Sudden Infant Death Syndrome: La sindrome della morte improvvisa nel lattante. Approcci preventivi ed educazione genitoriale” (2023).
- Resta, E.: “Valutazione dell’attivita’ antiglicante della frazione polifenolica estratta da scarti cerealicoli” (2023).
- Tavazzi, G.: “Screening preliminare sul potenziale antiglicante di estratti vegetali edibili” (2023).
- Boccaccini, A.M.: “Da veleno a rimedio: proprietà e future prospettive di impiego del veleno d’ape” (2024).
- Cagnoli, C.: “La malattia di Alzheimer e il microbiota intestinale: potenziale ruolo dei probiotici” (2024).
- Harhash, R.: “Forme farmaceutiche orali in pediatria: problematiche nello sviluppo di formulazioni adatte alle diverse età” (2024).
- Ibrahim, D.: “NANOTUBI DI CARBONIO: carrier farmaceutici che attraversano la BEE” (2024).
- Milani, N.: “Economia circolare per Pectina e Chitosano: da scarto alimentare a prodotto farmaceutico” (2024).
- Tiso, M.: “Innovazione e Performance: Biomateriali Avanzati nelle Protesi per Atleti” (2024).

PhD in Chemical and Pharmaceutical Sciences and Industrial Innovation

- Frosi, I.: “Gaining health and energy from Lombard agrifood waste” (2023).
- Ambrosetti, M.: “Alloy-based anodes for sustainable post Lithium batteries” (2024).
- Conti, D.M.: “Design of CNFs-supported self-standing cathodes for Sodium-ion batteries with enhanced performance at high C-rate” (2024).
- Colombi, C.: “Dye-Noble Metal Conjugates and Prussian Blue Nanoparticles for Visible Photothermal Inks” (2025).

PhD in Environmental and Industrial Engineering

- Caccamo, F.M.: “Economia circolare applicata al trattamento delle acque” (2023).
- Bellazzi, S.: “Messa a punto di strumenti gestionali per l'ottimizzazione di sistemi biologici avanzati” (2024).

Post-lauream Master II level “Nutraceutics and food supplements: from raw ingredient to marketing and their use in practical clinic”

- Boccia, G.: “Fattori di rischio cardiovascolare: Nutraceutici per il controllo del colesterolo e il consiglio del farmacista sui social” (2023).
- Corona, R.; “Caratterizzazione di ceppi per lo sviluppo di nuovi prodotti probiotici a base di spore: Bacillus subtilis SF106 e Bacillus clausii SF174” (2023).
- Crepaldi, L.: “Innovativa associazione nutraceutica di estratti vegetali per la protezione dai danni indotti dall’esposizione solare” (2023).
- De Leonardis, C.: “Gli inositoli: proprietà chimiche e farmacologiche e impiego nella pratica ostetrico-ginecologica” (2023).

- Di Bari, M.C.: “Green extraction: tecniche tradizionali e innovazioni tecnologiche” (2023).
- Manfrè, S.: “Melatonina e probiotici: integrazione innovativa per una migliore qualità del sonno” (2023).
- Michelli, S.: “Le Plant-derived Extracellular Nanovesicles: il cross-talking kingdom come approccio Nutraceutico” (2023).
- Perri, M.: “Il ruolo della nattokinasi nella prevenzione delle patologie cardiovascolari” (2023).
- Spagnoli, A.: “Dalla tradizione all'innovazione: set up del processo di estrazione dell'aglio nero invecchiato (Allium sativum)” (2023).
- Vallelonga, D.: “Estratto di buccia di melone come fonte di attivi ad attività antiglicante” (2023).
- Balduzzi, A.: “Progettazione e sviluppo di un integratore alimentare a base di L. rhamnosus TOM 22.8 per il trattamento delle infezioni vaginali: CANDILACT E4” (2024).
- Bettini, F.: “La formulazione di prodotti nutraceutici per una platea di giovani adulti” (2024).
- Biagini, P.: “L’Effetto del microbiota intestinale sulla funzione renale ed in particolare sul rene trapiantato. Breve focus sul possibile utilizzo di postbiotici nella malattia renale cronica” (2024).
- Bozorgzad Imani, A.: “Come approcciare l’integrazione nutraceutica in ambito sportivo” (2024).
- Ferrari, M.: “Sviluppo di un integratore alimentare in forma liquida a base di diosmina e flavonoidi per il benessere del microcircolo” (2024).
- Furfaro, L.: “Armonizzazione del piano di autocontrollo relativo alla presenza di residui di fitofarmaci nelle droghe vegetali impiegate negli estratti EPO” (2024).
- Giordani, E.: “Test in vitro di inibizione dell’attività metabolica di probiotici per il design di integratori alimentari” (2024).
- Giurici, M.C.: “Sviluppo di un Integratore Alimentare costituito di due forme farmaceutiche (compresse e stick pack) a base di Estratti vegetali, Vitamine, L-carnitina, L-arginina, Cromo e Probiotici” (2024).
- Mangione, B.: “Sindrome Metabolica: Approcci Nutraceutici per la Prevenzione e il Trattamento” (2024).
- Massimo, M.: “Botanicals per migliorare il benessere mentale e i disturbi del sonno” (2024).
- Riccardi, E.L.: “BERBERINA, VITAMINE DEL GRUPPO B e UBICHINOLO – Proprietà biologiche e applicazioni cliniche” (2024).
- Sammartini, F.: “Sviluppo in farmacia di un nuovo integratore a base di berberina per la gestione dell’infiammazione cronica di basso grado. La tecnologia fitosoma® come strumento per aumentare la biodisponibilità” (2024).
- Stucchi, F.: “Sviluppo di un integratore alimentare per il declino cognitivo: dallo studio del razionale alla progettazione del prodotto finito” (2024).
- Tempesta, F.: “Trattamento delle dislipidemie: classico approccio terapeutico e l’uso dei nutraceutici” (2024).
- Vatieri, C.: “Curcumina: un nutraceutico e la sua bassa biodisponibilità” (2024).
- Vecchiato, C.: “Studio formulativo di una nanoemulsione a base di CBD e possibili applicazioni come nutraceutico” (2024).

- Consoli Gentile, N.: "Strategie Nutraceutiche per il supporto alla guarigione tendinea: evidenze scientifiche e proposta teorica di una formulazione" (2025).
- Di Biase, E.: "Benessere naturale: Proprietà e applicazioni di Bromelina, Papaina e Licopene" (2025).
- Guacci, C.: "MaquiBright®, estratto standardizzato di bacca di maqui (Aristotelia chilensis): un approccio nutraceutico alternativo per la gestione dei disturbi della secchezza oculare" (2025).
- Michelini, G.F.: "Strategie di Micronizzazione per il miglioramento delle proprietà funzionali e tecnologiche dei prodotti Nutraceutici" (2025).
- Pistolesi, E.: "Il flusso produttivo di un integratore" (2025).
- Sala, L.: "Aspetti tecnici e regolatori per l'immissione nel mercato europeo di un nuovo alimento: il caso delle foglie di vitis vinifera fermentate" (2025).
- Urso Russo, M.: "Conformità normativa nel settore Nutraceutico: l'esperienza di IMS nella Micronizzazione conto terzi" (2025).

U.O. Perugia

Bachelor in Biology (Laurea triennale)

- Dolci, S.: "Quando il pH modella le proteine: il caso dell' albumina bovina serica" (2025).
- Marziali, R.: "Caratterizzazione spettroscopica di lisozima in funzione di pH" (2025).

Master in Chemistry Sciences (Laurea magistrale)

- Puleo, M.: "Sintesi e caratterizzazione di materiali nanostrutturati per la fotodegradazione di farmaci" (2023).
- Sambucari, G.: "Studio delle proprietà di luminescenza di sistemi nanostrutturati a base di argento in matrici inorganiche" (2023).
- Cozzali, E.: "Studio delle proprietà di luminescenza di sistemi nanostrutturati in matrici complesse" (2024).
- Duri, A.: "Effetto delle condizioni di sintesi sulle proprietà termocromiche di materiali nanostrutturati a base di VO_2" (2024).
- Giansanti, S.: "Synthesis and characterization of Gd-doped carbon dots and their functionalization for MRI" (2024).
- Ranieri, D.: "Synthesis and characterization of DNA-stabilized silver nanoclusters for bioimaging applications" (2024).
- Visca, G.: "Sintesi e caratterizzazione di materiali a base di MOF per applicazioni colorimetriche" (2025).

PhD in Chemistry Sciences (Dottorato)

- Cambiotti, E.: "Radiation up-conversion through nanostructured materials" (2024).
- Bondi, R. "Synthesis and Characterization of Nanoparticles for Sustainable Lighting and Mitigation of Urban Heat Island" (2025).
- Grigoras, M.A. "Exploring the potential of Bi-based photocatalysts: How preparation conditions affect performances" (2025).

RDT-a

- Quaglia, G.: “Functionalization and formulation of nanomaterials” (2024-2027).

U.O. Siena

Bachelor in Chemical Sciences (Laurea triennale)

- Angileri, C. “Caratterizzazione chimico-fisica di nano-emulsioni caricate con estratti vegetali” (2023).
- Bindi, V. “Idrogel a base di polimeri biocompatibili ed estratti di brassicacee per la disinfezione di suoli agricoli: efficienza di caricamento e profili di rilascio del principio attivo” (2023).
- Calosi, L.: “Contenuto di sostanze antiossidanti in panificati fortificati in funzione della shelf-life” (2023).
- Del Monaco, L. “Analisi Chemiometrica della Dinamica Intertemporale degli Idrocarburi Policiclici Aromatici (PAH) in Taranto e Zone Limitrofe” (2023).
- Formiggini, G.: “Analisi ICP-MS di metalli in tracce in terreni e foglie d'olivo da oliveti toscani” (2023).
- Frusta, E. “Analisi dei Trend Interannuali e Stagionali di Arsenico nel Lago di Piediluco” (2023).
- Maroni, C. “Sviluppo e caratterizzazione di idrogel a rilascio controllato di microemulsioni a base di isotiocianati per la disinfezione di suoli agricoli” (2023).
- Nuti, A. “Ottimizzazione di un Metodo HPLC-DAD per l'analisi di Esteri dell'acido Ftalico in Campioni di Acqua Marina” (2023).
- Paggetti, S.: “Analisi delle proprietà antiossidanti delle componenti anatomiche della drupa di Coffea arabica” (2023).
- Sinibaldi, A.: “Sviluppo e caratterizzazione di bio-adesivi a base di chitosano” (2023).
- Turchi, G. “Caratterizzazione chimico-fisica di liposomi e cubosomi caricati con curcumina” (2023).
- Barnabà, A.: “Caratterizzazione chimica di olio da semi di pomodoro” (2024).
- Bettarini, A. “Analisi di metalli tramite ICP-MS per lo studio dell'origine geografica di oli d'oliva toscani” (2024).
- Ferruzzi, L.A. “Design e sintesi microfluidica di nanoparticelle lipidiche” (2024).
- Fratello, V.A. “Distribuzione Spazio-Temporale del CDOM e dei Metalli Presenti nel Fiume Orcia” (2024).
- Grazzi, T. “Analisi metabolomica tramite NMR e spettrometria di fluorescenza per lo studio dell'origine geografica di oli d'oliva toscani” (2024).
- Ibricic, A. “Sintesi e caratterizzazione chimico-fisica di liposomi e solid lipid nanoparticles come sistemi per il drug delivery” (2024).
- Marciante, R.: “Analisi comparativa delle proprietà chimico-fisiche di miscele Amido/Chitosano/PVA con lignina ottenute tramite solvent casting ed estrusione” (2024).
- Mari, R. “Dinamiche spazio-temporali della materia organica e dei metalli nel fiume Merse” (2024).
- Martino, L.: “Variabilità delle proprietà nutraceutiche in campioni di drupe di Olea europaea da oliveti toscani” (2024).

- Mascaretti, A. “Caratterizzazione chimico-fisica di sistemi per il drug delivery” (2024).
- Melluso, A. “Modelli sulla Dinamica di Triptofano in Ambienti Fluviali” (2024).
- Moraru, M. “Georeferenziazione dei vini rossi della regione toscana attraverso l'analisi dei campioni con ICP-MS e fluorescenza” (2024).
- Pecorini, R.: “Sviluppo di matrici polimeriche a base di PVA contenenti metal-organic framework” (2024).
- Rizzo, C.: “Proprietà nutraceutiche di Medicago sativa L. per il suo utilizzo come ingrediente fortificante” (2024).
- Sacchini, E.: “Liposomi cationici caricati con triamcinolone utilizzati per la sintesi di un gel oculare a base di acido ialuronico” (2024).
- Scuteri, S.: “Valutazione e caratterizzazione di materiali polimerici alternativi al PVC per la realizzazione di sacche medicali per farmaci liquidi iniettabili” (2024).
- Sicuro, L.: “Ottimizzazione di sintesi microfluidica di solid lipid nanoparticles” (2024).
- Vizziello, I.: “Studio della Dinamica dei Fosfati nelle Zone Costiere del Lago Tanganyika” (2024).
- Arrigucci, M.: “Ottimizzazione di un sensore ottico low-cost per il monitoraggio di nitrati e fosfati negli ecosistemi” (2025).
- Bonucci, R.: “Nutrienti e sostanza organica disciolta: analisi spazio-temporale sulla qualità delle acque nel fiume” (2025).
- Salinaro, J.: “Studio dell'origine geografica di oli d'oliva extravergini tramite spettrometria di massa ad alta risoluzione HPLC-HRMS” (2025).
- Sciortino, N.: “Dinamica dei macronutrienti nel fiume Mara: un’analisi transfrontaliera tra Kenya e Tanzania” (2025).

Master in Chemistry (Laurea magistrale)

- Caria, A.M.: “Chemical composition of anatomical parts of coffee beans” (2024).
- Colamarino, R.: “Geographical origin characterization of olive oil production chain via excitation-emission matrix (EEM) fluorescence spectroscopy combined with multivariate analysis” (2024).
- Cordovani, S.: “Performance evaluation of the removal efficiency of total nitrogen, COD, BOD5, and other parameter in aqueous liquid waste using a thermophilic industrial SBR biological treatment plant followed by refinement with a pilot MBR system” (2024).
- D'Anna, R.: “Combining secondary metabolites and trace metals levels for the geographical identification of olives from Tuscany orchards” (2024).
- Fornarini, P.: “Effects of dopants on spiro-ometad in perovskite solar cells: device preparation, characterization and sustainability aspects” (2023).
- Frullani, C.: “Determination of trace and ultra-trace metal(loid)s for the geographical identification of vineyard samples” (2024).
- Gabbricci, G.: “Optimization of Thymol Loaded Solid lipid nanoparticles for Home-care applications” (2023).
- Adelaide Colamarino, A.: “Assessing metal concentrations and fluorescent dissolved organic matter using participatory approaches” (2024).
- Maccari, N.: “NMR tools for multi-attribute quantification methods of polysaccharides in vaccine formulations” (2024).

- Mattia Carbone, M.: “Organic matter dynamics by PARAFAC and NMR analysis of an Italian river” (2024).
- Sapenova, A.: “Evaluating Water Quality Dynamics Using Chemometrics Approaches” (2024).
- Torresi, L.: “Tomato waste as a sustainable source of bioactive compounds” (2024).
- Ghiro, S.: “Life cycle assessment of bio-packaging production from chestnut burrs residues” (2025).
- Rotondi, L.: “Establishing the link between flow uniformity and overpotential in electrocatalytic flow cell” (2025).

Master in Pharmacy or Pharmaceutical Chemistry and Technologies (Laurea magistrale)

- Albertini, G.: “Sintesi microfluidica di nanoparticelle di chitosano ottimizzata tramite design sperimentale” (2025).
- Chigozie, L.E.: “Sintesi e Caratterizzazione di Nanoparticelle Magnetiche Attraverso l’uso di estratti di foglie d’ulivo” (2025).

Master in Sustainable Industrial Pharmaceutical Biotechnology (Laurea magistrale)

- Danja, M.: “The development of a circular bioeconomy model for the extraction of biofuel for energy production purposes from macro-algal biomass taken from the Orbetello lagoon” (2023).
- Dongryung, K.: “Vaccines immunological assessments: a case study with sars-cov-2 vaccine” (2023).
- Gonzalez Monroy, M. A.: “Life Cycle Assessment of protein production process: attributional comparison between conventional stainless-steel and single-use fermentation technologies” (2023).
- Iannibelli, V.: “Advancing business efficiency: integrating document automation with machine learning and analyzing ai regulatory frameworks in healthcare” (2023).
- Munir, I.: “Maintenance manual of a robotized filling machine: drafting of the document and evaluation of future implementation for interactive content to avoid paper copy of the document” (2023).
- Nencetti, E.: “A new dimension of learning: integrating VR and AR into GMP training for sustainable pharmaceutical manufacturing” (2023).
- Da Vela, L.: “Sustainable Management of Invasive Algae: Life Cycle Assessment of Biochar and Paper Products Derived from Orbetello Lagoon” (2024).
- Ghaith, J.: “Assessing and Enhancing Sustainability towards Greening Ibuprofen Production Line: A Comparative Phase-By-Phase Evaluation Study of Synthesizing, Compacting, Packaging and Transporting for Environmental Efficiency” (2024).
- Redi, R.: “Integrating Machine Learning with Density Functional Theory to Uncover New Organic Dyes for Indoor DSSCs” (2024).
- Upano, M.: “A Comprehensive Life Cycle Assessment of Perovskite Solar Modules applied on Buildings: A Prospective Approach” (2024).
- Campaniello, A.: “Study of the camaleonicity and phisiochemical properties of protacs targetting CK2” (2025).
- Darbandi, A.: “Nanostructured QCM-Based Biosensor for Diagnostic Applications” (2025).

- Narisetty, S.: “Novel Magnetic Iron Oxide Nanoparticles: Eco-Inspired Synthesis and Applications in Wastewater Treatment” (2025).

Degree in Pharmacy (Laurea a ciclo unico)

- Jahai, S.: “Comparazione di nanovettori lipidici per incapsulamento di idrochinone a uso topico” (2024).

PhD in Chemical and Pharmaceutical Sciences

- Cangeloni, L.: “Identification and characterization of natural bioactive molecules and their liposomal formulation” (2024).
- Pepi, S: “Polymeric and metal-organic frameworks for drug delivery” (2024).
- Bisozzi, F.: “Nutraceuticals: chemical characterization and delivery systems” (2025).
- Boldrini, A. “Advanced Chemical and Optical Sensors to Reduce Diffuse Pollution in Urban Waters” (2025).
- Talarico, L: “Advanced Carriers for Active Compounds and Enhancers for Sensing Technologies” (2025).

PhD Student in “Sustainable Agricultural-Forestry Systems” XL cycle

- Melkamu Tiru Gelaw: “Novel Antifungal substances against Fomitiporia mediterranea of Grapevine” (Vitis vinifera).

U.O. Venezia

Post Doc

- Segato, J. “Fish waste valorization” (01/02/2023-15/11/2024).
- Massari, D. “Fish waste valorization” (01/01/2025-31/12/2025).
- Pajer, N. “Study of the structure of biorefinery residues” (01/02/2023-31/01/2025).
- Peroni, G. “Encapsulate” (15/01/2023-15/07/2025).
- Bressanelli, L. “Development of innovative materials from renewable resources” (15/02/2025-15/02/2026).

RESEARCH PROJECTS

1A – Activated carbon from biomasses: a route for green energy storage and environmental sustainability?

C. Milanese, A. Girella, S. Paraboschi, E. Conti, Y.A. Diaz Fernandez, F. Ridi

Aims

Preparation and characterization of novel carbon-based nanostructures and innovative hybrid hydrides-carbon structures for solid-state H_2 storage from industrial and agricultural wastes; evaluation of their hydrogen sorption properties; determination of the thermodynamic and kinetics parameters of the sorption reactions.

Results

Circular economy and energy storage are very hot topics concerning scientific and technological research and economy. In this framework, our activities develop regarding solid state hydrogen storage.

Biochar, the carbon side-product in the pyrolysis/gasification of residual waste biomasses, started to receive a widespread attention in the field of energy-storage, thanks to its hierarchical porous structure inherited from biomass precursors, its excellent chemical and electrochemical stability, high conductivity, high surface area and inexpensiveness. In particular, activated carbon (SSA > 1000 m^2/g) obtained from biomasses through a chemical treatment with H_3PO_4 and subsequent thermal treatment or through pyrolysis and KOH physical activation appears to be a new cost-effective and environmental-friendly material with great application prospect in the field of energy-storage. In this regard, we were able to prepare novel hierarchically-porous super-activated carbon materials originating from original biomasses such as melon, pumpkin, potatoes and orange peels, asparagus stems and walnut or peanuts shells with surface area higher than 2000 m^2/g. The chemical activation process proved to be efficient to remove most impurities, stabilizing highly porous hierarchical structures with local graphene-like morphology.

Biomasses are mainly constituted by hemicellulose, cellulose and lignin, with the last one being highly stable and difficult to decompose. For the first time in hydrogen storage topic, we performed a biological pretreatment of the biomasses with different White-Rot Fungi species from Pavia University collection to start the polymer degradation before the thermal treatment, obtaining an improvement in the biochar production yield (double efficiency) at lower temperatures (450°C vs 650°C) and times (4 h vs 6h) , going towards a better sustainability of the pyrolysis processes.

The obtained activated carbon materials are able to adsorb up to 5 wt% of hydrogen at 77K and 10 bar in around 1 min and to desorb the same amount in 1.5 min under vacuum. This result is superior with respect to the values reported in literature for the conventional activated carbon or graphitic materials.

Decoration of these materials with metallic nanoparticles (Ni, Fe, Cu) has been performed through chemical impregnation starting from nitrate and chloride salts,

followed by a thermal reduction under Ar/hydrogen atmosphere. Nanoparticles with size lower than 10 nm have been deposited, leading to better adsorption performance (+0.5 wt%) with respect to the undecorated ones.
To obtain systems working in chemisorption mode, the activated and the decorated carbon materials have been mixed with Mg hydride, the first generation absorber, having the drawback of high working temperature (> 320 °C). The activated carbon has been demonstrated, for the first time in literature, to promote desorption, leading to faster kinetics with respect to the plain hydride, and to improve its reversibility.
Work is in progress to perform a deep characterization of the C based materials obtained from the different biomasses and to explore the role of the metallic nanoparticles in the sorption behavior of C and of the Mg hydride. Moreover, complex and intermetallic hydrides with promising working temperature will be mixed with the C materials to investigate a possible catalytic effect.
The porous compounds obtained by asparagus stems and orange peels demonstrated to behave as excellent electrode materials for high-performance symmetric supercapacitors (SCs), reaching interestingly high specific capacitance and specific energy. Work is in progress to prepare a fully green supercapacitors by using pectin obtained from orange wastes as an electrolyte component.
Finally, the as prepared biochar has been demonstrated to be promising for water remediation, working with high efficiency as adsorbents for pollutants (active principles, drugs, hormones) present in wastewater, opening another green route for preserving our environment.

References

[1] Cignolo, D.; Rizzi, V.; Fini, P.; Petrella, A.; Milanese, C.; Cosma, P.; Gubitosa, J. “Composite Chitosan-Biochar-based sponges for the removal of Direct Blue-78 from water: Physical and chemical parameters affecting the adsorption process”, Colloids and Surfaces A: Physicochemical and Engineering Aspects, 724, 137518 (2025).
[2] Ahmad, N.; Rinaldi, A.; Sidoli, M.; Magnani, G.; Vezzoni, V.; Scaravonati, S.; Pasetti, L.; Fornasini, L.; Gupta, H.; Tamagnone, M.; Ridi, F.; Milanese, C.; Riccò, M.; Pontiroli, D. “Pre-treated biomass waste melon peels for high energy density semi solid-state supercapacitors”, Journal of Power Sources, 624, 235511 (2024).
[3] Bianchini, P.; Merlo, F.; Quarta, V.; Ferrari, L.; Milanese, C.; Profumo, A.; Speltini, A. “Improving sample preparation by biochar-coated sampling tubes: proof-of-concept extraction of sex hormones from real waters”, Advances in Sample Preparation 12, 100129 (2024).
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1A – Antioxidant cerium oxide nanozymes

N. Gallucci, I. De Cristofaro, A. Cangiano, G. Vitiello, L. Paduano
(U.O. of Naples, University of Naples Federico II)

Aims

Recently, cerium oxide nanoparticles (CeO_2 NPs) have been considered as promising nanozymes, due to their excellent catalytic properties. This peculiarity is due to the coexistence, in the crystal structure, of cerium (III) and cerium (IV); this guarantees a continuous redox cycle and therefore the ability to acquire or lose electrons (Bai et al., 2024). The Ce(III)/Ce (IV) ratio is therefore the one that establishes whether NPs have pro-oxidant or antioxidant properties. The presence of defects and the Ce(III)/Ce(IV) ratio on the surface are addicted to the NPs shape and size and, therefore, they can be opportunely modulated by varying the synthesis conditions, such as temperature, pressure, nature of the inorganic precursor and/or the capping agent. For this reason, this project aims to synthesize and characterize CeO_2 NPs, varying temperature and length of the alkyl chain of the capping agent, to obtain the best system, in terms of size and shape, that can be tested as nanozymes.

Results

The properties of nanoparticles depend on their shape and size, which can be modulated during synthesis. For this reason, we synthesized cerium oxide nanoparticles by thermal decomposition of cerium(III) nitrate hexahydrate at varying temperatures (150, 200, and 250 °C) and using primary amines with different alkyl chain lengths (from C8 to C18). As can be observed from Figure 1, as the temperature and length of the alkyl chain increase, the size of the inorganic core decreases, the morphology becomes increasingly regular and spherical, and the tendency towards self-aggregation decreases, so much so that the nanoparticles synthesized at 250 °C with oleylamine (C18) are monodisperse in chloroform (see DLS curve).

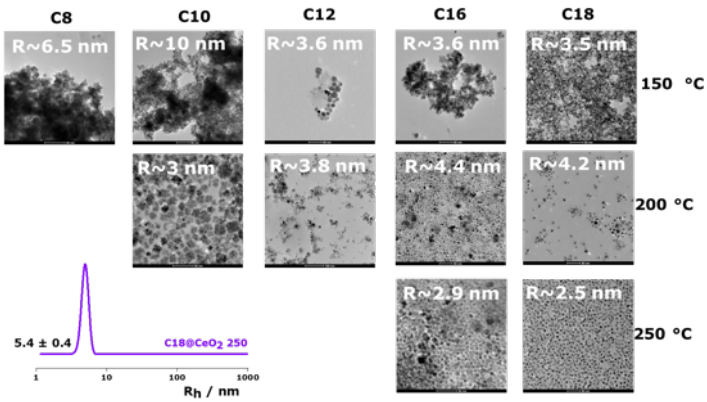

Figure 1: TEM images of CeO_2 NPs synthesized at different temperatures and with different capping agents; Hydrodynamic radius distribution of C18@CeO2 250 NPs in chloroform.

To utilize these nanoparticles as nanozymes, we chose to functionalize only the nanoparticles synthesized at 250 °C with oleylamine. We used two functionalization approaches, encapsulation in a bilayer using sodium oleate as a functionalizing molecule, and ligand substitution using, instead, a modified dopamine. In both cases, the functionalization occurred successfully, although sodium oleate allows to obtain the co-presence of functionalized single nanoparticles and small functionalized aggregates (about 20 nm of hydrodynamic radius), while the exchange of ligands leads to the formation of functionalized single nanoparticles. Finally, the obtained nanoparticles were found to be non-toxic and antioxidant, as shown in Figure 2 (Gallucci et al. 2021).

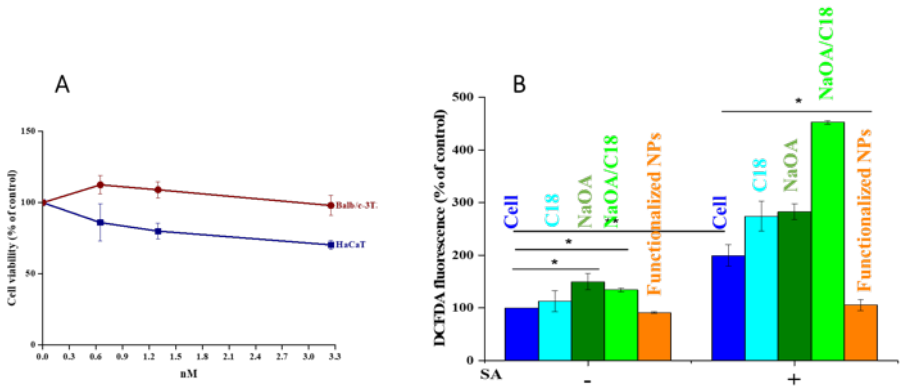

Figure 2. MTT assay (A), DCFDA Assay (B).

References

[1]Bai, Y.; Li, Y.; Tian, L. “Advanced Biological Applications of Cerium Oxide Nanozymes in Disease Related to Oxidative Damage”, ACS Omega, 9, 8601-8614 (2024).

[2]Gallucci, N.; Vitiello, G.; Di Girolamo, R.; Imbimbo, P.; Monti, D. M.; Tarallo, O.; Vergara, A.; Russo Krauss, I.; Paduano L. “Towards the Development of Antioxidant Cerium Oxide Nanoparticles for Biomedical Applications: Controlling the Properties by Tuning Synthesis Conditions”, Nanomaterials, 11, 542 (2021).

1A – Chemical pickling treatment to improve the corrosion resistance of additively manufactured Ti-6Al-4V

L. Nani, S. Lorenzi, T. Persico, D. Fiorona, M. Cabrini, T. Pastore (Department of Engineering and Applied Sciences, University of Bergamo, Dalmine (Bg), Italy)

Aims

This study aims to investigate the influence of chemical pickling on the corrosion performance of Ti-6Al-4V alloy produced by additive manufacturing through laser powder bed fusion (LPBF) and electron beam melting (EBM). Although these processes allow for high design flexibility and improved osseointegration due to the inherent surface roughness, residual partially melted particles adhered to the surface may detach, leading to metal ion release and potential inflammatory reactions in biomedical applications. The work therefore focuses on optimizing a pickling treatment capable of removing loosely bonded surface particles while preserving the topological features beneficial for osseointegration. Comparative analyses were carried out on as-built and heat-treated specimens, in polished and pickled conditions, by employing electrochemical methods in simulated body fluid.

Results

The optimized pickling procedure, consisting of five cycles of immersion in a nitric and hydrofluoric acid solution, effectively reduced the number of loosely attached particles present on the as-built surfaces without eliminating the surface roughness required for osseointegration. Surface analyses revealed that the treatment decreased the Sa parameter by approximately 20% in EBM and nearly 50% in LPBF specimens, while confocal reconstructions confirmed the removal of weakly bonded spherical particles (figure 1). Electrochemical investigations demonstrated that pickled samples exhibited the lowest steady-state current densities during long-term potentiostatic polarization, indicating reduced ion release rates (irr) (figure 2). In contrast, polished specimens showed higher currents due to the exposure of subsurface porosities, while as-built surfaces displayed localized spiking events linked to residual unmelted particles. Electrochemical impedance spectroscopy corroborated the potentiostatic findings, showing an increase in impedance modulus over time and confirming passive film growth. A strong correlation between EIS data and potentiostatic measurements suggested that non-destructive impedance tests can reliably estimate ion release behavior. Importantly, no significant differences in long-term corrosion performance were observed between LPBF and EBM samples, nor between as-built and heat-treated conditions, emphasizing that surface topology rather than microstructure dominated the corrosion response.

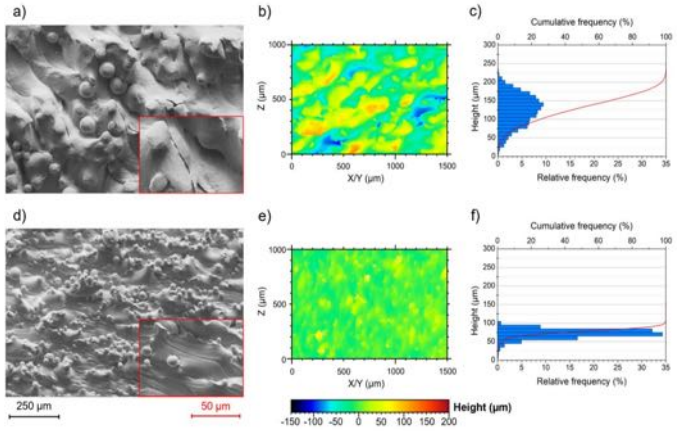

Figure 1: The estimated long-term ion release rates suggested that the values measured after one week of exposure would only be reached again after 11÷14 years in service, underlining the relevance of pickling as an effective surface modification to mitigate early-stage inflammatory risks.

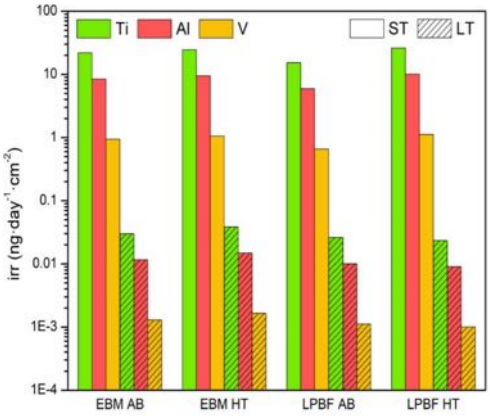

Figure 2

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1A – Development of Innovative Strategies for Controlling the Size and Stability of Amorphous Calcium Phosphate Particles

R. Gelli, D. Briganti, F. Ridi

Aims

Controlling nanoparticle size is critical for their effectiveness in nanomedicine applications such as drug delivery, targeting, and imaging. This is primarily because particle size significantly influences in vivo transport behavior, due to various physiological size thresholds and size-dependent interactions within biological systems. In this context, amorphous calcium phosphate (ACP)-based nanoparticles emerge as a promising platform, thanks to their biocompatibility, biodegradability, biological relevance, low cost, pH sensitivity, and porous structure—features that support the loading of therapeutic agents. However, their biomedical potential is limited by a strong tendency to aggregate in aqueous environments, often forming micron-sized particles prone to crystallization. As a result, achieving stable ACP-based nanoparticles with controlled size and preserved amorphous phase remains a significant challenge.

In this scenario, we are developing different strategies to control size and stability of ACP nanoparticles, mainly relying on proteins (Fetuin-A and Albumin), polymers (polyacrylates) and bisphosphonate molecules.

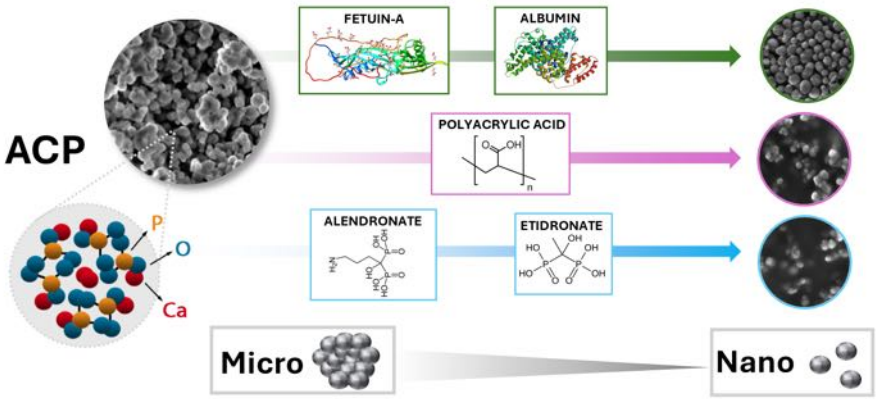
Results

We demonstrated that the glycoprotein Fetuin-A, either on its own or in combination with albumin, can significantly reduce the size of ACP particles—from several microns down to a few hundred nanometers—and can also delay the transition from the amorphous to crystalline phase in a concentration-dependent manner.

Nanoparticles with excellent redispersibility were also obtained using polyacrylates of different molecular weight. The presence of such polymers in the ACP-formation medium lead to nanoparticles with tunable size. Different Ca/Mg ratios were also tested, showing that the ratio between the two ions in the final nanoparticle can be controlled and results in a different stability of the amorphous phase in solution.

Concerning bisphosphonates, molecules such as alendronate, etidronate, zolendronate and ibandronate can control the assembly of ACP clusters in solution. The size of the obtained particles is strongly related to the concentration and type of bisphosphonate, leading to functionalized nanoparticles which could potentially be further functionalized with targeting agents or fluorophores.

The described systems were investigated using a comprehensive multi-technique approach, including dynamic light scattering for size analysis in solution, transmission and scanning electron microscopy for morphological characterization, X-ray diffraction and IR spectroscopy for crystallinity assessment, and thermal analysis. Altogether, our findings offer valuable insights into the controlled synthesis of ACP-based nanoparticles with tunable size and crystallinity, supporting their potential use in nanomedicine.



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1A – EPR spectroscopy on complex matrices: from the soil, through the leaves to the final product oil and wine, for traceability, quality and shelf-life analyses

J. Costa, M.C. Baratto*, F. Borghini*, R. Nardin*, A. Riccaboni°, R. Pogni**

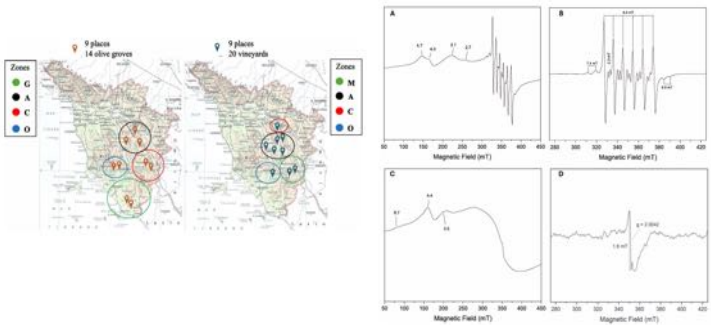
**Department of Biotechnology, Chemistry and Pharmacy*
°Department of Business and Law, University of Siena, Italy)

Aims

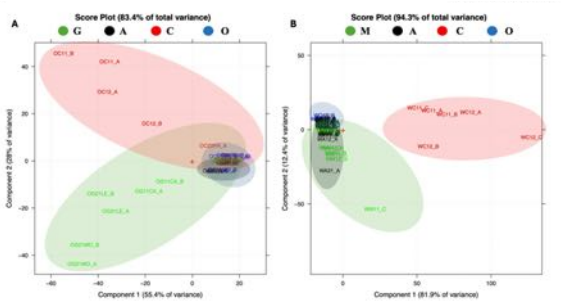
Electron Paramagnetic Resonance (EPR) spectroscopy is an accepted technique for studying agricultural complex matrices. This presents a significant advantage, as it enables the characterization of complex matrices without the need for purification processes, maintaining the sample intact and reducing experimental time compared to other techniques. The technique has been employed to analyze soils and leaves from vineyards and groves at room temperature. 33 soil samples and 31 leaf samples from olive groves and 53 soil samples and 19 leave samples from vineyards, were collected from different areas in Tuscany. The samples were examined on the basis of the principal signal of manganese ion which was present in all samples and quantified. Furthermore, taking into account the characteristic lineshapes of the spectra and integrating these data with Principal Component Analysis (PCA), a new, innovative, and effective method for differentiating samples on the basis of their geographical origin was developed. EPR spectroscopy combined to spin trap approach, antioxidant assays and compositional analysis has also been used to comprehensively assess the oxidative stability of extra virgin olive oils (EVOOs).

Results

In the following figure EPR spectra from soil samples collected from different areas of Tuscany represented by various contributions of transition metal ions and radical species are reported.



The spectrometric data of soils from olive groves (A) and from vineyards (B) combined with a statistical analysis were used to highlight differences and similarities correlated with the sample origin. The integration of EPR analysis with multivariate techniques provides a robust tool for clustering soils and leaves from olive groves and vineyards.



The oxidative stability and quality were determined through EPR-spin trapping technique using the PBN and the scavenging assays towards Galvinoxyl and DPPH radicals. The antioxidant capacity was correlated with the polyphenol content, while tocopherols showed a strong association with shelf-life. A direct investigation of radical formation to assess the oxidative stability of extra-virgin oils should be complemented by a thorough analysis of their chemical composition, enabling meaningful correlations between oxidative reactivity and the presence of key bioactive compounds.

The research project has been funded under the PNRR-AGRITECH-Spoke9, Missione 4, Componente 2, Investimento 1.4 – D.D.1032 17/06/2022-CN00022.

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1A – Euramet project ConcenSus: Establishing traceable concentration measurements of particles for a more sustainable industry

Y.A. Diaz Fernandez, L.R. Doveri, P. Pallavicini

Aims

Transitioning to a sustainable industry requires advanced materials for priority sectors like energy, semiconductors, health and personal care. Advanced complex particles defy accurate measuring by current methods, therefore there is a need for updating current standards to include traceable evaluation of the number concentration of complex particles to address industry regulations. This requires development of accurate, harmonised methods for measuring the particle density and refractive index required by established industrial practices for number concentration determination. Proposals addressing this SRT should deliver methods and documentary standards that enable regulatory compliance and commercialisation of particle-based products of value to sustainable industry. The project started in June 2025 and will last for three years.

Results

The specific objectives are:

1. To develop relevant (for health and personal care, semiconductor or energy materials, or represent typical environmental pollutants such as nanoplastics) representative test materials (RTMs) for number concentration measurements of nano- and sub-micrometre particles. The RTMs shall cover relevant ranges of density, size and concentration (low for pollutants, high for industrial particles) and come with indications of refractive index, size, and density.

2. To verify the performance of established references and laboratory methods for measurements of the number concentration of relevant RTMs and to develop new, material-specific sample preparation protocols for, e.g., imaging methods. To run an interlaboratory comparison to compare the performance of particle (between 1 nm and 100 nm) counting methods and ensemble methods (e.g., SMLS, SAXS, MADLS, DCS, UV-Vis, Raman spectroscopy).

3. To develop traceable methods for particle material characterisation, aiming to reduce the uncertainty of concentration measurements by ensemble methods, and to define uncertainty requirements for density and refractive index as input parameters for number concentration measurements. For density measurements, to consider a selection of methods such as TGA, CLS, XRD, multi-velocity CLS and dry mass measurements. For refractive index measurements, to consider ensemble and single-particle methods such as FCM, UV-VIS, FFF-RI, light scattering, and laser diffraction.

4. To validate modelling of material parameters in the measurement processes and develop a roadmap for generating traceability and standardisation of particle refractive index measurements.
5. To collaborate with the technical committees CEN/TC 352, ISO/TC 24/SC 4 and ISO/TC 229 and ISO/TC 276 and the users of the standards they develop to ensure that the outputs of the project are aligned with their needs, including the revision of standards ISO TS/24672 on particle concentration.

1A –EURAMET project MetrINO-Metrology for innovative nanotherapeutics (22HLT04/h03-)

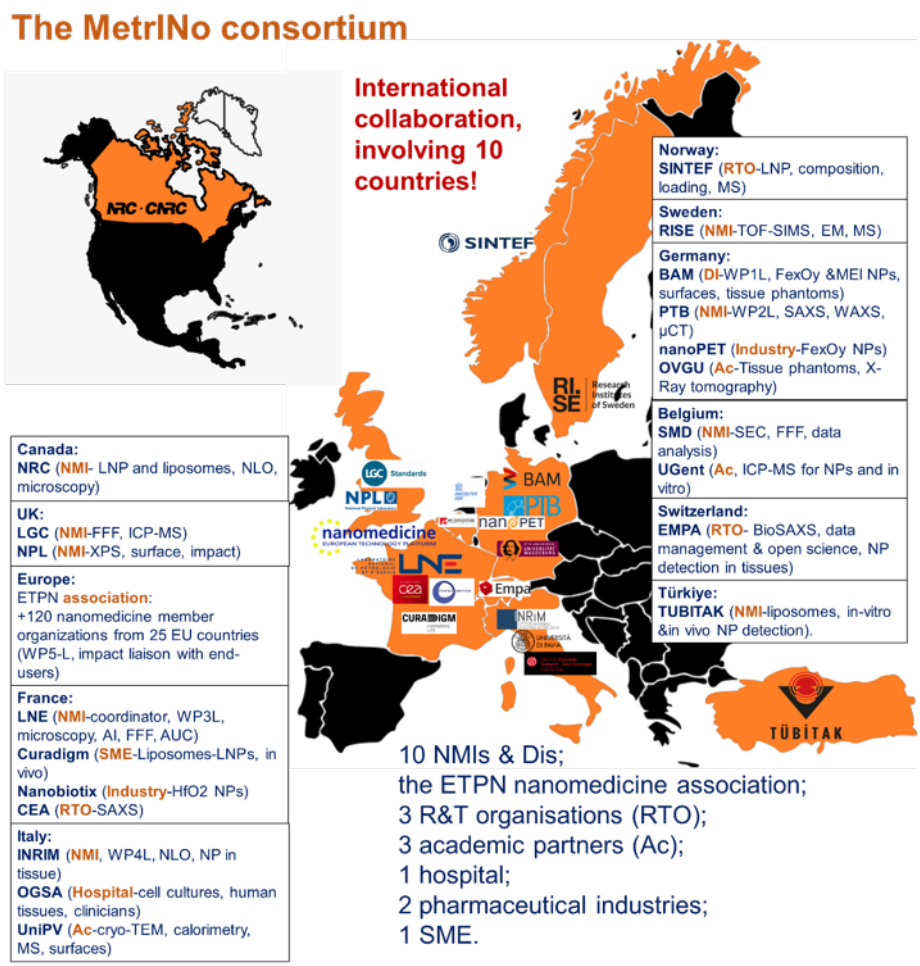
Y.A. Diaz Fernandez, L.R. Doveri, P. Pallavicini, C. Milanese

Aims

MetrINo responds to the immediate metrological needs expressed by industry, regulatory agencies and policymakers to develop, and validate traceable measurement methods and reference materials for the assessment of the critical quality attributes of nanotherapeutics. The project focus on clinical formulations, including synthetic lipid-based and metal oxide nanoparticles used for localised cancer treatment, gene therapy, vaccines (COVID-19) or as contrast agents. Candidate reference materials will be developed and used for measurement control. MetrINo will develop and validate traceable methods to measure nanoparticle physical properties, biotransformation in biological media, and methods for their identification and quantification in cells and tissues.

Results

The project is coordinated by the LNE, Laboratoire national de métrologie et d'essais. The international consortium involving 10 countries is composed by 10 national metrology institutes or designated institutes (LNE, BAM, PTB, RISE, SMD, TUBITAK, INRIM, LGC, NPL, NRC), the ETPN nanomedicine association; 3 research and technology organisations (SINTEF, EMPA, CEA), 3 academic partners (UPv, OVGU, UGent) 1 hospital (OGSA), 2 pharmaceutical industries (NanoPET, NanoBiotix) and 1 SME (Curadigm) that are key experts in the field of nanomedicine. MetrINo is further supported by more than 20 international stakeholders. The project will be completed by June 2026.



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1A – Fabrication of Carbon-based Perovskite solar celland Modules for Indoor and Outdoor applications with Eco Profile analysis using Life cycle assessment

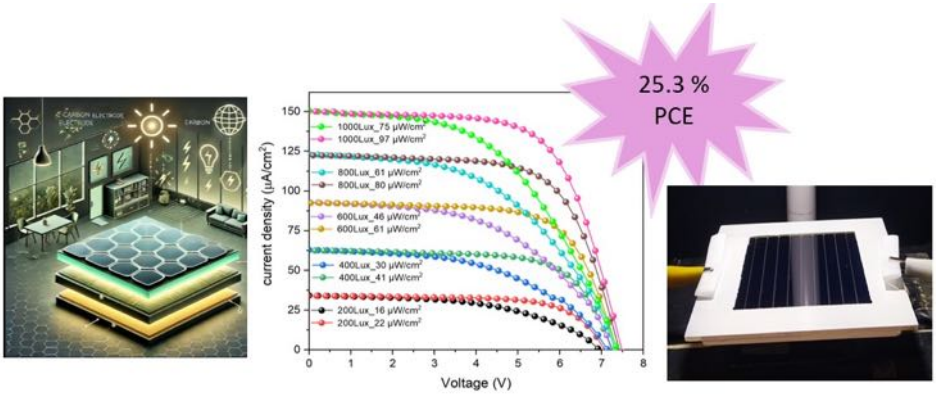
K. Pandurangan, M.L. Parisi, A. Sinicropi (Dept. of Biotechnology, Chemistry and Pharmacy, University of Siena, Italy), L. Vesce, A. Di Carlo (Centre for Hybrid and Organic Solar Energy (C.H.O.S.E.), Department of Electronic Engineering, University of Rome Tor Vergata, Italy)

Aims

Perovskite solar cells (PSCs) have emerged as a revolutionary photovoltaic technology owing to their exceptional power conversion efficiencies (PCEs), low manufacturing costs, and solution-processable fabrication methods [1]. Perovskite materials exhibit excellent optoelectronic properties, including strong light absorption, long carrier diffusion lengths, tunable bandgaps, and high defect tolerance. Since their first demonstration in 2009 with an efficiency of ~3.8%, PSCs have rapidly evolved, achieving certified efficiencies exceeding 27% in less than two decades. Compared to conventional technologies, PSCs offer reduced material usage, a lower carbon footprint, simple manufacturing processes (including roll-to-roll feasibility), low-temperature processing, and short energy payback times. With increased operational lifetimes, PSCs can reduce CO_2 emissions by up to 50% compared to silicon technology, depending on a country's energy mix. Life cycle assessment (LCA) studies of PSC modules reveal that over 70% of the total environmental impact originates from the metal top contact[2,3]. Replacing this with carbon electrodes improves environmental compatibility and enhances device stability by suppressing metal ion migration.
The aim of this work is to fabricate high-efficiency, carbon-based PSCs entirely outside a glovebox, under ambient air, using a scalable blade-coating technique.

Results

Through systematic optimization of all layers in the device stack, we have achieved cell efficiencies of 18% and module efficiencies of 17%, with only a 6% loss upon upscaling to lab-scale modules (120 cm^2). These solar cells exhibit excellent thermal stability with no performance loss after 1000-hour, T_{80} > 1600 hours in Maximum power point tracking. Carbon-based PSCs also demonstrate strong indoor performance, with PCEs exceeding 32% for cells and 25% for modules under indoor lighting. LCA was conducted from cradle to gate, focusing on the environmental impact of the manufacturing phase



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1A – Fluorine-doped ZnO quantum dots as smart nanoplatforms for optical biosensing

N. Gallucci, A. Cangiano, S. Russo, L. Paduano, G. Vitiello
(U.O. of Naples, University of Naples Federico II)

Aims

Bacterial infections cause numerous risks to human health. Gram(-) is a major source of infection due to the presence of endotoxins, such as lipopolysaccharides (LPS), within their outer membrane. For this reason, it is important to develop a biosensor that can specifically detect and quantify Gram(-) pathogens (McConnell et al. 2020). Biosensors combine a biorecognition mechanism with physical transduction, leading to selective and sensitive detection of analytes. This project aims to develop a biosensor by optimizing the matrix, consisting of F-doped zinc oxide quantum dots (F-ZnO QDs), and choosing the appropriate biomolecule (e.g., LA27 aptamer). In this way, the aptamer labeled with a fluorescence probe should act as the energy donor, and QDs as energy acceptor. By analyzing the optical response of the aptasensor, the presence of LPS and their quantification will be detected. Here, F-ZnO QDs at different F-concentration were synthetized and physico-chemically characterized to choose the best sample, in terms of size, morphology, and optical properties, to create the 2D platform for biosensor.

Results

ZnO QDs naturally present defects in their crystalline structure, such as oxygen vacancies or interstitial zinc. Thanks to this peculiar structure, these defects can be occupied and/or increased by doping agents introduced in the synthesis phase, which can amplify and/or modify the intrinsic properties of QDs. To amplify the fluorescence intensity of the ZnO QDs, different atomic concentrations of fluorine (0 to 20%) were tested. The physicochemical characterization of the obtained QDs showed that the doping agent does not alter their crystal structure, dimension and morphology, but has an effect on the optical properties of the nanomaterial of facts.

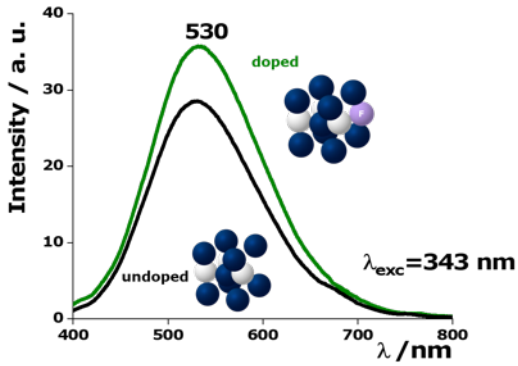

Figure 1: Fluorescence spectra of undoped (black line) and doped (green line) of ZnO QDs.

As shown in Figure 1, the fluorescence intensity is greater in the doped system than in the non-doped one and thanks to a quantitative analysis employing the determination of the quantum yield, it has been demonstrated that a doping of 1.5% at of fluorine increases the quantum yield of the ZnO QDs by 22% (Gallucci et al. 2024).
The QDs system with the best optical properties was chosen, and deposition conditions were optimized. To this end, both silicon and glass supports, and different deposition conditions were tested in terms of nanoparticle concentration and rotation speed. By combining ellipsometry and X-ray reflectivity measurements, it was demonstrated that the best support for obtaining a single thin film of nanoparticles is silicon (Figure 2). Furthermore, from the analysis of the different results, the best deposition conditions were determined, i.e., a suspension of QDs of 3.0 mg/mL and 3000 rpm as the best rotation speed in the spin coating process (Gallucci et al. 2025).

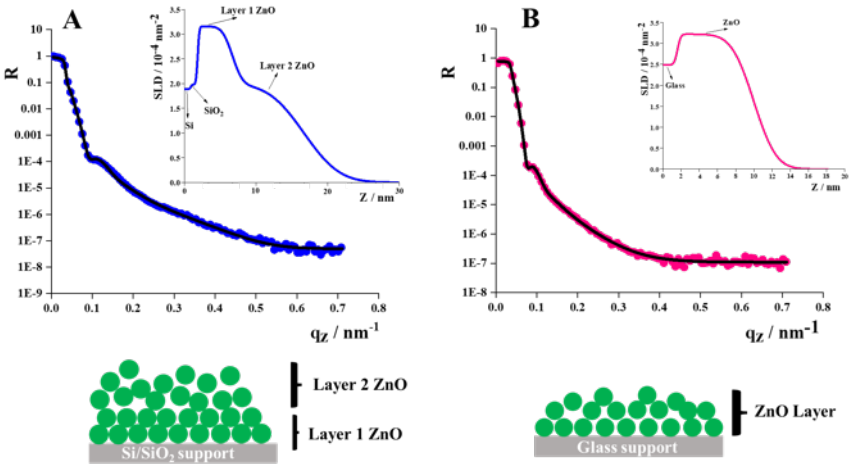

Figure 2: XRR experimental data (circles) and the best fit (black line) of ZnO QDs on silicon (A), and on glass (B) supports. The corresponding SLD curves are shown in the inserts.

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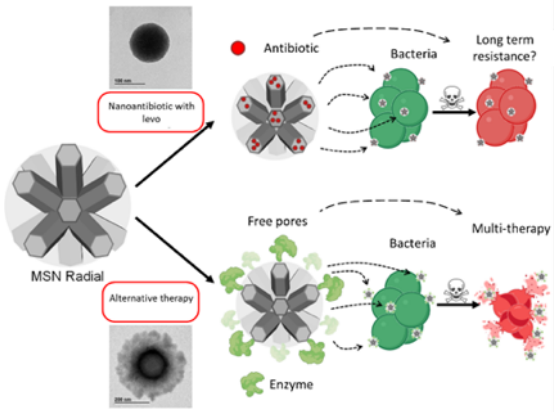
1A – Immobilized enzymes on radial mesoporous silica nanoparticles as bionanoantibiotics against Staphylococcus aureus bacteria

C. Carucci, A. Salis, M. Monduzzi, B. González, M. Colilla, I. Izquierdo Barba, M. Vallet Regí (Universidad Complutense de Madrid, UCM, Madrid, Spain)

Aims

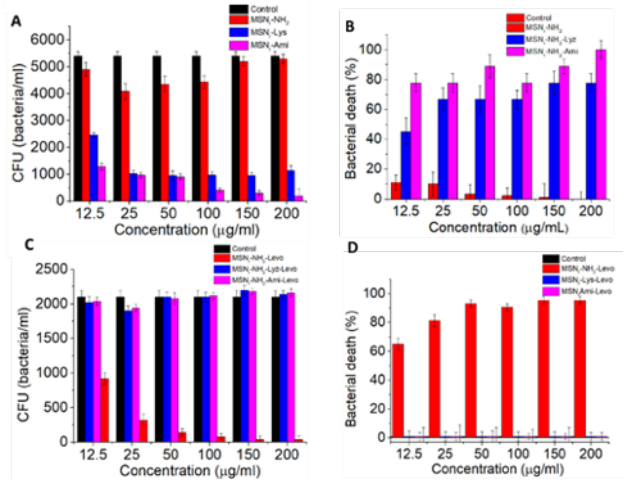
Antibiotic resistance poses a growing global health threat, particularly in implant-associated bone infections where implant surfaces promote colonization by Staphylococcus species. Conventional antibiotic therapies carry side effects and drive resistance, motivating alternatives such as antibacterial coatings and nanoscale drug carriers. Mesoporous silica nanoparticles offer high surface area and facile functionalization and have been used to deliver antibiotics including gentamicin, ampicillin, and levofloxacin. Enzymatic hydrolases that degrade bacterial cell wall components, such as glucosaminidases, muramidases (lysozyme, lyz), and transglycosylases, represent a promising nontraditional antimicrobial approach. Immobilization of enzymes on solid supports enhances stability and enables responsive delivery, and previous work has demonstrated antibacterial effects for lysozyme and other enzyme-functionalized MSNs. β-N-acetylglucosaminidase (dispersin B, Ami) hydrolyzes the glycan backbone of peptidoglycan and is effective in biofilm dispersion, yet its bactericidal performance when immobilized on MSNs remains unexplored. Here, β-N-acetylglucosaminidase was grafted onto radial amino-functionalized MSNs for the first time, lysozyme was immobilized in parallel for comparison, and selected particles were loaded with levofloxacin to evaluate potential synergistic or antagonistic effects against planktonic Staphylococcus aureus.



Results

Radial Mesoporous silica nanoparticles (MSNr) were characterized by TEM, DLS, ζ-potential, FTIR, TGA and elemental analysis, confirming successful enzyme

immobilization. MSNr were impregnated with levofloxacin (Levo) before enzyme grafting to test for synergistic or antagonistic interactions. Levo loading (0.069 mmol/g) was achieved despite small pore diameters, and release occurred primarily within 5 hours under physiological conditions. Enzymatic activity of the immobilized enzymes was also tested. MSN-enzyme nanosystems were verified in planktonic against Staphylococcus aureus Gram-positive bacteria. Bare MSNr and MSNr-NH2 were inactive, whereas MSNr-NH2-Lyz induced a concentration dependent bacterial death (45% at 12.5 µg/mL, 80% at 25 µg/mL). Despite lower enzyme loading, MSNr-NH2-Ami showed higher efficacy (79% death at 12.5 µg/mL, full removal at 200 µg/mL). MSNr-NH2-Levo exhibited antibacterial activity, but loading Levo with surface-grafted enzymes suppressed bacteria elimination, suggesting an antagonistic hydrolase inhibition by the drug. Overall, MSNr-NH2-Ami outperformed Levo-loaded systems at low doses, highlighting enzyme-functionalized MSNr as promising bionanoantibiotics.



Future directions include clarifying Levo induced enzyme inhibition, optimizing co-loading strategies to preserve activity, assessing cytotoxicity and in vivo safety, and developing regenerative agents to be loaded within pores, compatible with surface bound enzymes.

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1A – Investigating protein corona formation. BSA interactions with amino functionalized mesoporous silica nanoparticles are buffer specific.

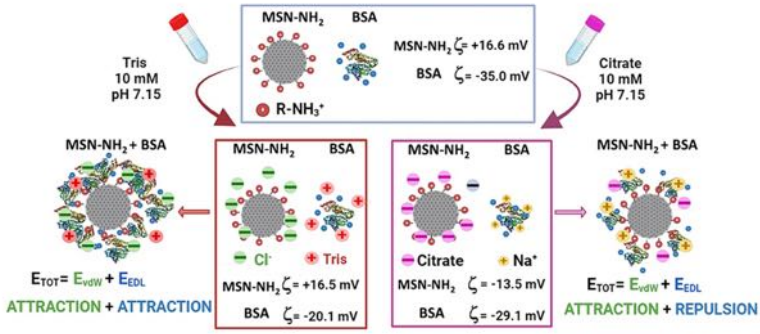
M. Mura, C. Carucci, E. Caddeo, D. Parsons, M. Piludu, A. Salis, Š. Sovová, M. Pekař (Brno University of Technology, Brno, Czechia), B. Jachimska (Jerzy Haber Institute of Catalysis and Surface Chemistry Polish Academy of Sciences, Krakow, Poland)

Aims

Hard matter based drug delivery systems have been studied for the loading and transport of several drugs due to their ability to overcome biological barriers and enhance drug targeting.[1] Among hard matters carriers mesoporous silica nanoparticles (MSN) present useful characteristics such as high surface area (> 700 m^2/g), tunable pore size for high drug loading and easiness in surface functionalization. [2] Once in contact with biological fluids, the MSN undergoes to the formation of protein layers, known as *"protein corona"*, which alters their physicochemical properties. Among the adsorbed proteins, dysopsonins such as albumin can prolong MSN circulation time, retarding clearance, and making their adsorption of particular interest.[3] In this work, the adsorption of bovine serum albumin (BSA) onto amino functionalized nanoparticles (MSN-NH_2) at physiological pH 7.5. In this work, we investigated how different buffer compositions affect the formation of the BSA protein corona around amino-functionalized mesoporous silica nanoparticles (MSN-NH_2). Specifically, Tris, BES, cacodylate, phosphate, and citrate buffers were compared at fixed pH 7.15 and at concentrations of 10, 50, and 100 mM, to elucidate their influence on both the amount of adsorbed BSA and on the electrostatic/dispersion energies of the nanoparticles.

Results

BSA adsorption was strongly buffer-dependent: at 100 mM, Tris promoted a maximum loading of 184 ± 3 mg BSA per g of MSN-NH_2, almost 4.4-fold higher than that observed in citrate (42 ± 2 mg/g). This difference cannot be explained solely by classical adsorption theories; the proposed mechanism combines electrostatic double-layer energy (E_{EDL}) with dispersive contributions (E_{vdW}). Zeta potential measurements further confirmed that MSN-NH_2 acquired positive potentials in Tris but negative ones in citrate, reversing the expected trend. This inversion is rationalized by including dispersion forces (dipole-induced interactions and polarizability) into the global energetic model, which effectively modulates electrostatic responses depending on the buffer. Overall, these results demonstrate that beyond pH and surface charge, the choice of buffer critically dictates nanoparticle–protein interactions, thereby directly influencing protein corona formation. [4]



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1A – Metal-Organic Frameworks and hierarchical MFI zeolite as support for Laccase Immobilisation

D. Tocco, R. Mastrangelo, E. Fratini, D. Chelazzi, P. Baglioni, A. Salis, M. Hartmann (Erlangen Centre for Interface Research and Catalysis FAU Erlangen–Nürnberg, Germany)

Aims

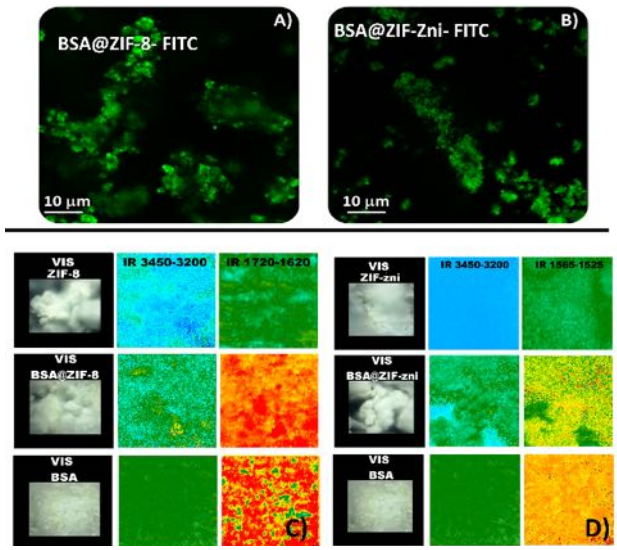
Laccase (LC) is highly efficient biocatalyst, but its use in industrial processes is often limited by harsh reaction conditions, such as extreme pH values and temperatures, which can lead to loss of catalytic activity. LC Immobilization on solid support can overcome these limitations by enhancing enzyme stability and enabling reuse. In the present research project, three trimesic acid–based MOFs (FeBTC, TbBTC, GdBTC), an imidazolate-based MOF (ZIF-zni), and a functionalised pure-silica hierarchical MFI zeolite (ZMFI, microporous–macroporous) were screened to find the support which allowed the best performance in terms of activity and stability to the immobilised *Aspergillus sp.* LC . Since the location of the enzyme can influence catalytic activity, the spatial distribution and conformational changes of BSA, used as a model protein, were investigated upon immobilisation within two different zeolitic imidazolate frameworks (ZIF-zni and ZIF-8).

Results

BSA protein and LC were immobilised *in situ* within FeBTC, TbBTC, GdBTC, ZIF-8 and ZIF-zni MOFs trough a mild reaction conditions (e.g. aqueous medium, neutral pH and room temperature). The LC immobilisation on MFI-Type Zeolite particles with embedded macropores was instead carried out post synthesis. A combination of WAXS, SAXS, SEM, TGA, FTIR, Raman and CLSM characterisation techniques were employed to investigate both pristine and bio-composite materials. Among the tested systems, LC@FeBTC showed the lowest activity (0.17 µmol min^{-1} mg^{-1}), while higher values were observed for LC@TbBTC (10.8 µmol min^{-1} mg^{-1}), LC@ZIF-zni (1.3 µmol min^{-1} mg^{-1}), and LC@GdBTC (6.6 µmol min^{-1} mg^{-1}). All MOF experiments were carried out at pH 5 due to the limited stability of MOFs under more acidic conditions. LC@ZIF-zni exhibited the lowest KM (21.6 µM) compared to LC@FeBTC (35.5 µM), LC@GdBTC (59.7 µM), and LC@TbBTC (97.9 µM), most likely due to mass-transfer limitations or conformational constraints related to the MOF environment. In contrast, experiments with the hierarchical pure-silica MFI zeolite (ZMFI), which is stable under acidic conditions, were carried out at pH 3. LC@ZMFI displayed a K_M of 10.3 µM and a V_{max} of 0.74 $\mu mol \cdot mg^{-1} \cdot min^{-1}$, highlighting the enhanced substrate affinity achievable under optimal pH conditions.

SAXS, CLSM analyses (A-B), and FTIR 2D imaging maps carried out on BSA@ZIF-8 and BSA@ZIF-zni (C-D) confirmed protein encapsulation and revealed conformational changes induced by immobilisation. BSA was found to be evenly distributed in micron-sized domains of 5–40 µm around the particles, while detailed SAXS analysis also suggested confinement within mesopores (4–8 nm), corresponding to cavities created by the protein itself. FTIR deconvolution revealed significant changes in protein

secondary structure: free BSA exhibited a high content of β-turns (~89%) and a low contribution of β-sheets (~4%). Upon immobilisation, the crystalline content increased markedly, with β-sheet and α-helix content rising to ~25% in BSA@ZIF-zni and ~40% in BSA@ZIF-8, accompanied by a drastic reduction in β-turns. These findings indicate that interaction with the MOF matrix promotes higher structural order in the protein.



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1A – Metallic nanocrystals: controlling optical properties through ligand density and solvent properties

A. Cangiano, N. Gallucci, L. Paduano
(U.O. of Naples, University of Naples Federico II)

Aims

This project aimed to synthesise and conduct a comprehensive physico-chemical characterisation of gold (Au-NCs), silver (Ag-NCs), and platinum (Pt-NCs) nanocrystals, which serve as the fundamental building blocks for creating supramolecular structures. The primary focus was to systematically investigate how the external solvent environment influences the nanocrystals' properties. Key solvent characteristics, specifically the dielectric constant and refractive index, were varied to understand their impact on the colloidal stability and optical response of the NCs. This foundational analysis is crucial for understanding and controlling the self-assembly behaviour of these nanocrystals into ordered aggregates.

Results

The metallic nanocrystals (M-NCs) were prepared using an oleylamine-mediated reduction method, where oleylamine acted as the solvent, reducing agent, and capping ligand. Transmission Electron Microscopy (TEM) analysis confirmed that the synthesis protocols yielded quasi-spherical nanocrystals for all three metal types. Statistical analysis of TEM images revealed mean core radii of 4.5 ± 0.8 nm for Au-NCs, 4.0 ± 0.9 nm for Ag-NCs, and 4.4 ± 0.8 nm for Pt-NCs. The consistent size and shape across the samples allow for a direct comparison of how different metal surfaces influence ligand interactions and subsequent assembly behaviour (Montanarella et al. 2022; Pansu et al. 2021). The oleylamine capping shell was analysed both qualitatively and quantitatively. Fourier-Transform Infrared (FTIR) spectroscopy confirmed the functionalisation of the metallic cores, showing characteristic vibrational modes for oleylamine on all three NC systems. A qualitative trend in the intensity of the FTIR peaks suggested a decreasing amount of oleylamine from Au-NCs to Ag-NCs and Pt-NCs. This observation was quantified using Thermogravimetric Analysis (TGA) to determine the ligand surface density (σ). The calculated ligand densities were 4.0 ± 0.2 chains/nm² for Au-NCs, 2.8 ± 0.5 chains/nm² for Ag-NCs, and 1.4 ± 0.4 chains/nm² for Pt-NCs. This confirms that oleylamine has a stronger affinity for gold surfaces compared to silver, and a significantly lower affinity for platinum surfaces.

The influence of the solvent environment on colloidal stability was investigated using Dynamic Light Scattering (DLS) by dispersing the NCs in four solvents with increasing dielectric constants: cyclohexane, toluene, ethyl ether, and chloroform. A consistent trend was observed for all M-NCs: the hydrodynamic radius (R_h) systematically decreased as the solvent's dielectric constant increased. For instance, the R_h of Au-NCs decreased from 7.1 ± 0.1 nm in cyclohexane to 5.8 ± 0.1 nm in chloroform (Figure 1). This is attributed to a change in the oleylamine ligand conformation, from an

extended state in low-dielectric solvents to a more compact one in high-dielectric solvents.

The optical properties of the M-NCs were also found to be dependent on the solvent environment. UV-Visible spectroscopy revealed that the maximum wavelength of the localized surface plasmon resonance (λ_{max}) experienced a red shift as the refractive index of the dispersing solvent increased. The refractive index sensitivity (S), defined as the change in λ_{max} per refractive index unit (nm/RIU), was determined by a linear fit of the data. Pt-NCs exhibited the highest sensitivity (S = 214 nm/RIU), followed by Ag-NCs (S = 102 ± 5 nm/RIU), while Au-NCs showed the lowest sensitivity (S = 54 ± 2 nm/RIU). These results are consistent with theoretical predictions and validate the experimental approach (Schulz et al., 2020; Cangiano et al. 2025).

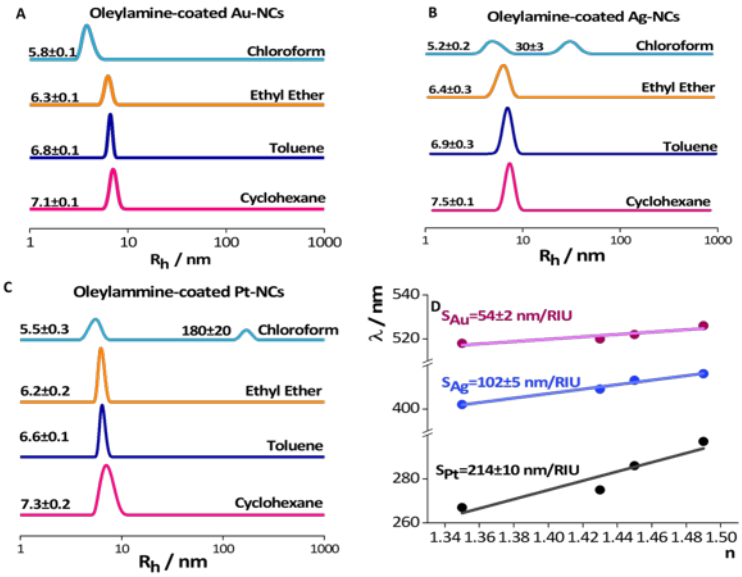

Figure 1: Solvent-dependent properties of metallic nanocrystals. (A-C) DLS measurements showing the hydrodynamic radii of Au-NCs, Ag-NCs, and Pt-NCs in various organic solvents. (D) LSPR peak wavelength versus solvent refractive index, showing the linear fit used to determine the sensitivity (S) for each metal

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1A – Nanoparticle-Imprinted Silica Gel for the Capture of Nanoparticles from Water

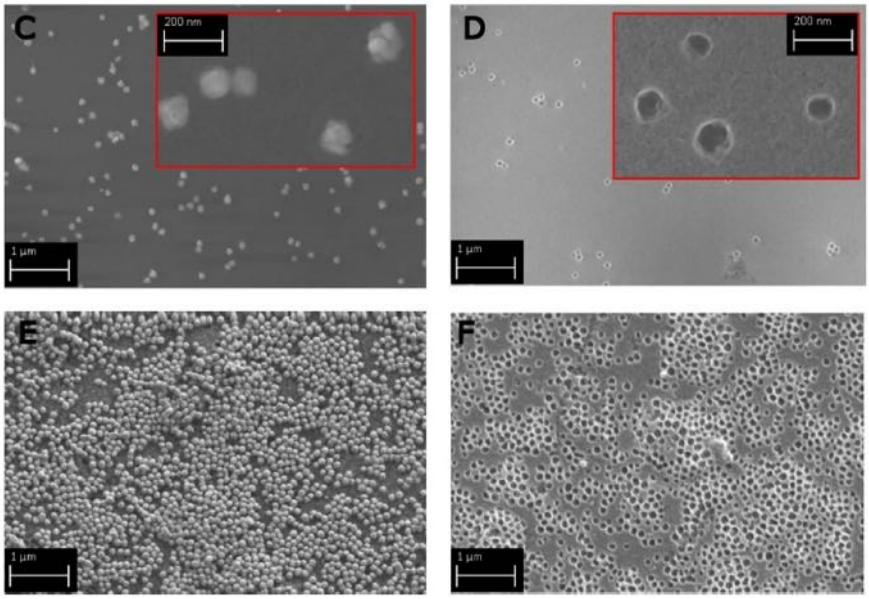
P. Pallavicini, Y.A. Diaz Fernandez, C. Milanese

Aims

Silica gel is an inert and relatively rigid material that can be prepared with embedded noble metal (Au, Ag) nanoparticles of different shapes and dimensions. Wet chemical oxidation, even with very strong oxidants (concentrated HNO_3, aqua regia) removes the particles without damaging the silica network, forming nanoimprinted materials with cavities of the same shape and dimensions of the oxidized nanoparticles. The nanoimprinted gels are to be used as remediation for nanoparticle-polluted waters, as they are able to reuptake nanoparticles with the same shape and dimensions of the cavities.

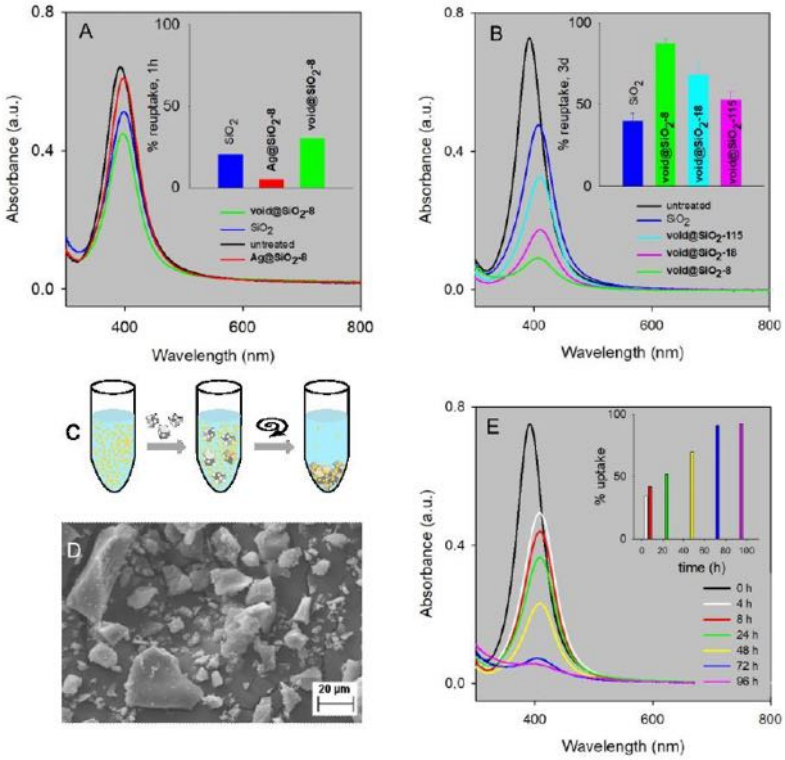
Results

Silica gel monoliths were prepared that embed well separated silver or gold spherical nanoparticles (NP), with diameters of 8, 18 and 115 nm. Fe^{3+}, O_2/cysteine and HNO_3 were all successfully used to oxidize and remove silver NP from silica, while aqua regia was necessary for gold NP. In all cases, NP-imprinted silica gel materials were obtained, with spherical voids of the same dimensions of the dissolved particles.



By grinding the monoliths, we prepared NP-imprinted silica powders that were able to efficiently reuptake silver ultrafine NP (Ag-ufNP, d = 8 nm) from aqueous solutions. Moreover, the NP-imprinted silica powders showed a remarkable size selectivity, based on the best match between NP radius and the curvature radius of the cavities, driven by the optimization of attractive Van der Waals forces between SiO_2 and NP.

Due to the latter observation, the reuptake process is expected to be poorly dependent on the type of material of the NPs to be reuptaken, so that these nanoimprinted materials are good candidates for the remediation of waters polluted with any kind of NPs



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1A – Optimized structural order and plasmonic enhancement in binary Au–CeO_2 superlattices

A. Cangiano, N. Gallucci, L. Paduano
(U.O. of Naples, University of Naples Federico II)

Aims

The self-assembly of different types of nanocrystals into binary superlattices is a powerful strategy for engineering the intrinsic properties of the constituent materials by exploiting collective interactions. This project investigates the co-assembly of plasmonic gold (Au-NCs) and semiconducting cerium oxide (CeO_2-NCs) nanocrystals. The primary goal is to establish a clear relationship between the nanoscale structural order, controlled by the Au-NC dopant concentration, and the resulting optical functionalities, specifically the plasmon-enhanced fluorescence of the CeO_2-NCs.

Results

In this work, we fabricated binary hierarchical assemblies by co-assembling CeO_2-NCs (~2.5 nm radius) with varying concentrations of Au-NCs (~4.0 nm radius), ranging from 0 to 3.0 mol%. The key finding is the discovery of an optimal dopant concentration at 1.6 mol% Au, which results in a maximum fluorescence enhancement of approximately 500% compared to disordered CeO_2 aggregates (Kim et al. 2023).

This remarkable optical enhancement is directly linked to a structural transition within the superlattice. Using Small-Angle X-ray Scattering (SAXS) and Cryo-Electron Microscopy (Cryo-EM), we determined that at the optimal 1.6 mol% Au concentration, the binary system assembles into highly ordered Frank-Kasper (FK) phases (Gallucci et al. 2024). In this specific architecture, the Au-NCs are successfully incorporated into the CeO_2-NCs host lattice. The enhancement mechanism is attributed to the Localised Surface Plasmon Resonance (LSPR) of the Au-NCs, which create intense electromagnetic hotspots that amplify the excitation and radiative decay rates of the surrounding CeO_2-NCs (Figure 1).

Conversely, at higher dopant concentrations (e.g., 3.0 mol% Au), the fluorescence enhancement decreases. Our structural analysis reveals that this is caused by a loss of long-range order due to phase segregation. The size mismatch between the two nanocrystal types introduces structural strain that, at high concentrations, leads to the exclusion of Au-NCs from the ordered domains. This frustration, supported by theoretical calculations of interparticle potentials, disrupts the precise architecture required for efficient plasmon-exciton coupling (Chen et al. 2023).

These results establish a definitive structure-property relationship, demonstrating that maximal functional enhancement in binary superlattices is achieved not just by adding a dopant, but by achieving a highly ordered, co-assembled state. This provides a clear design principle for fabricating advanced nanophotonic materials.

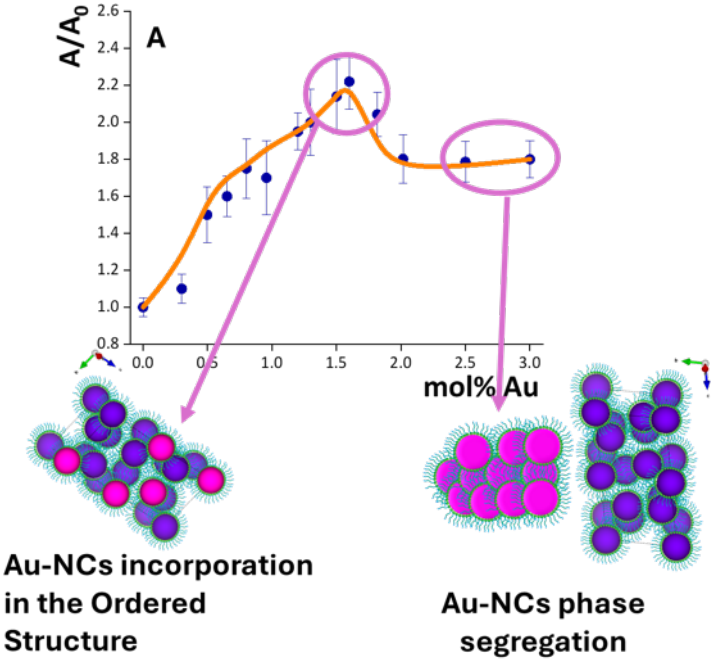

Figure 1: Normalised area below fluorescence emission spectra as a function of Au-NCs concentration with 3D schematic depiction of the Au-NCs incorporation into the CeO_2-NCs ordered structure, and the schematic depiction of the Au-NCs Phase segregation at higher doping concentrations.

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1A – Persistent Luminescent Hybrid Materials for Advanced Lighting Technologies

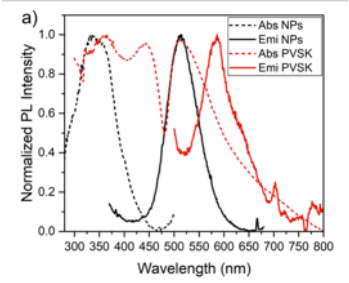
E. Cambiotti, R. Bondi, E. Fratini, L. Latterini

Aims

Persistent luminescence (PersL) is an optical process in which materials emit light for minutes or even hours after the excitation source is removed. PersL materials are highly promising for applications in bioimaging, biosensing, and advanced optoelectronic devices. In this study, we enhance the brightness of PersL nanoparticles by coupling them with lead-free perovskite nanocrystals (PVSK), which serve as efficient light-harvesting antennas and enable Förster-type energy transfer to maximize persistent emission. The resulting hybrid system is investigated both in solution and in solid-state within a stimuli-responsive polymer matrix (polydimethylsiloxane, PDMS) to fabricate luminescent, adaptive devices for potential applications.

Results

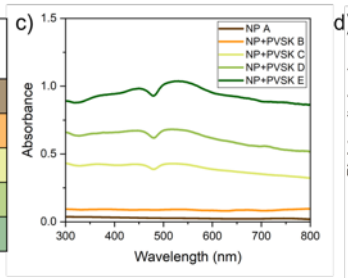
$SrAl_2O_4:Eu^{2+},Dy^{3+}$ PersL nanoparticles (NPs) exhibit absorption at 350 nm and emission at 510 nm, while $Cs_3Bi_2I_9$ perovskite nanocrystals with oleic acid ligands absorb across 350–550 nm and emit at 600 nm (Figure a). Coupling these nanostructures allows energy transfer from the PersL NPs donor to the PVSK acceptor upon excitation at 350 nm, increasing the overall luminescence efficiency.

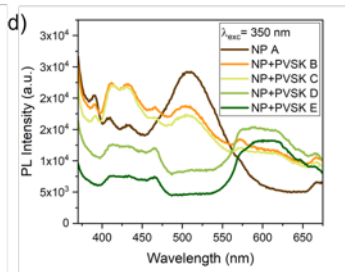


We first studied the hybrid system in chloroform dispersion, keeping the PersL NPs concentration constant and varying the PVSK content across five samples (Figure b). UV-Vis measurements indicate increasing absorption with higher PVSK concentrations (Figure c). Luminescence spectra show a progressive decrease in the PersL NPs emission at 510 nm as PVSK concentration increases (Figure d), confirming efficient energy transfer from the PersL NPs to the PVSK acceptor.

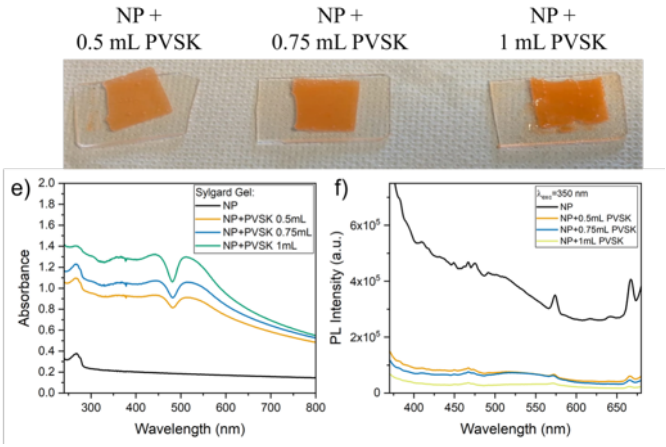
b)

Sample	NP:PVSK Ratio
A	Only PersL
B	2:1
C	1:1
D	1:1.5
E	1:2.3





Embedding the hybrid system in PDMS gels reproduces these trends. Absorbance increases with PVSK content, while PersL emission decreases (Figure e), demonstrating successful optical communication between the two species within a solid matrix. These results highlight the potential of PersL–PVSK hybrids for adaptive luminescent devices.



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1A – Photoactive biowaste-modified metal oxide nanoparticles for bacteria and microplastics treatment

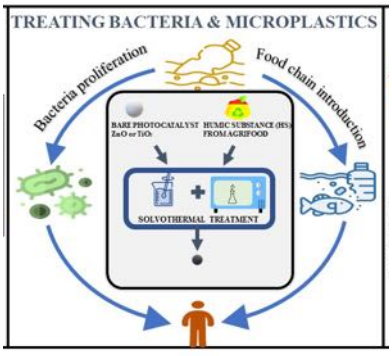
S. Russo, V. Venezia, R. Marotta (University of Naples Federico II), M. Cocca (CNR-IPCB, Pozzuoli), G. Vitiello (U.O. of Naples, University of Naples Federico II)

Aims

As a result of the accumulation in the environment, microplastics have become part of the food chain, boosting the resistance of fungi and bacteria which can easily meet human beings. Photocatalysis might be viewed as a potential strategy for the treatment of plastics and microplastic wastes as well as bacterial and fungi pathogens. The waste-to-wealth strategy is encouraging the design of functional hybrid organic-inorganic nanoparticles with enhanced photocatalytic and antimicrobial features, thus upholding the principles of the circular bioeconomy and environmental sustainability.

Results

A bottom-up synthetic strategy under solvothermal conditions was defined to combine at a molecular scale colloidal metal oxide nanoparticle (e.g. titanium dioxide, TiO2, and zinc oxide, ZnO) with humic substances (HS) extracted by agrifood biowastes. HS represent the alkali-soluble fraction of natural organic matter and are rich in functional groups, including carboxyl, phenol, hydroxyl, and quinone moieties, thus conferring them useful functional properties, such as metal ions chelation, organic pollutants absorption, paramagnetic and red-ox behaviour for generation and/or scavenging of Reactive Oxygen Species (ROS). This synthetic strategy lead to hybrid nanoparticles with an advanced ability in generating ROS and a significant multifunctionality acting as antimicrobial agents against different bacterial and fungal strains and as nano-photocatalysts (Venezia et al. 2023; Amato et al. 2023).



Specifically, physicochemical analyses indicated the formation of hybrid nanomaterials with morphology and size which were finely dependent by adopted synthetic conditions and nature of the inorganic component conjugated with HS. The hybrid nanomaterials showed an enhanced ability in producing •OH radicals in

aqueous environment after UVA/light irradiation greater than that of the bare ones. This effect was ascribed to the intrinsic free-radicals of HS, which played a key role in oxidating the polymeric chains and, simultaneously, in conferring an advanced biocide activity (Russo et al. 2024).

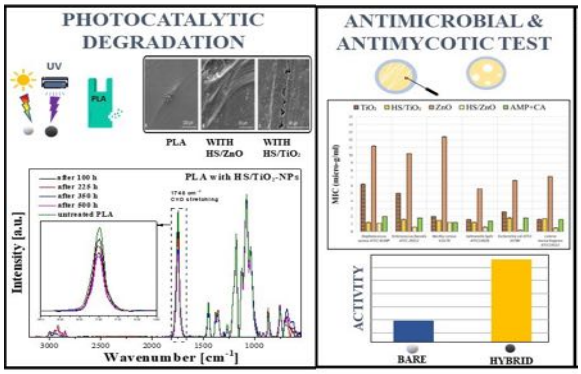


Figure 1: Photocatalytic degradation and antimicrobial/antimycotic tests of hybrid MeOx/HS nanoparticles without and under light irradiation.

Hybrid nanoparticles were able to favour the photodegradation of biodegradable polylactic acid (PLA) microplastics in water solution under both UVA and, alternatively, solar light at various intervals. At the same time, biological tests highlighted that the presence of HS strongly enhanced the antibacterial/antimycotic properties, since the diameter of the inhibition zone (DDK) increased, while the minimum inhibitory concentration (MIC) and the minimum bactericidal concentration (MCB) decreased (Figure 1). This approach represented a promising eco-sustainable strategy to design and apply advanced functional nanomaterials as photoactive nano-additives to be loaded into bioplastic films for food packaging for the simultaneous inhibition growth of bacteria and fungi and photodegradation of biopolymeric microplastics.

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1A – Physico-Chemical Properties of Pharmaceutical Systems

G. Bruni, D. Capsoni

Aims

In the pharmaceutical preformulation studies and in the quality control of pharmaceutical products a "polymorph screening" is required in order to collect as much information as possible on the existence of new crystalline forms of a given drug with the aim of identifying the thermodynamically stable form and the ways of interconversion between the forms. Unfortunately, it is not yet possible to achieve full control over the polymorph screening so much so that new solid forms are often obtained by chance rather than as the result of a systematic research. Furthermore, it is necessary to ensure that only the polymorph of interest is present in the dosage form. The regulatory agencies underline the importance of limiting the presence, in the pharmaceutical solids, of polymorphic impurities which, having different physico-chemical, technological and pharmaceutical properties, could compromise the efficacy, the stability and the safety of the product. Based on these considerations, the study of the crystalline polymorphism of the drugs is even more important than ever. This area includes the studies we conducted on ketoprofen and imepitoin.

Many drugs exhibit undesirable physicochemical properties which hinder the development of solid dosage forms. Among these properties, solubility is the most important, in fact it limits the potential bioavailability of molecules.

Salts and cocrystals are an efficient expedient to tailor the physico-chemical properties of drugs and in particular to enhance the solubility and dissolution rate of poorly water-soluble active principles so that their absorption from the GI tract can be improved and the desired therapeutic benefits can be reached in short times. The proper characterization of multicomponent crystalline systems of pharmaceutical interest is usually conducted by different investigation techniques among which DSC stands out as an excellent tool that can be used as a screening method for salts and cocrystals. One reason is that new binary crystalline entities can directly form from eutectic melting during the DSC experiment. DSC measurements are useful not only as a screening method to investigate the potential formation of new binary crystalline entities among specific components, but also to determine the composition and melting enthalpy of the new crystalline entity. Pimozide is the drug we considered to form a new multicomponent entity with improved pharmaceutical properties.

Results

Dexketoprofen shows a serious problem of polymorphic impurity and there was a strong industrial need to find a method that allows to quantify the presence of polymorphic impurity in batches of industrial production by the DSC technique. The main critical points of this system are constituted by the fact that the melting enthalpies of the two polymorphs (A and B) are very similar and the difference between the T_{onset} of their melting is just 2 °C. This second point makes it impossible to obtain an adequate resolution of the melting peaks, even when the experimental conditions are appropriately selected. A system characterized by this thermal

behaviour, in the scientific literature, is considered "impossible". The success of the method developed in our work is to be attributed, on the one side, to the methods adopted in the preparation of the physical mixtures of the two polymorphs, which need to have the composition as homogeneous as possible, and on the other side, to the idea of performing a conditioning of the samples that makes the low-melting temperature polymorph thermally inert. The polymorphic mixtures treated in this way show only the fusion of the high-temperature melting polymorph whose enthalpy decreases linearly with the increase of impurity. The method proposed here allows to detect the polymorphic impurity even when it is present in a very low percentage, equal to 0.3%, while it is possible to quantify it reliably for contents higher than 2%.
Scientific and industrial reasons dictated the study of the solid state of imepitoin. Our investigations allowed us to discover the existence of a new polymorph which finds itself in a monotropic relationship with the crystalline form (I) already known and present on the market. This form (II), obtained by crystallization from xylene, remains metastable under ambient conditions for at least 1 year. Both solid forms were characterized by thermal, spectroscopic, microscopic, and diffractometric techniques. The thermodynamic relationship between the two polymorphs (monotropic) is such that it is not possible to study the melting of polymorph II, not even by adopting appropriate experimental strategies. Our measurements highlighted that the melting peak of imepitoin actually also includes an onset of melt decomposition. The ab initio structure solution, obtained from synchrotron X-ray powder diffraction data collected, allowed us to determine the crystal structure of the new polymorph (II).
The in vivo efficacy of pimozide (*PMZ*) is limited by poor solubility. Therefore, adipic acid (*AAD*) was used as a coformer for the preparation of a binary product with improved pharmaceutical properties. The thermal behavior of the liquid-assisted grinding products of compositions included in the range $0.1 < X_{PMZ} < 0.9$ has been interpreted using a thermodynamic model according to which the two components originate a new crystalline entity in molar ratio *PMZ:AAD* 0.66:0.33, which forms an eutectic system with *AAD*. The model was confirmed using the quantitative analysis of the melting peaks and using PXRD and SXRD measurements. In particular, the latter have demonstrated that the new entity is actually salt [PMZH]2[adipate]. The crystalline product was characterized in terms of solubility and wettability. Then, a tablet formulation was developed, and its dissolution behavior was compared to a commercial product considered as a reference. The new entity showed improved solubility and wettability compared to the pure drug in both deionized water and bio-relevant fluids simulating oral administration in fed and fasted conditions.

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1A – Poly(3-hexylthiophene)-based smart biointerfaces for biomedical applications

G.M.L. Messina, P. Campione, R. Sciacca, L. Fabiano, G. Calabrese

Aims

In recent years, conductive polymers have raised as appealing materials in bioelectronics and tissue engineering because of their intriguing mixed ionic-electronic conductivity, biocompatibility, and adjustable physico-chemical characteristics. This study focused on bare P3HT and P3HT-based mixtures to connect with cells for biomedical purposes. The rise in electrical conductivity of P3HT-based blends is intriguing for potential integration with biological systems, promoting effective signal transduction between devices and cells, rendering it a suitable choice for bioelectronic interfaces. We investigated the morphological, nanomechanical, and physico-chemical characteristics of the surfaces. The highly promising findings emphasize the polymer's ability to influence cellular behavior via electrical, mechanical, and interfacial characteristics, promoting osteogenic differentiation even without specific growth medium or differentiation factors.

Results

Figure 1 shows the flat morphology of the P3HT pristine film (Fig. 1a), while the polymer blend exhibits a consistent distribution of the MWCNTs filler within the polymeric matrix throughout the sample (Fig. 1b). The roughness data (Fig. 1c) indicate that the addition of carbon nanotubes leads to a strongly increase in the average roughness of the samples. Furthermore, the formation of the mixture with MWCNTs affects the mechanical characteristics of the layer on the nanometer scale. The electrochemical characterization of the systems shows an increase of conductivity and capacitance of the polymer film with MWCNT as fillers. (Fig. 1d-f).

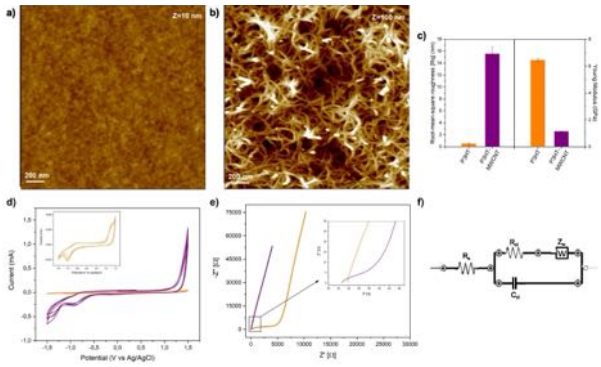

Figure 1

Given that substrate stiffness is crucial for how cells sense mechanical signals, the response of HT-22 cells on P3HT and P3HT-MWCNT thin films has been examined.

The results demonstrated a notable rise in cell viability and growth over time when compared to the glass control, emphasizing the influence of the cell-material interface on cell membrane properties, indicating that HT-22 responds actively to the surface nanostructures, facilitating the establishment of a neural cell network at the interface for use in neural interfacing and bioelectronics.

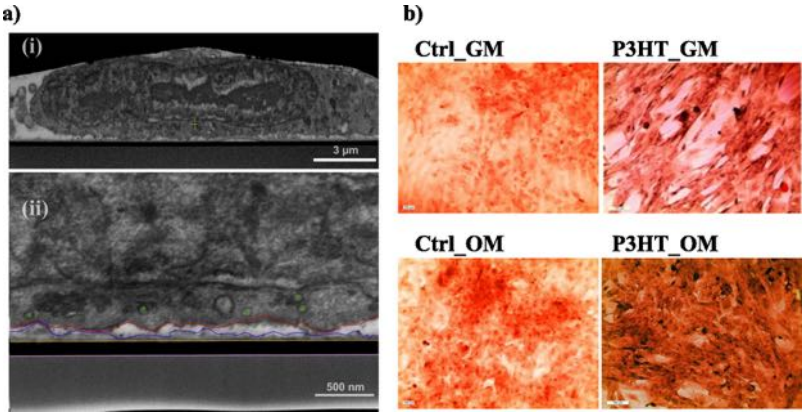

Figure 2

Additionally, the osteogenesis of human adipose-derived mesenchymal stem cells (hADMSCs) regarding cell behavior, cytoskeletal arrangement, and differentiation on electroactive thin polymer films (P3HT) was studied, utilizing both standard growth medium (GM) and osteogenic differentiation medium (OM).The findings indicated that the polymer surface is biologically compatible with hADMSCs and supports adhesion and proliferation in both GM and OM conditions. It is important to highlight that P3HT surfaces displayed a significantly high level of mineralization when exposed to both GM and OM, with the osteogenic differentiation medium specifically promoting calcium deposits, resulting in a noticeably stiffer extracellular matrix, as verified by Young's modulus assessments. In addition, elevated expression of osteoblastic markers on cells cultured on P3HT GM was more uniform than that observed on hADMSCs on P3HT OM. These encouraging findings showcase the remarkable osteoinductive characteristics of the thin polymeric film with semiconductive properties. These studies pave the way to further analysis for potential applications of this substrate in the field of biomaterials.
These investigations open the way to additional evaluations regarding possible uses of this substrate in biomaterials.

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1A – Spontaneous aggregation of soil organic matter and its interaction with iron oxide particles

E. Carretti, S. Baldini, F. Porpora, L. Dei, T. Duncan

Aims

Polydimethylsiloxane (PDMS) organogel sponges were prepared and studied in order tounderstand the role of pore size in an elastomeric network on the ability to uptake and release organic solvents. PDMS organogel sponges have been produced according to sugar leaching techniques by adding two sugar templates of different forms and grain sizes (a sugar cube template and a powdered sugar template), in order to obtain materials differing in porosity, pore size distribution, and solvent absorption and liquid retention capability.

Results

The sponges were characterized by Fourier-transform infrared spectroscopy with attenuated total reflectance (FTIR-ATR) and compared with PDMS slabs that do not contain pores. Scanning electron microscopy (SEM) provided information about their morphology. X-ray micro-tomography (XMT) allowed us to ascertain how the form of the sugar templating agent influences the porosity of the systems: when templated with sugar cubes, the porosity was 77% and the mean size of the pores was ca. 300 µm; when templated with powdered sugar, the porosity decreased to ca. 10% and the mean pore size was reduced to ca. 75 µm (Figure 1).

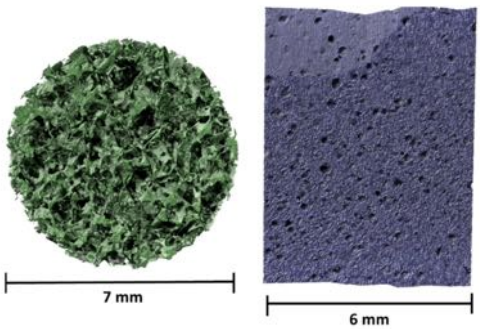

Figure 1: XMT 3D images for two different PDMS sponges: (left) PDMS_SugarCube; (right) PDMS_PowderedSugar.

A second approach was used, named “emulsion templating”. This method exploits the synthesis of water-in-oil (micro)emulsion to create cavities in the siloxane network with greater control over the pore size but pays in terms of difficulty of realization (the stability of a microemulsion is driven by a multitude of factors like temperature, volume, and mass ratio between the components and their purity) and in the expense of realization.

These materials, porous organic polymers (POPs), can absorb many solvents in different proportions as a function of their polarity (Figure 2). Absorption capacity, as

measured by swelling with eight solvents covering a wide range of polarities, was investigated.

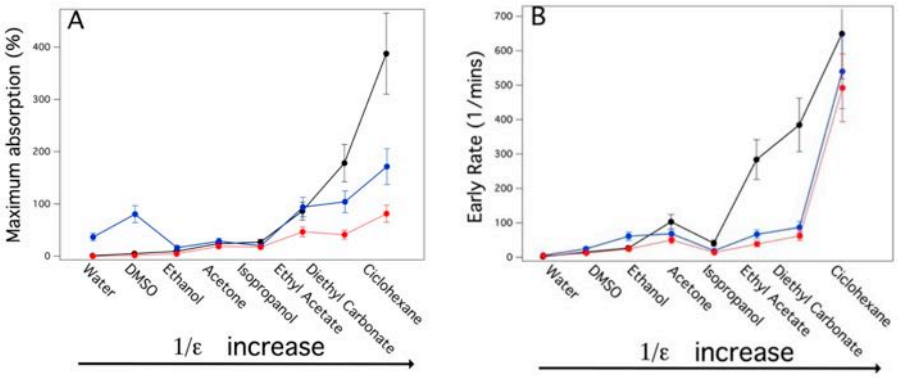

Figure 2: Maximum amount of organic solvent absorbed (A) and swelling rate (B) by PDMS slab (no porous) (red dots), PDMS_ PowderedSugar, (blue dots), PDMS_ SugarCube (black dots). The solvents on X axis are presented as a (red dots), PDMS_PS, (blue dots), PDMS_SC (black dots). The solvents on X axis are presented as function of 1/ε, where εis the dielectric constant of the solvents

Rheology data established that solvent absorption did not have an appreciable impact on the gel-like properties of the sponges, suggesting their potential for applications in cultural heritage conservation. Application tests were conducted on the surfaces of two different lab mock-ups that simulate real painted works of art. They demonstrated further that PDMS sponges are a potential innovative support for controlled and selective cleaning of works of art surfaces.

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1A - Study of low carbon formulations based on ground granulated blastfurnace slag

L. Campagiorni, F. Ridi

Aims

Using supplementary cementitious materials (SCMs) as cement replacement is a common practice to reduce carbon dioxide (CO_2) emissions and minimize the carbon footprint of global cement production, which accounts for 8% of all anthropogenic greenhouse gas emissions. [1] This research focuses on the study of the physico-chemical properties and hydration reactions of a low-carbon ternary blended cement, in collaboration with Ecocem company. Ternary blended cements are one of the most promising solutions to reduce the carbon footprint in the cement industry: these formulations are prepared by substituting a part of the classical Ordinary Portland Cement (OPC) with Supplementary Cementitious Materials (SCMs), powders coming from sustainable sources, that can provide binding properties, and with an inert filler. Being the development of these formulations very recent, their physico-chemical properties and the hydration kinetics are still not well understood.

Results

In this project the hydration kinetics, the rheological properties of the fresh pastes and the microstructure of cured samples have been investigated, studying the influence of three main parameters. In particular, several formulations have been prepared *i)* with fillers with different granulometry, *ii)* in the presence of different sulphate sources in the mix and *iii)* with superplasticizers having different chemical structure.

The results showed that the granulometry of the filler has an impact on the hydration kinetics and on the nature of the formed hydrated phases. Moreover, the sulphate source (calcium sulphates with different hydration degree) has been demonstrated particularly important in affecting the amount and the morphology of the aluminate hydrate phases. This result is particularly interesting as the characteristics of these phases determine the properties of the formulations at early stages and also the durability at longer time. Finally, superplasticizers characterized by different functional groups and chemical structure affect differently the fresh state properties of the formulations. These results, taken together, are particularly important because bring an advancement in the knowledge of the mechanisms that regulates the hydration reactions of these low carbon formulations, that are still in an infant stage with respect to those of the well-known Portland cement.

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1A – Synthesis and characterization of carriers for improved drugs' solubility and release

D. Capsoni, G. Bruni, C. Urru

Aims

Solubility of the drugs is a crucial parameter controlling oral drug adsorption in the gastrointestinal tract and its permeability through the gastrointestinal membrane. Poor soluble and permeable drugs often display insufficient and variable bioavailability, leading to negative concerns on safety and effectiveness. Several approaches are developed to enhance the bioavailability of these drugs. Among them, clay and nanoclay minerals as suitable hosts for drugs demonstrate high loading capacity and good control of dissolution rate and released amount of the drugs. Clay mineral materials, both natural and synthetic, display different morphologies and structures, and controllable size and porosity. Moreover, they are non-toxic and low cost.

In the present research project, we investigate the use of Layered Double Hydroxides (LDH), Halloysite nanotubes (HNTs), saponite (SAP) and laponite (LAP) as suitable carriers to control the loading and the release of some drugs belonging to the II Class of the Biopharmaceutics Classification System: zaltoprofen, carvedilol, meloxicam and perphenazine. The synthesized drug/clay hybrids were deeply investigated by several techniques (XRPD, SEM, EDS, TEM, FT-IR, Solid State NMR, TGA, DSC) to evaluate the drug loading and the drug-clay interactions. The pharmaceutical characterization (drug loading, wettability, solubility, and in vitro dissolution rate in different biorelevant fluids) put into evidence the promising feature of the hybrid systems, with improved dissolution rates.

Results

Firstly, we synthesize a new organic-inorganic adduct by insertion of the zaltoprofen active principle into the Zn/Al layered double hydroxide. The characterization techniques demonstrate the successful intercalation of the drug as carboxylate anion within the interplanar distance along the c axis of the LDH structure. The 13C and 27Al solid-state NMR demonstrates (i) the active principle strongly interacts with the host and the COO- and the OH moieties are involved respectively, (ii) zaltoprofen anions induce local structural changes in the host crystal structure, (iii) similar conformation of the molecules in the zaltoprofen crystal and those inserted into the LDH layers. Dissolution tests at pH 4.5 (gastric environment in fed state) and pH 6.8 (intestinal environment) show improved solubility and dissolution rate of the Zaltoprofen/LDH system (70-80% of the dose released in 2 hours in the two fluids). The results demonstrate the new composite promote both solubility and dissolution rate of zaltoprofen in different fluids simulating the gastro-intestinal environment, with great advantage for its bioavailability.

Carvedilol is a Class II poorly water-soluble drug employed to treat chronic heart failure. Our research points at developing new carvedilol-HNTs composites to enhance solubility and dissolution rate. Both commercial and etched (acidic and alkaline etching) HNT were used to synthesize the hybrids, to investigate how the applied

etching process affects the pharmaceutical behaviour of the drug. The simple and feasible impregnation method is used for carvedilol loading (30–37% weight). The etching and loading processes do not induce structural changes. The 27Al and 13C solid-state NMR and FT-IR results demonstrate that carvedilol interacts with the external siloxane surface of HNTs: in detail, the aliphatic carbons, the functional groups, and, by inductive effect, the adjacent aromatic carbons of the drug are involved in the interaction. All the carvedilol–halloysite composites display enhanced dissolution rate, wettability, and solubility, as compared to carvedilol. The carvedilol–halloysite system based on HNTs with the highest value of specific surface (HNT etched with HCl 8M) exhibits the best performance.

Meloxicam–halloysite nanotube composites were also explored as a viable approach to enhance the solubility and dissolution rate of meloxicam, a poorly water-soluble drug (BCS class II). Meloxicam is loaded via a solution method on both commercial and appositely modified halloysite (acidic and alkaline etching, or APTES and chitosan functionalization). All the drug–clay hybrids display high meloxicam loading (about 40 wt%). The halloysite modification processes and the drug loading do not alter the structure and morphology of both meloxicam and halloysite nanotubes, and weak drug–clay and drug-functionalizing agent interactions occur, involving the meloxicam amidic functional group. All the meloxicam–halloysite composites exhibit enhanced dissolution rates, as compared to meloxicam, and the meloxicam–halloysite composite obtained with chitosan-functionalized HNT showed the best performance both in water and in buffer at pH 7.5: this is explained by the chitosan grafting on the outer surface of halloysite nanotubes, which provides increased specific surface area disposable for drug adsorption/desorption.

Preliminary results were obtained by perphenazine-clay hybrids (clay: laponite, natural and synthetic saponite, and halloysite nanotubes), to enhance the Class II drug dissolution rate. All the hybrids exhibit weak drug-clay interactions, and fast dissolution rate at the pH of the gastrointestinal tract.

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1A – Synthesis of nanostructured materials for light harvesting and conversion

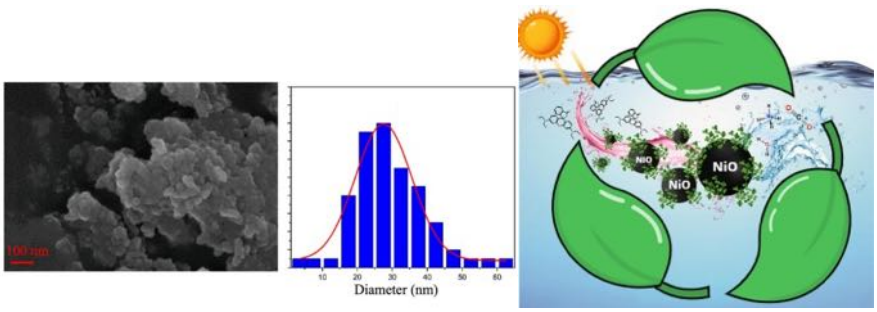
L. Latterini, G. Quaglia, A.M. Grigoras, R. Bondi, R. D'Amato

Aims

This project aimed to synthesize nanostructured materials with defined optical properties capable of absorbing electromagnetic radiation and converting it into light or photoproducts of significant optical value.
Formulation of bio-based smart hydrogels starting from protein denaturation. The product was functionalized with graphene to increase the hydrogel's electrical conductivity and with carbon dots, resulting in a hydrogel that exhibits stable luminescence properties over time. The results suggest the development of a versatile hydrogel, suitable for use as a matrix for the absorption of nanoscale materials. The optical properties of the material were investigated using UV-Vis, IR, Raman spectroscopy, and fluorimetry; while the mechanical properties were studied using a rheometer.

Results

• Preparation of semiconductor-based colloidal photocatalysts for environmental remediation.
• Preparation of luminescent materials with luminescence properties that can be adjusted in color and duration.



Molecular modelling results: (a) Overlapping helical structures formed by three subunits of the phenyl propanoid chain linked in a regular linear sequence, (b) Linear structure formed from two overlapped chains composed of six units, (c) 45–50 linear helix molecules looped spirally to form a ring-shaped structure. Finally, an experimental investigation performed through Transmission electron Microscopy (TEM), X-ray Diffraction (DRX) and Diffuse Reflectance Spectroscopy (DRS) was carried out to analyse the microstructure of synthetic iron coprecipitates in solid state and while their colloidal behavior as a function of pH was ascertained through Photon Correlation Spectroscopy and Laser Doppler electrophoresis.

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1A – Thermally Controlled Photon Upconversion thorough Phase Change Material in Solid-like Structures

E. Cambiotti, G. Quaglia, E. Fratini, L. Latterini

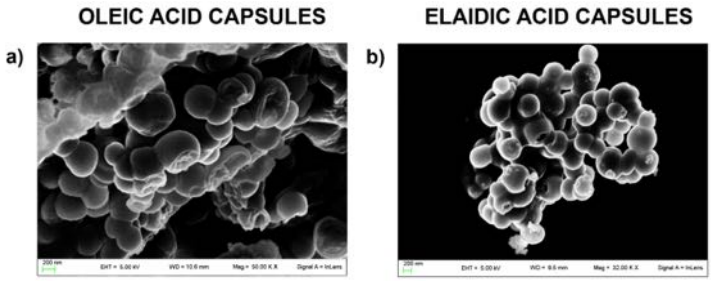
Aims

Triplet–triplet annihilation upconversion (TTA-UC) is a promising strategy to harvest low-energy photons, but its application in solid-state systems is still limited by inefficient molecular diffusion and oxygen-induced triplet quenching. Here, we demonstrate TTA-UC in solid silica-encapsulated systems containing Pt(II) octaethylporphyrin (PtOEP) and 9,10-diphenylanthracene (DPA) dissolved in phase change materials (PCMs). The silica shell acts as an effective physical barrier against oxygen and enables the fabrication of stable structures suitable for integration into optoelectronic devices. This work aims to control TTA-UC emission intensity via temperature under incoherent Xe-lamp excitation without external deoxygenation. We investigate the optical properties of the PtOEP/DPA pair both above and below the PCM melting points in silica capsules. The results highlight how phase-dependent molecular mobility and PCM-induced chromophore aggregation influence the overall upconversion efficiency.

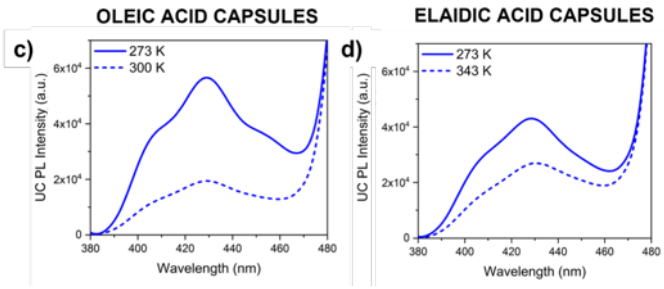
Results

Two syntheses were carried out to obtain oil-in-silica capsules using oleic acid (OA) and elaidic acid (EA) as oil phases. OA and EA are geometric isomers with the same chemical formula (C18H34O2) and can be classified as organic nonparaffin phase-change materials, with melting points at 289 K and 319-321 K. Due to the presence of an unsaturated bond, both fatty acids can contribute to protecting chromophores from molecular oxygen.

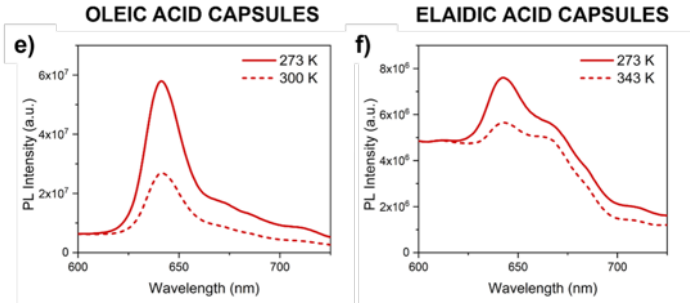
Figures a and b show SEM images of capsules containing OA and EA with average particle diameters of 520 ± 5 nm and 545 ± 5 nm, respectively.



Figures c and d show greater UC efficiency in OA than in EA-based capsules, with predominant UC emission observed in the solid phase for both media. This behavior indicates enhanced inter-chromophoric energy transfer at low temperatures, leading to a thermally regulated system.



The phosphorescence spectra of OA capsules exhibit spectral features of monomeric PtOEP, with a main emission band centered at 645 nm (Figure e). In contrast, EA capsules display an additional shoulder at 675 nm related to PtOEP aggregation (Figure f). The relative intensity of this shoulder increases above the melting temperature, indicating that porphyrin aggregation is promoted by increased molecular diffusion. Aggregate formation results in reduced PtOEP triplet availability and, consequently, to a lower overall UC efficiency in EA capsules compared with OA capsules. By controlling the nature of PCM and temperature, UC efficiency can be effectively modulated, enabling the development of air-tolerant, temperature-responsive TTA-UC systems suitable for sensing applications.



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1A – Valorization of marine natural products into biobased active materials: from crustacean waste to functional prototypes

J. Costa, M.C. Baratto, A.M. Atrei, R. Pogni
(Department of Biotechnology, Chemistry and Pharmacy, University of Siena, Italy)

Aims

The increasing demand for renewable, biodegradable, and multifunctional materials is driving innovation in sustainable polymer science. This work aims to develop bio-based active materials derived from seafood waste, focusing on the valorization of chitosan, obtained by deacetylation of chitin from crustacean shells. Chitosan's inherent antimicrobial, antioxidant, and film-forming properties make it a valuable candidate for food packaging, agriculture, and adhesive applications. To enhance its functional versatility and overcome limitations such as brittleness and low processability, chitosan was blended with starch to form biodegradable composites. The study explores two fabrication techniques, solvent casting and extrusion, to scale-up the process and evaluate their impact on mechanical, thermal, and structural performance. Additionally, the work investigates the incorporation of active biofillers to cover a wide range of applications.

Results

Biocomposites based on chitosan were successfully fabricated via both solvent casting and extrusion. Mechanical tests (Young's modulus, tensile strength), FT-IR spectroscopy, and DSC analysis showed good miscibility between the polymers and revealed the effect of processing method on material properties. The addition of lignin-based biofillers enhanced antioxidant activity and improved barrier properties, aligning with requirements for active food packaging. Within the FISH4FISH EU project, chitosan-based composites demonstrated excellent UV-shielding and antimicrobial performance, enabling the creation of home-compostable, allergen-free packaging that extends seafood shelf life. Chitosan also proved effective in developing bio-based adhesives with strong bonding, water resistance, and flame retardancy. In agriculture, it serves as a biopesticide and plant growth promoter, providing an eco-friendly alternative to conventional agrochemicals and supporting the development of innovative, bio-based solutions. Magnetic responsiveness was achieved by incorporating iron oxide MNPs synthesized through both classical and green routes. Olive leaf extract (OLE) was employed as a reducing agent in the green synthesis process. OLE-mediated synthesis produced stable nanoparticles due to the polyphenolic compounds acting as reducing and capping agents. Further surface functionalization was achieved through in-situ and ex-situ coating with olive leaf extract (OLE) and lignin, aiming to enhance interactions with the positively charged chitosan matrix and reduce nanoparticle aggregation. The MNPs were characterized using DLS, FT-IR, EPR, hysteresis analysis, and TEM, confirming their morphology,

surface chemistry, and magnetic properties. This work demonstrates a circular, scalable, and multifunctional approach to sustainable material design, showing how marine waste and eco-friendly nanotechnologies can be combined to produce next-generation bioplastics.

FISH4FISH project – Co-funded by the EU under the EASME/EMFF/Blue Economy-2018 program (grant no. 863697)
This work was also supported by the national infrastructure METROFOOD-IT (PNRR)

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1B – A tri(ethylene glycol)-tethered Morita–Baylis–Hillman dimer in the formationof macrocyclic crown ether-paracyclophane hybrid structures

M. Saletti, J. Venditti, G. Fattori, M. Paolino, A. Zacchei, G. Giuliani, G. Giorgi, C. Bonechi, A. Donati, C. Rossi, A. Cappelli (Department of Biotechnology, Chemistry and Pharmacy, University of Siena, Siena)

Aims

A Morita–Baylis–Hillman acetate was dimerized by a click-chemistry Copper(I)-Catalysed Azide–Alkyne Cycloaddition (CuAAC) reaction employing a tri(ethylene glycol) diazide derivative to obtain a dimeric MBHA derivative. The reaction of this dimeric MBHA derivative with n-butylamine afforded a photoisomerizable macrocyclic crown ether-paracyclophane hybrid architecture that is potentially useful in a large variety of applications as well as those already well-known for crown ethers.

Results

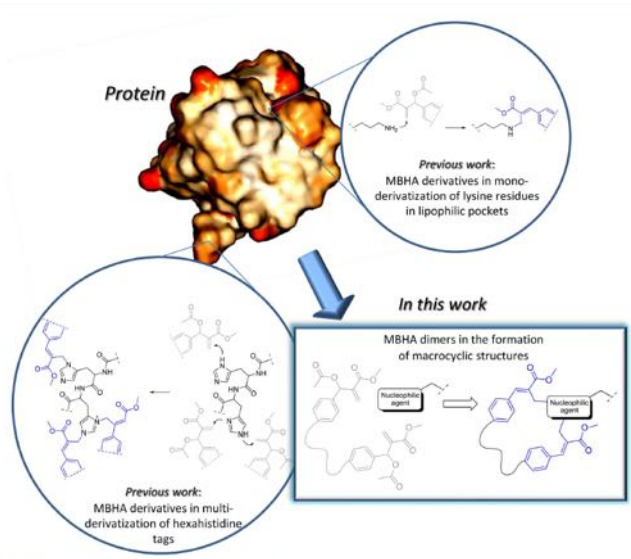
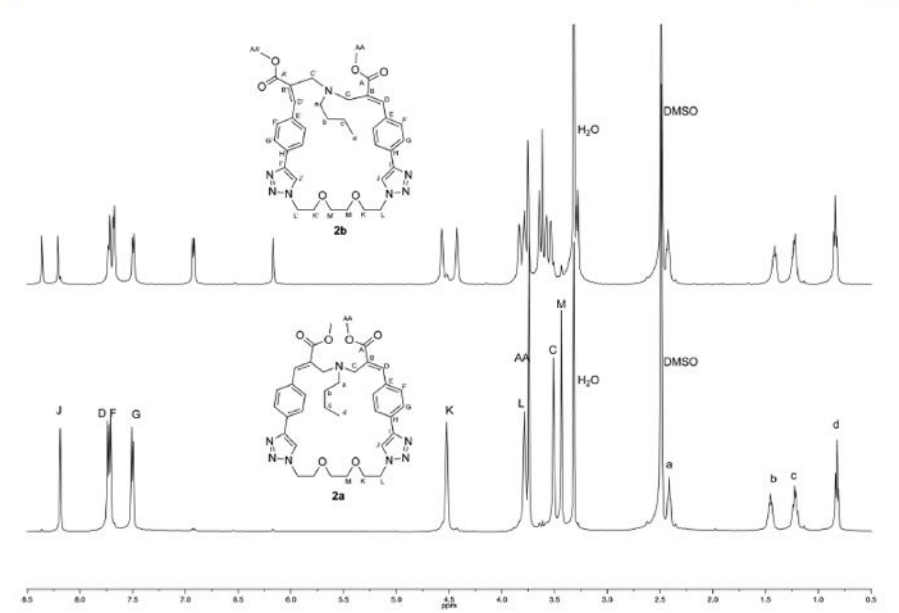


Figure reports the applications of MBHA derivatives to protein functionalization.

The photochemical features of the macrocyclic compounds were investigated by ^{1}H NMR spectroscopy studies starting from (E,E) diastereomer 2a owing to its well-established (i.e. by crystallography) symmetric structure, the simplicity of its ^{1}H NMR spectrum, and its solubility in deuterated solvents such as methanol and DMSO. Thus, compound 2a was dissolved in deuterated methanol into a 5 mm NMR tube and the resulting solutions were exposed to UV-B light into an appropriate photoreactor (Multirays, Helios Quartz). ^{1}H NMR spectra were registered at regular time intervals, elaborated, and compared (see ESI†). The comparison of the ^{1}H NMR spectra recorded

with the solution of 2a in deuterated methanol exposed to UV-B irradiation for increasing times (i.e. from 5 to 30 min) supported the liability of this (E,E) diastereomer to undergo photoisomerization with the formation of an almost insoluble compound, which precipitated from the reaction mixture.



In conclusion, a tri(ethylene glycol)-tethered MBHA dimer was synthesized and found to react with n-butylamine leading to the formation of macrocyclic crown ether-paracyclophane hybrid structures that could be modulated by light. Thus, reactive MBHA dimer could find applications in the functionalization of materials containing reactive basic groups with the formation of amphiphilic loops provided with a wide range of intriguing properties such as those shown by both crown ethers and paracyclophane derivatives. Deeper investigations are in progress to characterize the complex photoisomerization features of this interesting new family of macrocyclic derivatives, also in light of the little information on similar structures reported in the literature.

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1B – Biocompatible materials for biomedical applications

M. Bini, M. Ambrosetti, et al.

Aims

A biomaterial is "a substance employed to build objects capable of replacing original living parts of the human body" and, when inserted in the body, it should not produce adverse reactions, i.e. it should be biocompatible. The term biomaterials could be used for drug delivery systems, materials for prosthesis, surgical equipment or compounds used for the diagnosis. We synthesized mixed oxides, particularly zinc ferrites that can be applied in magneto-fluid hyperthermia and characterize them mainly by micro-Raman spectroscopy.

Results

The key property of $ZnFe_2O_4$ spinel is the superparamagnetic behaviour at room temperature, strictly dependent on particle sizes and cation distribution on the spinel sites. Raman spectroscopy was applied on nanostructured $ZnFe_2O_4$ system in order to correlate its structural, chemical, and vibrational properties to the functional behaviour, in view of the high sensitivity of the Raman probe to the cationic order in iron oxides. In particular, we investigated pure and Ga/Mg doped zinc ferrite nanoparticles synthesised by co-precipitation route by means of Raman spectroscopy, with a particular focus on the correlation between their structural and magnetic properties. We studied the homogeneity of the samples and their stability under laser irradiation disregarding the presence of spurious iron oxides in favour of a highly defective external shell of the nanoparticles. This hypothesis was corroborated by varying the incident laser wavelength therefore changing the investigated volume. Furthermore, we estimated the inversion degree of the spinel structure finding good agreements with the trend of the magnetic features. Raman spectroscopy evidences are supported by the results obtained with X-Ray Powder Diffraction, Electron Paramagnetic Resonance and SQUID magnetometry

We also studied the laser-induced transformations of pure and Mg-, Ga-doped $ZnFe_2O_4$ nanoparticles through micro-Raman spectroscopy thanks to its in-situ real-time monitoring of structural and phase changes in micrometer areas of the compounds, which were subjected to laser irradiation in high and low vacuum environments. We report the occurrence of magnetite after the in-vacuum irradiation that can be interpreted considering the sublimation of Zn cations and the subsequent reorganization of the Fe and O ions. We also determined that the presence of Mg and Ga co-doping blocks the depletion of Zn-ions therefore maintaining the spinel ferrite structure. This work provides indications for the design and the synthesis of more robust zinc ferrite nanostructures with low or no photoinduced degradation.

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1B – Bioresponsive Hyaluronic Acid-Based Hydrogel for Glioblastoma treatment

F. Barbugian[1], D. Salerno[1], E. Ballarini[1], L. Crippa[1], O. Francesconi[2], F. Mantegazza[1], G. Cavaletti[1], S. Roelens[2], G. Leone[3], S. Pepi[3], L. Talarico[3], G. Vigni[3], A. Magnani[3], C. Nativi[2], L. Russo[1]

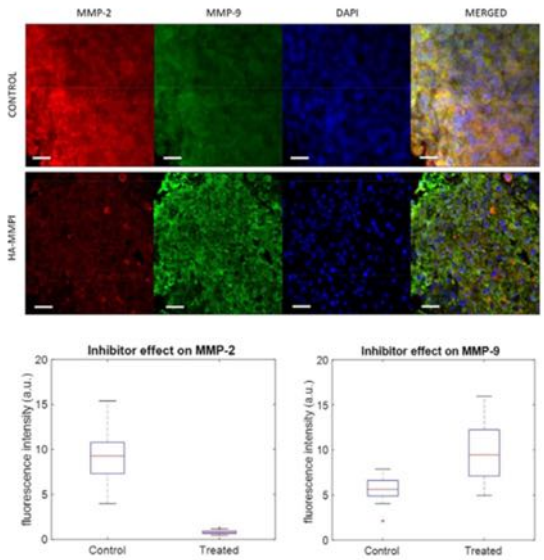
[1]School of Medicine and Surgery Università di Milano-Bicocca
[2]Department of Chemistry, University of Florence
[3]Department of Biotechnology, Chemistry and Pharmacy, University of Siena)

Aims

Glioblastoma multiforme (GBM) is an extremely malignant cancer, resistant to standard therapies. A bioresponsive hydrogel based on hyaluronic acid (HA) cross-linked with a branched metalloproteinase (MMP) inhibitor (MMPI) is proposed.

Results

The HA-based hydrogel is cross-linked with a branched MMPI. It is nontoxic and more stable to hyaluronidases than the native HA. The new hydrogel resulted suitable to fill the resection site after GBM surgical resection, and able to inhibit GBM spread, selectively inhibiting MMP-2 in situ. Experiments withU89 spheroids showed that cells migration, responsible for metastasis, was inhibited in presence of HA-MMPI. HA-MMPI hydrogel appears as a promising tool for the mitigation of tumor relapse and spread [1].



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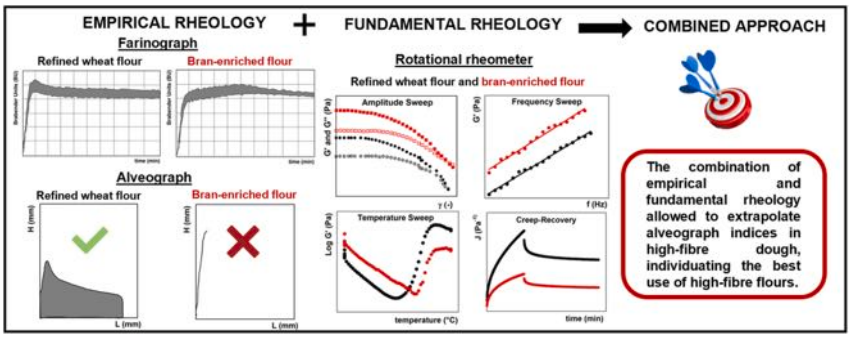
1B – Combination of empirical and fundamental rheology for the characterization of dough from wheat flours with different extraction rate

F. Cuomo, M.C. Trivisonno, S. Iacovino , M.C. Messia
E. Marconi

Aims

Empirical rheological techniques (assessed through Farinograph and Alveograph) conventionally used for evaluating wheat flour dough can be coupled to fundamental rheology, especially when viscoelastic properties of dough, like those with high bran content, cannot be readily investigated using empirical rheology alone. A correlation between the obtained parameters has not yet been reported. Hence, in this study, dough from different types of flours, ranging from the more refined flours to whole grain ones, were analyzed through dynamic oscillation measurements, farinograph and alveograph analyses, and the correlations between empirical and fundamental rheology were used to determine empirical indices of bran-enriched flours that could not be identified by official standard methods.



Results

The combined approach to dough characterisation revealed a strong correlation between empirical and fundamental rheology. Empirical rheology indicated that the higher protein and fibre content of less refined flours was associated with greater water absorption, a longer dough development time, and greater stability. This was in parallel with the dough having higher tenacity and lower extensibility. Fundamental rheology evidenced the predominantly solid-like nature of the samples, confirming the results of empirical rheology. Since the two approaches provide complementary information, combining empirical and fundamental rheology enables a comprehensive study of dough rheological properties. This also enabled the limitations of the empirical methods with respect to the samples considered to be overcome. In particular, the integrated approach proved highly applicable to the extrapolation of alveograph indices of white, refined, soft wheat flours enriched with wheat bran, which are difficult to analyse using the standard official protocol.

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1B – Confinement- and ion-mediated modulation of Bacillus subtilis motility: A Statistical Approach to Early-Stage Interactions

G. Bassu, M. Izzi, A. Castellani, F. Soto-Bustamante, R.A. Picca, E. Fratini, M. Laurati, N. Cioffi

Aims

Understanding the active behaviour of complex living systems is a topic of great interest in fundamental science and technological applications. From medicine to the bioactive materials industry, many crucial phenomena depend on bacterial migration and interaction with heterogeneous three-dimensional materials. In this research, biocompatible polyethylene glycol hydrogels with tunable porosity on a micron scale and a high degree of transparency allowed the direct investigation, by confocal laser scanning microscopy, of the motility behaviour of the micro-swimmer *B. subtilis [1]*. In order to better understand the early stages of interaction between inorganic antimicrobial agents and microorganisms, the short-term motility of bacteria after 30 minutes of contact with ZnO-based bioactive surfaces was examined using the same instrumental configuration, proposing an innovative statistical method for studying the bacteriostatic/bactericidal activity of antimicrobials [2].

Results

The average Mean Squared Displacements (MSDs) obtained for bacteria confined in hydrogels of different porosity shown in Fig. 1a allows to characterize the motility at different degree of confinement length ξ, defined as the ratio between the bacterial length and the average pore diameter. The characteristic run-and-tumble motility of unconfined flagellated bacteria turns into anomalous sub-diffusive motion with the increase of confinement. The single-trajectory analysis highlights the matrix-induced transition in the bacterial motility with the progressive decrease of average transport coefficient and the exponent n related to the nature of the motion. The transition from active to the sub-diffusive motion reported in in Fig. 1b was interpreted as the transient trapping of the micro-swimmers in the hydrogel network with excel agreement the hopping-between-trapping model.

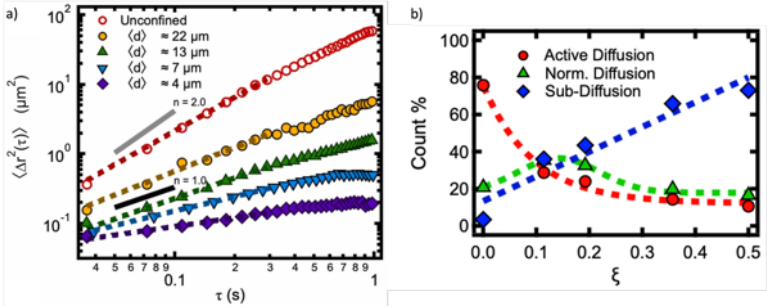

Figure 1: (a) Mean Squared Displacements of bacteria in unconfined conditions (empty markers) and loaded in the different porous hydrogels (full markers), and (b) normalized populations of trajectory segments classified as active, diffusive or sub-diffusive, as a function of the confining length (ξ).

Based on the presented statistical method, the short-time motility of bacteria after 30 min of contact with ZnO-based bioactive surfaces was inspected. Two stabilizers, Sodium Dodecyl Sulphate and Poly-Diallyl-Dimethyl-Ammonium chlorid, were employed to produce elongated and flower-like ZnO NSs morphologies. Inorganic antimicrobials were embedded into three polymeric matrices (polyethylene oxide, polylactic acid, and poly-vinyl-methyl-ketone) to produce nanocomposite coatings providing different release of Zn^{2+} ions, ranging from 20 to 120 ppm over time (i.e. tunable bioactivity). The time-dependent diffusion coefficient D(τ) extrapolated from MSDs revealed that the run-and-tumble dynamics of native *B. subtilis* turns into sub-diffusive motion under the effect of Zn^{2+} ions release indicating a strong biostatic effect already in the first minutes of contact (see Fig. 2a). Direct LSCM imaging of live-dead bacteria was additionally used to assess viability as a function of bioactive ion release revealing that even for the larger ions release less than 20 % of the cells were damaged the exposure (Fig. 2b), i.e. the bioactive surfaces have a biostatic rather than bactericidal effect. This direct approach offers a new paradigm in the development of bacteriostatic vs bactericidal strategies, allowing for a precise engineering of antimicrobial coatings to achieve a desired spatio-temporal effect.

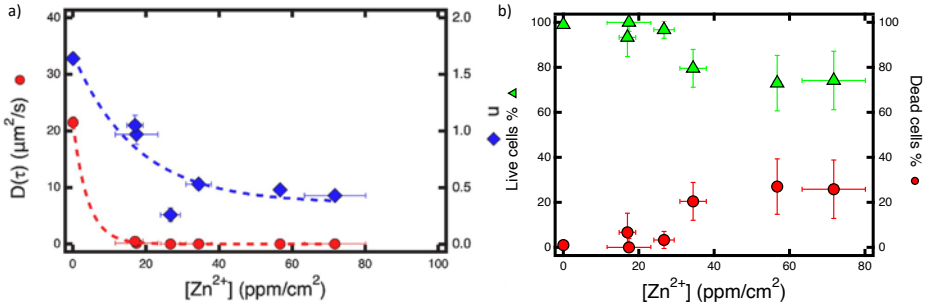

Figure 2: Characteristic transport parameters D(τ) and power-law exponent n obtained from the average MSD of the bacterial dispersions as a function of the Zn^{2+} concentration released after contact with NSs-loaded matrices (a), and percentage of live and dead bacterial cells of the investigated systems (b).

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1B – Design and Optimization of Solid Lipid Nanoparticles Loaded with Triamcinolone Acetonide

L. Talarico, S. Pepi, S. Susino, G. Leone, C. Bonechi, M. Consumi, I. Clemente, S. Costantini, A. Donati, C. Rossi, A. Magnani (Department of Biotechnology, Chemistry and Pharmacy, University of Siena, Siena)

Aims

Principles of quality by design and design of experiments are acquiring more importance in the discovery and application of new drug carriers, such as solid lipid nanoparticles. An optimized synthesis of solid lipid nanoparticles loaded with Triamcinolone Acetonide is presented using an approach that involves stearic acid as a lipid, soy PC as an ionic surfactant, and Tween 80 as a nonionic surfactant. The constructed circumscribed Central Composite Design considers the lipid and nonionic surfactant quantities and the sonication amplitude in order to optimize particle size and zeta potential, both measured by means of Dynamic Light Scattering, while the separation of unentrapped drug from the optimized triamcinolone acetonide-loaded solid lipid nanoparticles formulation is performed by Size Exclusion Chromatography and, subsequently, the encapsulation efficiency is determined by HPLC-DAD. The proposed optimized formulation with the goal of maximizing zeta potential and minimizing particle size has shown good accordance with predicted values of zeta potential and dimensions, as well as a high value of encapsulated triamcinolone acetonide.

Results

This work reports the optimization of the synthetical process for triamcinolone acetonide-loaded solid lipid nanoparticles using Stearic Acid as a lipid, and Tween 80 and soy PC as nonionic and ionic surfactants, respectively, in compliance with quality by design principles. The Central Composite experimental design implemented has shown a linear dependence between the tested independent variables and zeta average, with the major influence given by lipid and surfactant quantities, while the relationship of independent variables with zeta potential follows a quadratic model. The zeta potential is strongly influenced by the quantity of nonionic surfactants in relationship to lipid quantity and sonication power, due to different ratios between anionic and non-ionic surfactants in the formulation, while the minimum positive contribution is given by the AC term (combination of lipid quantity and sonication power) due to the possible presence of some stearic acid in the form of stearate anions on the particle surface. From the construction of response surfaces, an optimized synthetical pathway is obtained using 5% (w/v) of stearic scid, 2.45% (w/v) of Tween 80, and the fixed sonication power of 35%. This solution has the highest desirability index when assigning more relative importance to reduction of zeta average with respect to maximizing of zeta potential.

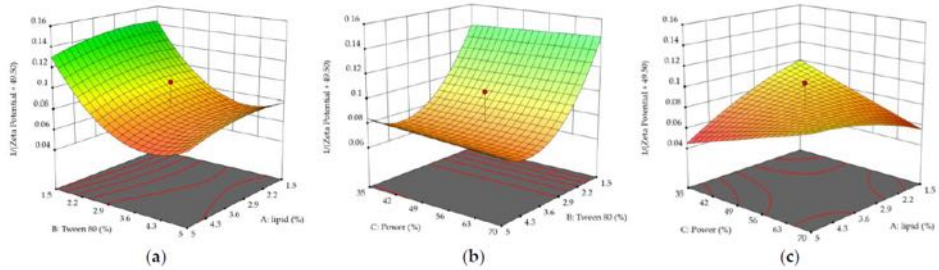

Figure reports the 3Dplots of the AB (Lipid/Tween 80 Figure 3a), BC (Tween80/power, Figure 3b), and AC (Lipid/Power, Figure 3c) terms for zeta potential. For each figure, the missing factor is fixed at its mean level.

Experimental values obtained from the optimized synthesis reports a dimension of 683 ± 5 nm, which differs by 3% from the predicted value, and a zeta potential of -38.0 ± 7.6 mV (12% difference from the predicted value).

Experimental values of zeta average and zeta potential are replicable and in good accordance with predicted results. When the solid lipid nanoparticles are purified via Size Exclusion Chromatography, this optimized synthesis has also shown a very high encapsulation efficiency, demonstrating that the proposed synthesis of solid lipid nanoparticles is capable of encapsulating triamcinolone acetonide in high quantities, yet permeation studies for the optimized formulation are required to classify this optimized formulation as drug delivery systems.

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1B – Development of photoactivatable liquid-crystalline nanoparticles for the therapy of NSCLC (SOLAR)

S. Murgia, C. Sinico, M. Schlich, C. Caltagirone, G. Picci, E. Lai, A. Pittiu

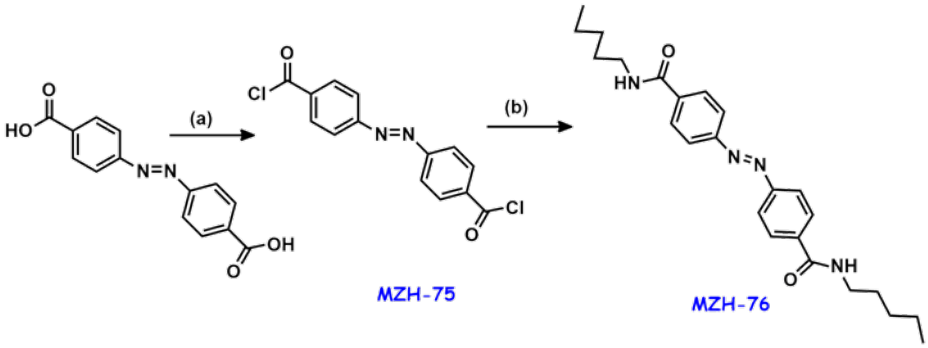
Aims

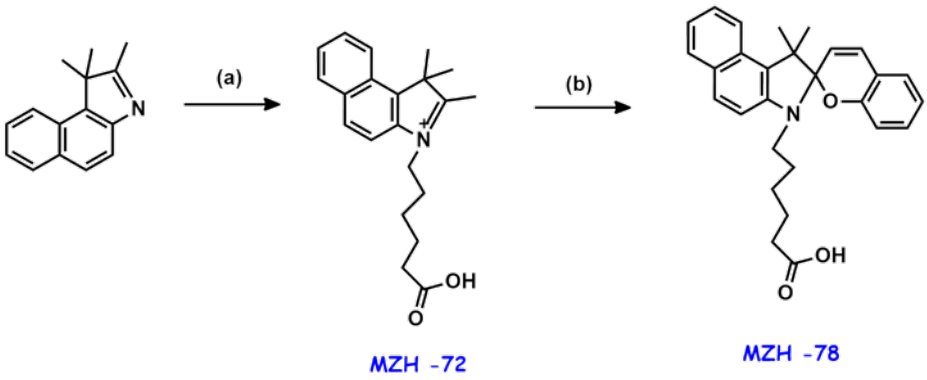
The SOLAR project aims to enhance the efficacy and safety of photodynamic therapy (PDT), a promising cancer treatment based on light-activated cytotoxicity. Despite its high specificity, current photosensitizers (PS) suffer from poor solubility, stability, and tumor selectivity. SOLAR addresses these limitations by developing biocompatible nanoparticles (cubosomes and hexosomes) with cubic or hexagonal structures to improve PS delivery. The project has two main objectives: (I) to overcome current challenges in the scalability and reproducibility of cubosome and hexosome production, and (II) to design novel formulations incorporating photo-activable switches, enabling light-triggered drug release. The physicochemical properties of the developed nanoparticles will be thoroughly characterized using complementary analytical techniques, while their therapeutic potential will be evaluated in vitro on lung adenocarcinoma models.

Results

The initial phase of the project was marked by notable achievements, including the successful synthesis of various novel photoactive species (PASs), representing a crucial milestone toward fulfilling the project's primary objectives. In parallel, the microfluidic protocol for formulating lipid-based liquid crystalline nanoparticles was optimized, allowing for precise control over particle size, morphology, and stability, key parameters for their effectiveness in biomedical applications. Cubosomes and hexosomes, engineered as advanced carriers for enhanced drug delivery, were successfully loaded with photoactive compounds and photosensitizers, and underwent comprehensive physicochemical and photophysical characterization.

The progress achieved during this initial period has established a strong scientific and technical foundation for the next phases of the project. The successful synthesis of target molecules and the refinement of nanoparticle formulation protocols demonstrate both the feasibility and the innovative potential of the proposed approach. These results not only confirm the project's alignment with its original objectives but also position it well for upcoming activities, including the integration of therapeutic agents into nanocarriers and their subsequent in vitro evaluation. Overall, the work completed thus far reflects a coherent and forward-looking strategy, ensuring the scientific relevance of the project.





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1B – Efficacy of lignin nanocapsules for delivering natural pesticides to Eruca sativa plants against Plutella xylostella

S. Falsini, C. Gonnelli, A. Papini, M.C. Salvatici, S. Ristori
(University of Florence and ICCOM CNR, Florence, Italy)

Aims

Over the past 50-60 years, pesticides have been largely used in agriculture, causing adverse effects on the ecosystem and humans. For this reason, antiparasites administered in the form of finely dispersed particles, the so-called nanopesticides, have recently gained attention. In this context, nanoparticles and other soft matter formulations based on natural lipids have been proposed.
In this contribution, we report on the design, preparation and physico-chemical characterization of nanosystems based on kraft lignin for the transport of neem oil and capsaicin as insect repellents. These are examples of natural antiparasites, with activity against the common insect Plutella xylostella whose usage is limited by low solubility in water media, which results in poor bioavailability and high loss of the active principles. The present formulations were applied by foliar spray

Results

The following samples were prepared starting from 5% w/w lignin in KOH solution:

Sample name	pH of starting lignin solution	Composition	final pH
N13	13.5	NCs + neem	9.5
NC13	13.5	NCs + neem + Capsaicin	9.0
N11	11.5	NCs + neem oil	7.9
NC11	11.5	NCs + neem + Capsaicin	6.4

Neem oil and Capsaicin content were 4.5% v/v and 6 10^{-3} mg/mL, respectively. To bring the final pH at values fully compatible with plants, a 2% HCl 0.1 M was added dropwise. The physicochemical characterization showed that particles with different mean diameter, from 20nm to approximately 800 nm, were present in solution. However, the size distribution could be reduced by filtering with 800 nm pore membranes and brief ultracentrifugation (three 5' cycles at 14000 rpm), as shown by DLS (Figure 1)

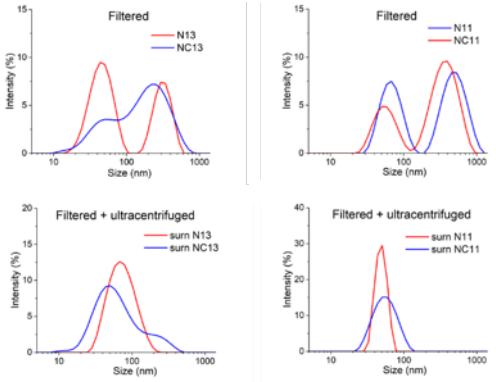

Figure 1

The Zeta Potential values were -35 mV and -50 mV for the N11 and N13 sample, respectively, and were substantially unchanged after addition of neem and capsaicin, suggesting that the host substances are located inside lignin capsules.
High resolution techniques, i.e. TEM and SAXS, confirmed the presence of more than one nanoparticle population. In particular, TEM micrographs showed that elongated structures are formed in samples prepared at higher starting pH (N13 and N13C), while only spheres were observed in N11 and N11C.
SAXS intensity profiles of N11 and N11C were fitted by considering core-shell cylinders and core-shell spheres, whereas only spherical aggregates were considered for in the fitting of N13 and N13C profiles.
The antifeedant activity of plain and loaded lignin nanocapsules was established by exposing Eruca sativa to *Plutella xylostella* insects. The results of this treatment are shown in figure 2 and 3

Figure 2: Control plants (left) and treated plants (right) of *Eruca sativa* after 7 days exposure to *Plutella xylostella* insects

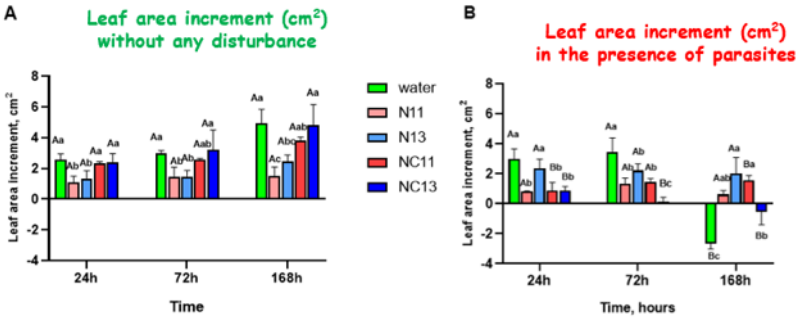

Figure 3

In conclusion, this work provides a case study of how sustainable nanotechnology can be used to counteract insecticide resistance, showing that formulations from natural sources are a viable strategy for plant protection.

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1B – Elucidating the action mechanism of PEG-120 methyl glucose dioleate (ANTIL 127) in model surfactant systems

I. De Cristofaro, L. Paduano
(U.O. of Naples, University of Naples Federico II)

Aims

Aqueous surfactant-based formulations are at the core of personal care products. These multicomponent systems typically consist of mixtures of anionic, zwitterionic, or nonionic surfactants, salts, and functional additives such as polymers. Their macroscopic properties arise from a complex interplay of supramolecular interactions that govern self-assembly behavior (Gradzielski, 2023). Among functional additives, hydrophobically modified water-soluble polymers—known as associative thickeners (ATs)—play a key structural role (Larson et al. 2022). In this project, we investigate the role of PEG-120 Methyl Glucose Dioleate (ANTIL 127), a sugar-based nonionic AT, within a model surfactant system composed of Sodium Laureth-1 Sulfate (SLE1S), and Cocamidopropyl Betaine (CapB). To disentangle individual and combined effects, we first characterized the surfactant mixture, with and without sodium chloride (NaCl), a common viscosity enhancer. The self-assembly behavior of ANTIL 127 in water was investigated and, finally, examined the full formulation containing both ANTIL 127 and the surfactant system under ionic screening conditions through Dynamic Light Scattering (DLS) and Small-Angle X-ray Scattering (SAXS) to gain insight into component-driven structural changes and the role of ANTIL 127 in tuning surfactant self-assembly.

Results

The aggregation behavior of the individual surfactants SLE1S, and CapB, as well as their binary mixture, was investigated in aqueous solution. DLS measurements showed that CapB forms a single, well-defined micellar population, consistent with its zwitterionic nature and low inter-headgroup repulsion. In contrast, SLE1S exhibited a polydisperse profile with a multi-exponential decay, indicative of micellar instability and transient supramicellar aggregates resulting from electrostatic repulsion among sulfate headgroups. The surfactant mixture (SM) retained this polydispersity, suggesting that CapB alone provided limited electrostatic screening. Upon addition of NaCl, both SLE1S and the SM formed single, stable micellar populations, indicating enhanced structural stability (Fig. 1a-b). SAXS measurements further revealed a morphological transition from spherical to rod-like micelles upon salt addition, attributed to increased ionic strength, which reduces headgroup repulsion and increases the Critical Packing Parameter (Fig. 1c). Building upon this understanding, we examined the aggregation properties of ANTIL 127 in water. The autocorrelation function displayed a single exponential decay, and the size distribution revealed a single population with a hydrodynamic radius of 7.3 ± 0.2 nm, confirming spontaneous aggregation driven by the amphiphilic nature of the polymer (Fig. 2a-b). The SAXS profile supported the formation of compact, globular aggregates, with a symmetric P(r) (Fig. 2c). To evaluate

how ANTIL 127 modulates surfactant self-assembly under formulation-relevant conditions, we analyzed its interaction with the SM in the presence of NaCl (SM@NaCl@ANTIL 127). The resulting aggregates exhibited a hydrodynamic radius of 5.6 ± 0.3 nm, larger than the micellar aggregates but smaller than ANTIL 127 alone (Fig. 2a-b). The P(r) function retained a micellar core–shell profile but also showed a pronounced high-r shoulder, indicative of long-range internal correlations (Fig. 2d). This structural signature suggests the formation of dumbbell-like aggregates. Such an interpretation was supported by ab initio shape reconstruction based on SAXS data using DAMMIF. The models were averaged with DAMAVER and refined with DAMMIN, yielding a 3D bead model consistent with a dumbbell-like morphology, in which the hydrophobic dioleate moieties of ANTIL 127 insert into the cores of the micelles, while the hydrophilic PEG backbone spans the aqueous phase, bridging the micellar domains (Fig. 2e).

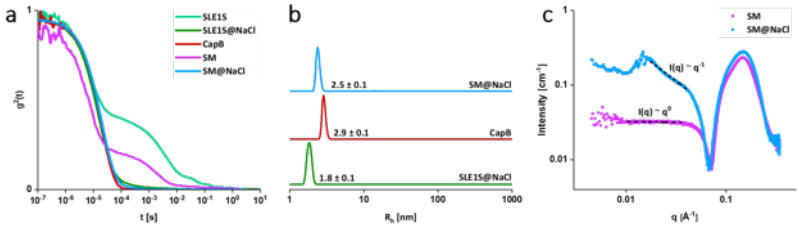

Figure 1: Autocorrelation functions of SLE1S, CapB, SM, SLE1S@NaCl, and SM@NaCl in water (a); distribution curve of hydrodynamic radius for SLE1S + NaCl, and SLE1S + CapB + NaCl in water (b); SAXS curves and linear fittings in the low q-regions for SLE1S + CapB and SLE1S + CapB + NaCl in water (c).

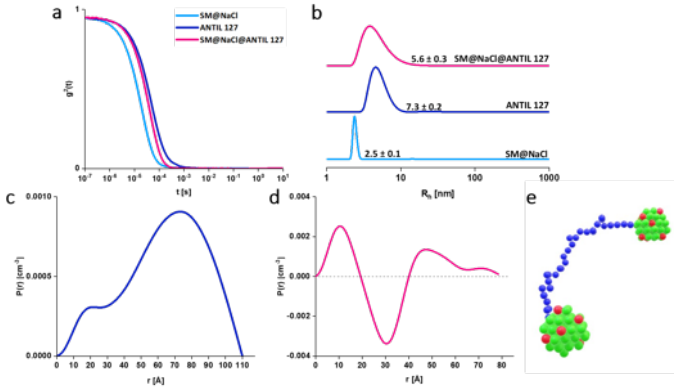

Figure 2: Autocorrelation functions (a), distribution curves of hydrodynamic radius (b) for ANTIL 127, SM@NaCl, and SM@NaCl@ANTIL 127 in water; P(r) of ANTIL 127 (c), and SM@NaCl@ANTIL 127 (d); 3D bead model obtained for SM@NaCl@ANTIL 127 (e).

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1B – Enrichment of olive oil emulsions with antioxidant compounds

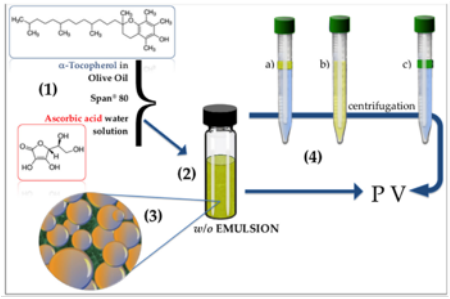
G. Cinelli, F. Cuomo, F. Lopez , F. Venditti, A. Ceglie

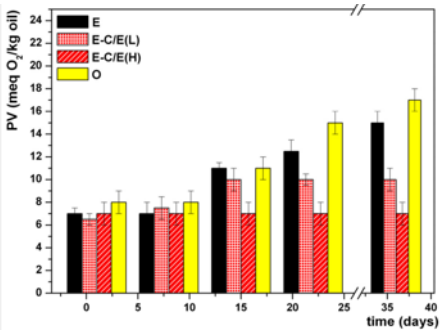
Aims

Water-in oil (w/o) emulsions are heterogeneous systems able to solubilize both hydrophilic and hydrophobic compounds. Thus, hydrophilic vitamin C, lipophilic vitamin E and red wine dry extract (WDE) were loaded in (w/o) emulsions at 1% (w/w) water stabilized by 1% (w/w) Span 80.

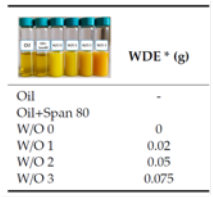
Results

The antioxidant effect of vitamins in emulsions was studied considering the variation of the peroxide values during storage. The oxidation reaction was slowed down in emulsions containing vitamin C, but it was faster by the loading of vitamin E for its high concentration. In emulsions containing vitamin E, indeed, the peroxide values were higher than in emulsions prepared in the absence of vitamins or in oil. The antioxidant activity generated by the co-loading of vitamin C and E was very effective to the point that in presence of high amounts of vitamins the peroxide values did not change in about 40 days of storage, due to the vitamin E regeneration by vitamin C.

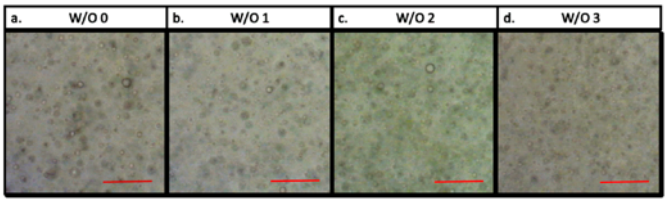


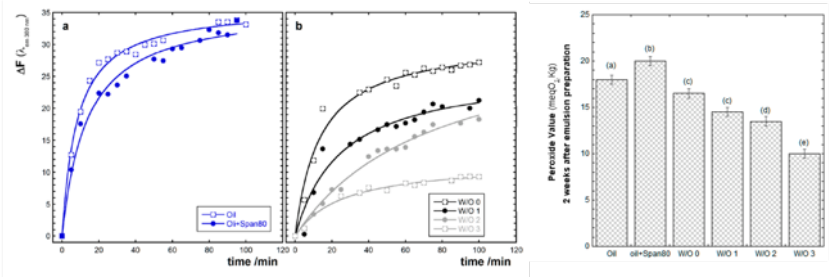


Kinetics of oil oxidation carried out in oil and emulsions in the presence of an increasing amount of WDE, revealed that the presence of WDE slowed down the oxidation rate. The oxidation reaction was monitored in two ways; i.e., with the classical method that consists of the determination of the peroxide value, and with an accelerated test made using the radical initiator (AMVN) and a fluorescent probe revealing the hydroperoxides development (DPPP). Moreover, by comparing the emulsion structures observed by optical microscopy, no differences in term of size of the dispersed aqueous phase were detected with the increase of the wine dry extract concentration.



	WDE * (g)
Oil	-
Oil+Span 80	
W/O 0	0
W/O 1	0.02
W/O 2	0.05
W/O 3	0.075





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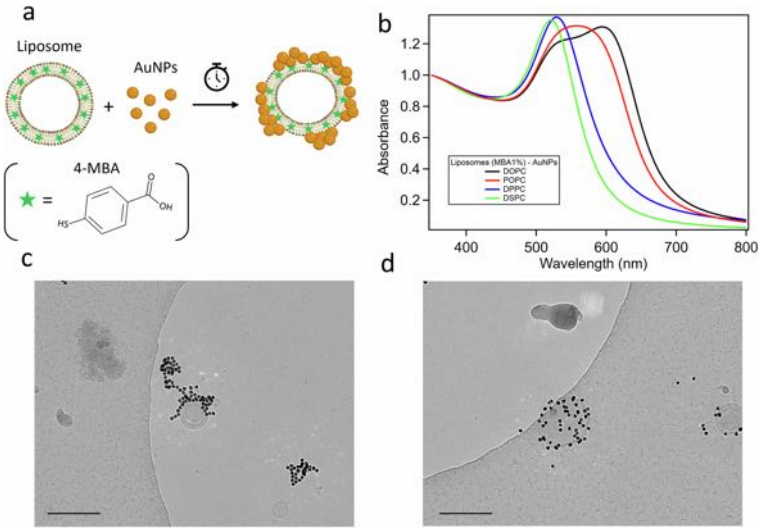
1B – Exploring and exploiting nano-bio interfaces for developing plasmonic and SERS applied nanocomposites

J. Cardellini, L. Caselli, A. Balestri, I. De Santis, C. Montis, D. Berti

Aims

In recent years, achieving a thorough understanding of the interactions between inorganic nanoparticles and lipid interfaces has been recognized as a key factor in advancing research on nano–bio interfaces, from both fundamental and applied perspectives. Associating inorganic nanoparticles with soft lipid scaffolds represents an attractive strategy for creating functional materials that combine the unique properties of inorganic nanomaterials with the biocompatibility, self-assembly capabilities, and chemical and structural tunability of lipid systems. Over the years, numerous examples of lipid–nanoparticle hybrids have been reported, including magnetoliposomes and, more recently, lipid-camouflaged nanoparticles. However, the fabrication of hybrid systems with well-controlled and tailored characteristics often requires complex synthetic routes and/or extensive post-synthetic manipulation. The aim of our contribution to this field is to understand, control, and exploit the factors governing nano–bio interface interactions for a range of applications.



Results

In this field, we have contributed through several complementary studies. The unique plasmonic properties of gold nanoparticles (AuNPs) and their lipid membrane–templated clustering behavior were disentangled and exploited for analytical applications, particularly in the context of biogenic extracellular vesicles. In addition, a variety of lipid–nanoparticle hybrid systems were designed, in which functional

nanoparticles (magnetic, plasmonic, or magnetoplasmonic) were associated with lipid assemblies of different compositions and geometries via simple self-assembly processes. By deliberately tailoring lipid–nanoparticle interfacial interactions—such as ligand exchange and/or hydrophobic effects—we achieved fine control over the structural, morphological, colloidal, and ultimately functional properties of the hybrids. Using this approach, several hybrid systems were developed, including: (i) lipid vesicle–nanoparticle assemblies with discriminating colloidal properties of potential interest for the separation of mixed vesicle dispersions; (ii) controlled clusters of gold nanoparticles on lipid vesicles with enhanced plasmonic properties, relevant for Raman imaging applications; and (iii) ternary systems composed of magnetite and gold/magnetite core–shell nanoparticles hybridized with lipid vesicles, exhibiting combined magnetic and plasmonic functionalities. Overall, these results demonstrate a facile strategy based on the controlled self-assembly of inorganic nanoparticles at lipid interfaces to produce complex, biocompatible functional materials with broad applicability.

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[5]https://www.sciencedirect.com/science/article/pii/S0021979723002564

1B – Flowless multiangle dynamic light scattering for detection on asymmetric flow field flow fractionation

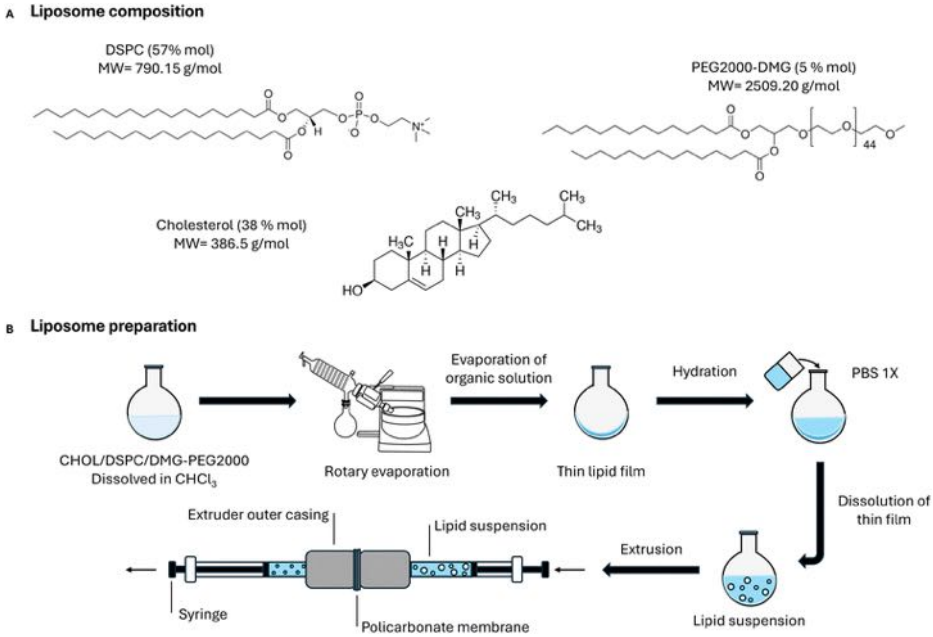
L.R. Doveri, G. Dal Pan, G. Tomaselli, T. Muñoz Santoro, P. Pallavicini, C. Ortiz de Solorzano, Y.A. Diaz Fernandez
In collaboration with University of Navarra, Spain

Aims

Nanomedicine is an emerging field of research, demanding new analytical methods to respond to stringent regulatory and safety requirements. Particle size and size distributions are critical quality attributes that require accurate and affordable measurements suitable for both R&D activities and routine quality control in production pipelines. Here we propose a new approach combining multidetector asymmetric flow field flow fractionation (MD-AF4) with multiangle dynamic light scattering (MADLS) for determination of particle size on bioinspired colloids and on polymeric particles, without the need for calibration materials. We benchmarked our results against established analytical methods, using a set of model liposome formulations to cover a wide range of particle sizes. Our approach could be extended to any kind of colloid suitable for light scattering methods and paves the way for the revisitation of AF4-DLS instrumentation that may become widely available in the future, expanding the set of analytical tools for nanomedicine applications.

Results

The liposomes, prepared by the traditional lipid thin-film extrusion method, were characterized by cryogenic transmission electron microscopy (cryoTEM) and MADLS, showing high monodispersity and long-term stability. These model samples allowed us to evaluate the effect of key variables on the performance of AF4 coupled to in-flow dynamic light scattering, identifying the influence of sample concentration on analytical bias for size determination. We extended the analysis to other types of particles (i.e. polystyrene and polymethyl methacrylate), which are relevant for environmental and drug delivery applications. Our results demonstrate that the analytical bias for in-flow DLS measurements follows a universal law, nearly independent of the chemical nature of the nanoparticles investigated. Subsequently, we combined MADLS and AF4 techniques, exploiting a programmable fraction collection system, enabling the accurate determination of particle size and number concentration in the absence of flow, and providing higher resolution for the size distributions.



We observed a universal trend between analytical bias and scattering count rate, nearly independent of particle size and chemical composition. The bias of in-flow DLS determination can be overcome by the new approach proposed, combining a programmable sample collection system and batch MADLS measurements at the end of the AF4 detector line. The results from this approach are in good agreement with cryoTEM and conventional DLS measurements on the original samples, suggesting that our strategy could be used for validation of the new analytical method in the future. Although the proposed system is not fully automated, we hope that the interesting findings presented here will shift the interest of the scientific community and of instrument manufacturers to reconsider AF4-MADLS as a promising calibration-free and bias-free tool to face the emerging challenges of the nanomedicine revolution.

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1B – Fluorine-Free Bio-Based Coatings for Durable Water-Repellent Textiles

V. Trovato, A. Safarshargh, G. Rosace, R. Palucci Rosa, M. Hadhri, A. D'Agostino
(Department of Engineering and Applied Sciences, University of Bergamo, Italy)

Aims

Water repellency is a key functionality for textiles, important for both technical applications and everyday clothing. For decades, this property has relied on per- and polyfluoroalkyl substances (PFAS), whose effectiveness has been overshadowed by concerns about their persistence, bioaccumulation, and health risks. As a result, research has shifted toward fluorine-free options, such as silicone-based finishes, short-chain non-fluorinated repellents, and bio-based polymeric coatings. In this study, two fluorine-free, bio-based acrylate copolymers were applied to cotton and polyester fabrics using a pad-dry-cure method, with crosslinkers to promote network formation and improve wash durability (ISO 105-C10). Coatings were characterized to confirm the uniformity of the polymer films, while hydrophobicity was measured through static water contact angle measurements and spray tests (ISO 4920). The results showed that bio-based resins are sustainable options to replace PFAS, compatible with standard textile finishing methods.

Results

FTIR analysis confirmed successful crosslinking on both textile substrates. On treated cotton, compared to pristine cotton, characteristic changes were observed in the asymmetric and symmetric CH stretching at 2917 and 2850 cm^{-1}, together with absorption bands at 1732, 1686, and 1539 cm^{-1}, assigned to C=O stretching and NH deformation of the crosslinked network (a). Similar infrared absorptions were also detected on polyester, confirming effective coating depositions (b). SEM images revealed the formation of uniform, ultrathin films on both cotton and polyester fabrics, without significantly affecting their original morphology (c, d).

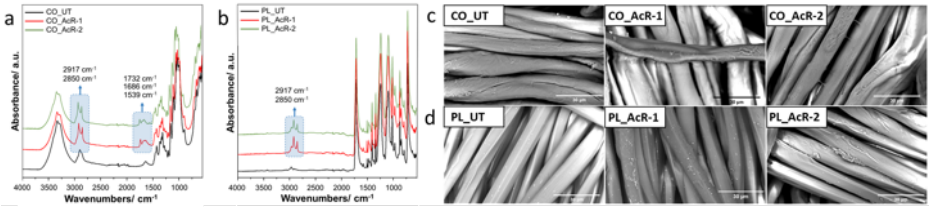
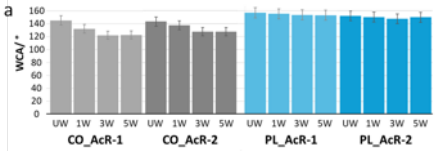


Figure 1: Characterization of fabrics treated with the two fluorine-free bio-based resins (AcR-1 and AcR-2) and comparison with untreated samples (UT): FTIR of cotton (a) and polyester (b); SEM images of cotton (c) and polyester (d) fabrics.

The hydrophobic performance of the fluorine-free bio-based crosslinked networks was assessed through static water contact angle (WCA) measurements (a) and ISO 4920 spray tests (b). Treated cotton fabrics before washing exhibited WCAs close to

140°. Although a decrease was observed after the first laundering cycle, WCA values stabilized after three washes and remained constant up to five (around 120°), demonstrating the maintenance of water repellency properties. On polyester, both bio-based coatings achieved WCAs above 140°, approaching superhydrophobic behavior and comparable to conventional fluorinated finishes. These high values were maintained after repeated washing, confirming the strong adhesion of the crosslinked network. The spray test supported these findings, with polyester consistently outperforming cotton.

a



b

Sample	Unwashed	After 1W	After 3W	After 5W
CO_AcR-1	100	70	50	50
CO_AcR-2	100	70	50	50
PL_AcR-1	100	100	100	100
PL_AcR-2	100	100	100	100

Water repellency performance of cotton and polyester fabrics before (UW) and after the washing cycles (1W, 3W, 5W): (a) Static water contact angle; (b) ISO 4920 spray test.

In conclusion, the fluorine-free, bio-based crosslinked coatings exhibited durable water repellency while preserving the fiber morphology and ensuring stability through multiple washing cycles, particularly on polyester. Their bio-based origin and ultrathin film deposition are compatible with conventional textile processing, also representing a significant step toward aligning with circular economy strategies. These results highlight the potential of bio-based coatings as sustainable and scalable alternatives to PFAS-based treatments, offering a combination of functional performance and environmental responsibility.

This study was carried out within the MICS (Made in Italy – Circular and Sustainable) Extended Partnership and received funding from the European Union Next-GenerationEU (PIANO NAZIONALE DI RIPRESA E RESILIENZA (PNRR) – MISSIONE 4 COMPONENTE 2, INVESTIMENTO 1.3 – D.D. 1551.11-10-2022, PE00000004).

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1B – Functionalized lipid nanocarriers for targeting intracellular delivery of siRNA

I. De Cristofaro, N. Gallucci, L. Paduano
(U.O. of Naples, University of Naples Federico II)

Aims

Gene therapy by RNA interference offers an innovative approach to cancer treatment by silencing disease-causing genes. Effective small interfering RNA (siRNA) delivery requires Lipid Nanocarriers (LNCs) to protect it from degradation (Tenchov et al. 2021). In this project, LNCs were developed using POPC, DOTAP, and PEGylated lipids (DOPE-PEG2000-COOH and DOPE-PEG2000-maleimide). To enable targeted delivery, a T7-modified peptide (CGSG-HAIYPRH), which binds to the human Transferrin Receptor (hTfR) overexpressed on cancer cells, was synthesized and conjugated to the LNCs via thiol-maleimide reaction (Han et al. 2024). The designed LNCs were characterized using Dynamic Light Scattering (DLS), Small Angle Neutron Scattering (SANS), and ζ-potential measurements. Their interaction with vesicle-mimicking tumor cell membrane (TCMVs) was verified using SANS, Fluorescence Correlation Spectroscopy (FCS), and Transmission Electron Microscopy (TEM). Finally, Flow Cytometry experiments were performed to evaluate cellular uptake in the MCF-7 cell line.

Results

LNCs exhibited a suitable hydrodynamic radius for systemic delivery (91 ± 1 nm, Fig. 1a) and a positive ζ-potential value (+50 ± 1 mV) confirming their potential as effective siRNA carriers. Accordingly, CGSG-T7@LNCs@siRNA were prepared by first encapsulating siRNA through hydration of the lipid thin film with a 1 µM siRNA solution in 150 mM PBS. The resulting LNCs@siRNA were then functionalized with CGSG-T7. The characterization of LNCs and CGSG-T7@LNCs@siRNA was performed using SANS. The curves were fitted using the lamellar model, and a noticeable increase in bilayer thickness was observed upon functionalization, suggesting the presence of CGSG-T7 on the LNCs surface (Fig. 1b).

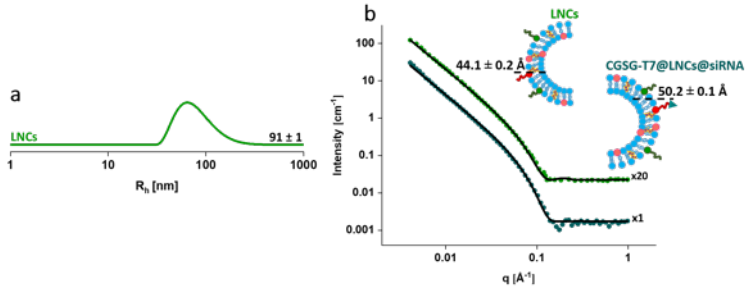

Figure 1: Hydrodynamic distribution curve of LNCs in PBS 150 mM at 37 °C (a); SANS profiles and fittings of LNCs, CGSG-T7@LNCs@siRNA in D2O at 37 °C (b).

To investigate the potential interaction of CGSG-T7@LNCs@siRNA with tumor-mimicking cell membranes, CGSG-T7@LNCs@siRNA were incubated for 24 h with

TCMVs composed of POPC, POPS, and cholesterol. The interaction sample, CGSG-T7@LNCs@siRNA_TCMVs, displayed a bilayer thickness of 42.4 ± 0.1 Å, which is intermediate between the values of the two individual systems, suggesting effective interaction and possible membrane fusion (Fig. 2a). TEM images provided morphological evidence of this process (Fig. 2c). LNCs appeared as well-defined spherical structures. In contrast, LNCs_TCMVs revealed irregularly shaped aggregates. These features are consistent with membrane fusion or strong lipid exchange events between the LNCs and the tumor-mimicking LUVs. Additional confirmation was provided by FCS measurements (Fig. 2b). Free Rhodamine B exhibited a faster diffusion time, while LNCs labeled with Rhodamine B and the interaction sample with TCMVs showed progressively slower diffusion, indicating increased particle size and membrane association. Finally, to assess the cellular uptake of the CGSG-T7@LNCs@siRNA, Flow Cytometry experiments were performed using Rhodamine B labelled CGSG-T7@LNCs@siRNA (Fig. 2d). At the highest tested concentration (100 µM), a high percentage of Rhodamine-positive cells was detected (~94%), indicating efficient interaction and internalization. Uptake was concentration-dependent, decreasing gradually at lower doses.

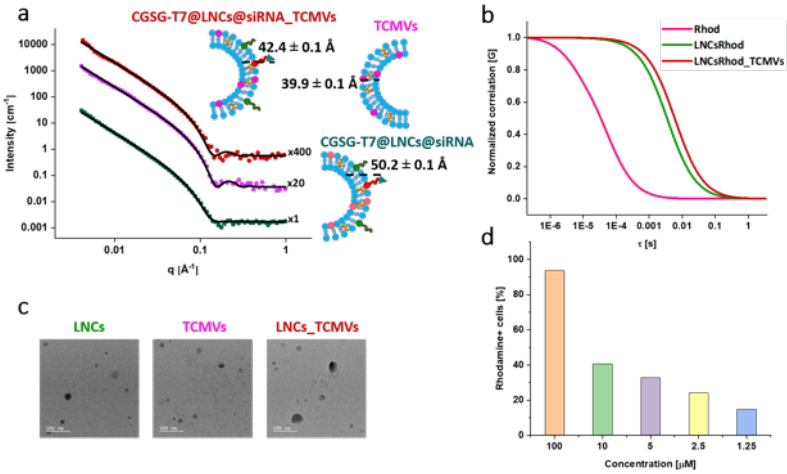

Figure 2: SANS profiles and fittings of CGSG-T7@LNCs@siRNA, TCMVs, and their interaction in D2O at 37 °C (a); FCS data comparing diffusion times of free Rhodamine B, LNCsRhod, and LNCsRhod_TCMVs in PBS 150 mM (b); TEM images of LNCs, TCMVs, and LNCs_TCMVs in PBS 150 mM (c). Flow Cytometry quantification of cellular uptake of CGSG-T7@LNCs@siRNA in MCF-7 cells (d).

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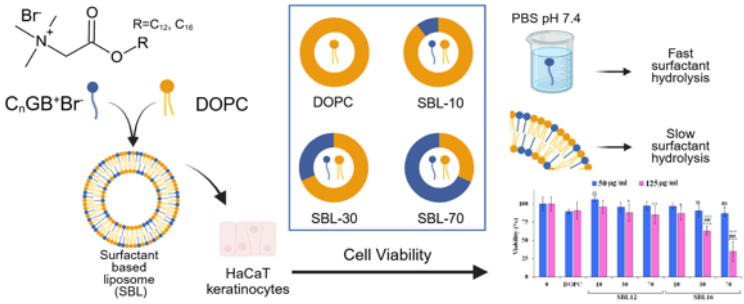
1B – Glycine betaine surfactant-based liposomes: Physicochemical characterization and cytocompatibility assessment

M. Tozzi[a], F. Piras[b], A. Rosa[b], M. Piludu[b], A. Frongia[a], V. Sogos[b], C. Carucci[a], A. Salis[a], F. Cesare Marincola[a]

[a]*Department of Chemical and Geological Sciences - CSGI, University of Cagliari, Italy*
[b]*Department of Biomedical Sciences, University of Cagliari, CA, Italy)*

Aims

Recently there has been an interest in the formulation of drug delivery systems (DDS) that are stable and non-toxic. In particular, a new type of DDS have emerged from the combination of a phospholipid and a surfactant to yield a particular liposome that shows increased flexibility and is ideal for transdermal drug delivery. Some studies synthesized a cationic surfactant using naturally derived compounds like glycine betaine (GB) and fatty alcohols to yield betaine esters surfactant (C_nGB^+). C_nGB^+ are interesting as they belong to the cleavable surfactant category and are hence easily hydrolyzed and more environmentally friendly. C_nGB^+ in particular, are easily hydrolyzed in neutral and basic environment, while they are stable in acidic environment. In this work two betaine esters have been synthesized using dodecyl alcohol ($C_{12}GB^+$) and hexadecyl alcohol ($C_{16}GB^+$). These surfactants have been combined with 1,2-dioleoyl-sn-glycero-3-phosphocholine (DOPC) in different molar percentages (10, 30 and 70 mol % of surfactant) to yield surfactant-based liposomes (SBLs).



To prepare SBLs, different media have been used (MilliQ water, NaCl 10 mM, NaCl 100 mM and PBS 150 mM). Using dynamic light scattering (DLS) and electrophoretic light scattering (ELS), the hydrodynamic diameter (D_H) and the zeta potential (ζ) of the obtained liposomes have been studied and compared to pure DOPC liposomes. DLS and ELS measurements have been repeated in the span of one month to assess the stability of the formulations. Nuclear magnetic resonance (NMR) spectroscopy has been employed on free surfactants as well as on surfactants embedded in the SBLs, to determine the kinetic of hydrolysis of the betaine esters. Transmission electron microscopy (TEM) was employed to obtain an image of the stained and dried suspensions of SBLs. Finally, in vitro citotoxicity of the SBLs prepared in PBS was studied through MTT assay using HaCaT cell line.

Results

Compared to DOPC liposomes, SBLs present a more consistent D_H when changing the solution used to prepare them, showing a milder influence of the dispersant's ionic strength on their size. ζ increases for all SBLs as the molar percentage of surfactant increases, and it is higher for weaker ionic strength of the dispersant. All formulations showed good storage stability in the span of one month. Kinetic hydrolysis in PBS pH 7.4 showed that $C_{12}GB^+$ was completely hydrolyzed after 10.5 hours, while $C_{16}GB^+$ degradation took place in only 5 hours. Interestingly, when both were embedded in the SBLs, their hydrolysis was significantly hindered. SBLs with 10 mol % of surfactants showed no sign of degradation after 24 hours from the formulation. SBLs with 30 mol % of C_nGB^+ showed a 19% and 15% of hydrolysis for shorter and longer alkyl chain respectively. Finally, SBLs with 70 mol % of surfactants, displayed the highest hydrolysis: 31% and 39% for $C_{12}GB^+$ and $C_{16}GB^+$ respectively. Lastly, MTT assay on HaCaT cells showed that all SBLs besides SBL with 70% of $C_{16}GB^+$ did not affect cell viability compared to untreated cells, when analyzed at 50 µg/mL. Increasing the concentration of SBLs to 125 µg/mL brought to a decrease in cell viability for most SBLs, while SBL12 with 10% of the shorter chain surfactant showed no citotoxicity even at the highest concentration tested. Overall, this study showed the possibility of formulating surfactant-based liposomes with a naturally derived surfactant that can be easily hydrolyzed at neutral pH while being stable in storage for at least one month when present within the SBLs. These systems can be prepared easily and are characterized by a stable D_H while they can be tuned adjusting the surfactant content. SBLs demonstrated low citotoxicity with SBL12-10 in particular, showing no citotoxicity even at high concentrations, representing a good candidate for a future application in drug delivery. Future studies will take place to study the capability of these systems to load and release an hydrophilic drug. Permeability tests on a model membrane using a Franz cell will also be performed to assess SBLs potential to be used in transdermal drug delivery.

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1B – Green Protein-Based Nanohybrids as Adaptive Surfactants – GrASs project (PRIN2022 PNRR - P2022PKRWA)

I. Russo Krauss[a], G. Li Destri[b]
[a] *University of Naples Federico II, CSGI U.O. Naples*
[b] *University of Catania, CSGI U.O. Catania*

Aims

Stabilization of soft interfaces under dynamic conditions represents still a challenge for formulation of stable dispersed systems, such as emulsions and foams. As a possible approach GrASs project plans to exploit proteins as surface active agents, because thanks to their large dimensions and hierarchical structure, characterized by high flexibility and adaptability to environmental conditions, they are promising adaptive surfactants; moreover, they are more eco-sustainable and biocompatible than canonical oil-based surfactants. However, to truly unlock their potential it is necessary to stabilize protein films under dynamical conditions. The project aims to leverage the high desorption energy of NPs to achieve this result, by thoroughly investigating protein-NP interactions and NP-induced protein structural changes in bulk solution, which are expected to play a crucial role in guiding adsorption at interface and determining interfacial film behavior.

Results

To develop protein-nanoparticle nanohybrids (PNH) endowed with surface activity for stabilization of air/liquid and liquid/liquid interfaces in a variety of different environmental conditions, we have chosen commercially available silica NPs and a variety of model proteins characterized by different structure, flexibility, and isoelectric point, namely Bovine Serum Albumin (BSA), β-lactoglobulin (BLG), and β-casein (BCN).

The GrASs project has been organized along two main research lines: i) the detailed characterization of PNH behavior in i) bulk solution, ii) at fluid interfaces.

As for the first research line, we focused on possible protein structural reorganization and stability within PNH and on protein-NP interaction, using a variety of spectroscopic techniques including circular dichroism and fluorescence spectroscopy, as well as on the structural characterization of PNHs and their colloidal stability, employing scattering techniques such as Dynamic and Electrophoretic light scattering and Small Angle Neutron Scattering. We also analyzed the effects of different environmental parameters such as pH and ionic strength on formation and stability of PNHs.

As for the second research line, surface activity of proteins and PNHs at increasing NP content was analyzed in static and dynamic conditions by means of dynamic surface tension and by recording compression isotherms in a Langmuir trough, highlighting how NP addition significantly modifies protein behavior. Structural features of PNH monolayers were investigated in detail by means of synchrotron Grazing Incidence

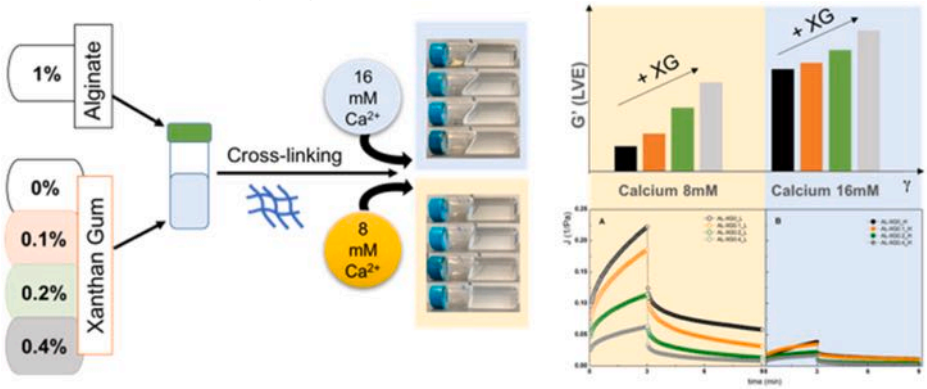
Small Angle X-ray Scattering (GISAXS), as well as by Neutron Reflectometry (NR), during compression in a Langmuir trough.
Overall, we found that the interfacial properties of PNHs, in terms of surface tension reduction, monolayer structure, and response to compression, strongly depends on composition, opening the way to the leverage of tailored protein-NP formulations for the design of thin films with tunable interfacial properties.

1B – How xanthan gum affects the flow and deformation properties of alginate gels

M. Cofelice, M.C. Messia, E. Marconi, F. Cuomo, F. Lopez

Aims

The selection of biopolymers as constituents of hydrogels is of great importance to enable their use in a variety of fields. The present study proposes a mixed hydrogel of alginate (AL) and xanthan gum (XG) prepared by the in-situ gelation method promoted by Ca^{2+} at two different concentrations, using a fixed concentration of AL and variable quantities of XG. The main goal was to evaluate how the presence of XG could affect the properties of crosslinked AL through the study of rheology by small and large amplitude oscillatory shear tests, steady shear flow and time dependent properties of the obtained blended hydrogels.



Results

The results showed that the hydrogels behaved like shear-thinning materials and Carreau fluids. The overall viscosity of the hydrogels depended on the concentrations of both Ca^{2+} and XG. The length of the linear viscoelastic range was only influenced by xanthan gum content at low calcium concentrations, while storage modulus (G') increased with xanthan gum and calcium content. Interpolating the mechanical spectra using a power law showed that G' and G'' depended slightly on frequency, and that G' became less frequency-dependent with the addition of xanthan gum. Although the elastic contribution of the hydrogel increased with calcium and xanthan concentrations, the hydrogels obtained could not fully recover their original structure after a high load was applied. Behaviour at large amplitude oscillatory strain, which mimics real processing conditions, showed that hydrogels crosslinked with a low calcium concentration were affected by xanthan gum at lower concentrations than hydrogels crosslinked with a high calcium content. Such hydrogel mixtures could be used in food industry research.

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1B – Hybrid materials for drug-delivery

M. Bini, G. Bruni, et al.

Aims

A large part of the drugs on the market is poorly soluble in the gastro-intestinal tract, so requiring the administration of high dosages to reach the minimum effective daily dose. The development of systems or methods allowing improving the drug solubility is a forefront topic for the pharmaceutical market. The available methods are numerous, including salt formation, co-crystal production, excipients addition or the micronization. In this field, we propose the synthesis of hybrid organic (drug) and inorganic (Layered Double Hydroxides (LDH) or Hydroxyapatite (HAP)) systems to improve the wettability, solubility and drug dissolution rate with respect to the drug alone. We also prepared bone cements (phosphate based) loaded with anti-inflammatory drugs as injectable cements to solve bone injuries.

Results

We mainly focused on the synthesis of HAP pure and properly doped as a drug delivery system for poorly water-soluble anti-inflammatory or diuretic drugs. We applied this strategy to Bumetanide, Meloxicam, Tenoxicam and Piretanide drugs (see references). The hybrids, in which the drug and HAP are linked by weak bonds, were characterized by the physical-chemical techniques such as X-ray powder diffraction, FT-IR spectroscopy, SEM and EDS analysis demonstrating the successful synthesis of the hybrids, and, in case of doping, the stoichiometry of the samples. Pharmaceutical measurements are mandatory in these cases to determine the possible improvement of dissolution rate and solubility of the hybrids with respect to the drug alone. We could determine that the hybrids' wettability was improved with respect to the separated entities, so justifying the excellent dissolution rates measured in different media at various pH values.

Calcium phosphate cements (CPCs), thanks to some amazing features such as the ability to harden in vivo, bioactivity, and resorbability, are promising candidates to treat musculoskeletal disorders, notwithstanding their poor mechanical properties. We synthesise pure and barium- or silicon-doped brushite-based CPCs loaded with piroxicam to study the effects of the substitution on physical-chemical and pharmaceutical properties before and after cement immersion in phosphate buffer for different times. Our results demonstrated that piroxicam became amorphous in the hardened cements. The dopants did not change the brushite structure or its lamellar morphology, while both Ba and Si additions improved the initial Young modulus compared to the pure cement, and the opposite trend was observed for compressive strength. Both the compressive strength and the elastic modulus decreased for the samples immersed in solution compared to the non-immersed samples, with stabilisation as the number of days increased. After 7 days, the whole drug amount was released, with a slower and constant kinetic for the Ba-doped cements compared to the pure and Si-doped ones.

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1B – Hybrid synthetic biogenic lipid particles

L. Caselli, J. Cardellini, A. Balestri, V. Pacciani, D. Berti

Aims

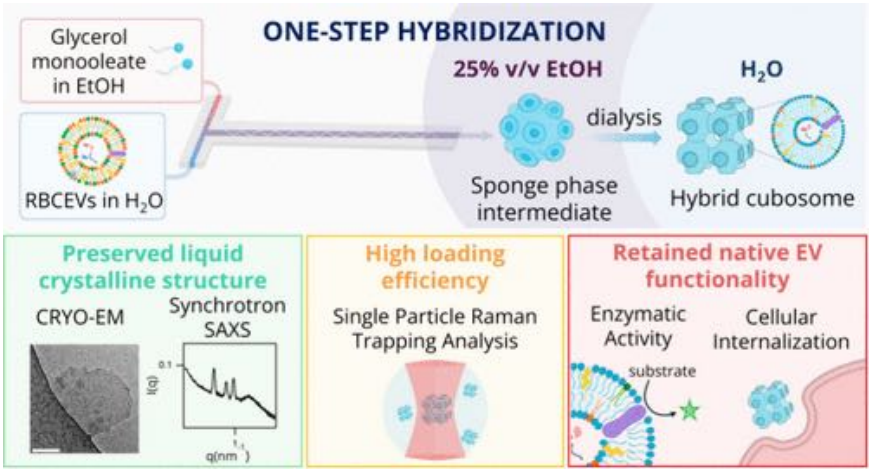
Lipid-based nanoparticles (LNPs), ranging from lamellar structures like liposomes to non-lamellar liquid crystalline nanoparticles like cubosomes and hexosomes, are attracting growing interest as next-generation drug delivery platforms, as demonstrated by the widespread success of nucleic acid vaccine formulations. However, synthetic LNPs still face important challenges in biological environments, including poor cell uptake and tissue targeting. A promising strategy to overcome these limitations is the hybridization of synthetic nanocarriers with biogenic materials—naturally derived components such as extracellular vesicles (EVs), purified cell membrane–derived components, and bioactive proteins or peptides. EVs, lipid bilayer-enclosed particles released by all types of cells, are particularly attractive in this context. These vesicles carry a variety of cellular components and play key roles in cell–cell communication and many biological processes. Their native protein–lipid composition enables prolonged circulation, immune evasion, and selective interactions with target cells, making them ideal candidates for enhancing the biological performance of synthetic LNPs.

Results

In this work, we introduce a single-step microfluidic strategy to engineer hybrid nonlamellar LNPs, specifically cubosomes, with prototypical EVs, namely, red-blood-cell-derived EVs (RBCEVs). Uniquely, in this approach, hybridization occurs *in situ* during LCNP formation via ethanol-assisted microfluidic preparation. Inspired by the microfluidic-based ethanol injection method used for mRNA encapsulation in LNP formulations, our process involves mixing an ethanol phase (containing synthetic lipids in monomeric form) with an aqueous phase containing EVs (in place of mRNA), followed by ethanol removal.

This process not only yields colloidally stable hybrid LCNPs with precise structural and compositional control but for the first time preserves the internal liquid-crystalline architecture of synthetic LCNPs following RBCEV hybridization. Synchrotron small-angle X-ray scattering (SAXS) and cryoelectron microscopy (cryo-EM) revealed hybrid nanoparticles featuring well-defined cubic internal structure alongside phase-separated amorphous nanodomains enriched in native RBCEV-associated proteins. Hybridization efficiency was quantified using single particle automated Raman trapping analysis (SPARTA), while enzymatic assays confirmed retention of the bioactivity of the RBCEV acetylcholinesterase membrane protein. Additionally, the hybrids exhibited enhanced cellular uptake in HEK293t cells.

From a mechanistic perspective, we demonstrate that the presence of ethanol during microfluidic is critical for both retaining the LCNP structure and enabling efficient encapsulation of RBCEV components.



This finding aligns with recent studies that increasingly highlight the role of ethanol in LNP formulation, though its mechanistic contribution remains largely unexplored. Ethanol is universally employed in LNP microfluidic preparation, where the water/ethanol volume ratio during mixing modulates LNP self-assembly and nucleic acid encapsulation. At the same time, the presence of ethanol in LNP preparations has been shown to destabilize lipid assemblies by altering membrane permeability and fluidity, promoting particle aggregation and potentially enhancing membrane fusion propensity. Beyond these empirical observations, however, the influence of ethanol on LNP-related processes, particularly particle fusion, remains poorly understood.
Addressing this gap, we here elucidate for the first time the mechanism of ethanol-assisted hybridization, revealing ethanol-mediated structural rearrangements within LNPs that drive RBCEV loading and impart long-term structural stability.
This proof-of-concept study establishes a high-throughput, scalable platform for generating hybrid biogenic LCNPs with high structural and compositional precision, potentially translatable to a broad range of synthetic/biogenic hybrids.

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1B – Intrinsically chiral organic functional materials

F. Fontana , I. Natali Sora , R. Pelosato
(Department of Engineering and Applied Sciences, University of Bergamo, Dalmine (Bg), Italy)

Aims

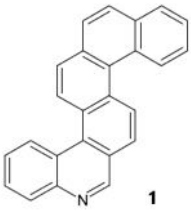
Preparation of organic materials extensively conjugated and intrinsically chiral. Helicenes with 6 or more fused aromatic rings, homocyclic or bearing one or more heteroatoms, such as nitrogen or sulfur, will be synthesized and modified, by either side chains or functional groups or by quaternarization of the nitrogen atom. These structures will be characterized and applied to

a) the preparation of SERS-active noble metal surfaces for the detection of chiral biomolecules
b) intrinsically chiral substances to be used as additives in ionic liquids for the chiral discrimination of biomolecules in electroanalytical processes

Results

A study on phenanthro[3,2-*k*]phenanthridine (**1**) obtained as byproduct during the synthesis of an aza[6]helicene illustrates the potential of SERS in characterizing novel aza-aromatic derivatives with complex structures. The present application is performed on samples in a strongly diluted solution due to the extreme sensitivity of the SERS technique, thus avoiding intermolecular interactions that can affect the Raman spectra of crystalline samples.

Remarkably, thanks to these experimental conditions, even fine details in the SERS spectrum of 2 can be assigned by DFT calculations, thus allowing the complete identification of the molecular structure. The weak interaction of 2 with the Au surface does not dramatically affect its intrinsic molecular and vibrational structures. Hence, we can identify in the SERS spectra recorded on 2 reliable vibrational fingerprints characteristic of the isolated molecule. Moreover, the analysis of the frontier molecular orbitals explains the charge transfer mechanism at the basis of the chemical mechanism of SERS.



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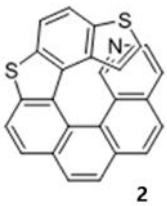

2

A new dithiaaza[7]helicene (**2**) of remarkably multifaceted nature and functional properties is introduced and studied by comparison with a pool of simpler thia- or azahelicenes and related model molecules. Its helical conjugated backbone endows it with interesting spectroscopic and electrochemical features as well as with powerful inherent chirality. In addition, the new molecule has terminals of opposite character which endow it with push-pull features (along the backbone and across 3D space) as

well as with a remarkable pool of functional properties: (i) an electron poor pyridine-based terminal, which can be involved in acid/base equilibria or enable conversion into molecular salts by alkylation; and (ii) an electron rich (benzodi)thiophene-based terminal, which allows reproducible electrodeposition of electroactive films, thus enabling to transfer the above pool of properties from single molecule to nanostructured inherently chiral electroactive material

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1B – Investigation of the gelation mode of agarose and application of its hydrogels as 3D-confined cell microenvironments

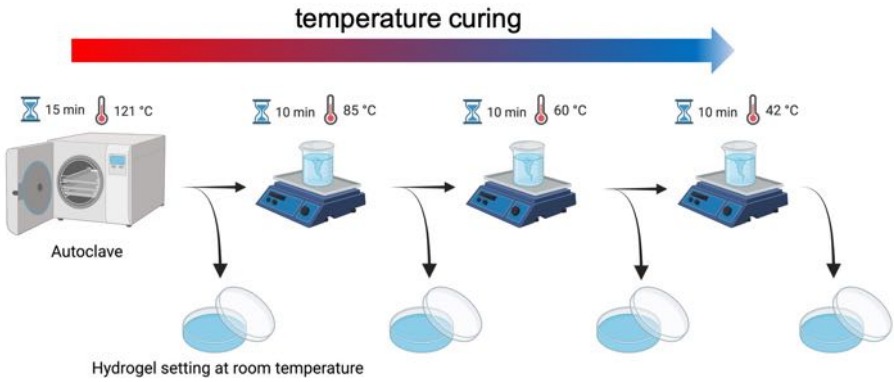
L. Mio , F. Piazza , E. Fratini , F. Lopez , I. Donati, P. Sacco

Aims

Agarose undergoes thermally reversible gelation when hydrogen bond-controlled cross-links are formed between the biopolymer chains leading to their aggregation, sustained by the entropy gain associated to the release of water molecules from the biopolymer, leading to the aggregation of polysaccharide chains. Final agarose hydrogels appear as slightly turbid, rigid and viscoplastic networks whose mechanics can be well tailored depending on the molecular weight and chemical composition of the agarose, its concentration, the temperature quenching of the solutions and the thermal history of the final hydrogels. Final agarose hydrogels can be used for the development of cell spheroids or in the context of tissue engineering and mechanobiology.

Results

With respect to temperature quenching of the agarose solutions, we have reported a material strategy for the fine modulation of quenching that involves temperature-curing steps of agarose. Combining microscopy techniques, standard and advanced macro/nanomechanical tools, we revealed that agarose accumulates on the surface when the curing temperature is set at 121 °C. The inhomogeneity can be mostly recovered when it is reduced to 42 °C. This has a drastic effect on the stiffness of the surface, but not on the viscoelasticity, roughness and wettability. When hydrogels are strained at small/large deformations, the curing temperature has no effect on the viscoelastic response of the hydrogel bulk, but does play a role in the onset of non-linear region. Cells cultured on these hydrogels exhibit surface stiffness-sensing that affects cell adhesion, spreading, F-actin fiber tension and maturation of vinculin-rich focal adhesions. Collectively, our results indicate that the temperature curing of agarose is an efficient strategy to produce networks with tunable mechanics and suitable for mechanobiology studies. In recent experiments we have used a combined approach of oscillatory rheology, low-field NMR, small-angle X-ray scattering (SAXS) and cryo-SEM to investigate the gelation stage of agarose. The data have revealed a two-phase gelation process that can be efficiently tuned by using anions with different degrees of hydration, changing the biopolymer entanglement or applying mechanical shear stimulation. This could have an impact on the final topology of the network, which is crucial in the context of cell mechanobiology.



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1B – In Vitro Effects of Charged and Zwitterionic Liposomes on Human Spermatozoa and Supplementation with Liposomes and Chlorogenic Acid during Sperm Freezing

E. Moretti, C. Bonechi, A. Donati, C. Rossi, S. Costantini, C. Signorini, R. Corsano, L. Micheli, L. Liguori, G. Centini, G. Collodel

(Department of Molecular and Developmental Medicine, Department of Biotechnology, Chemistry and Pharmacy and Department of Medicine, Surgery and Neuroscience, University of Siena, Siena)

Aims

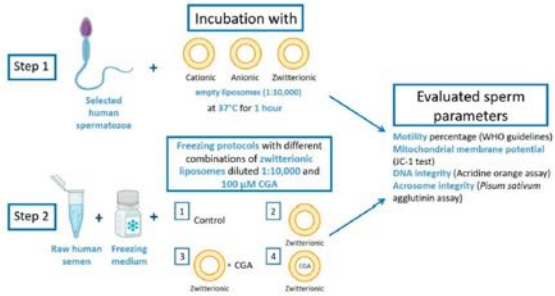
Semen handling and cryopreservation cause oxidative stress, which must be minimized. This study tested human semen supplementation during cryopreservation with handmade liposomes and chlorogenic acid (CGA), an antioxidant. Zwitterionic (ZL), anionic (AL), and cationic (CL) liposomes were synthesized. Swim-up sperm aliquots were incubated with each liposome type (1:10,000). Sperm motility, mitochondrial membrane potential (MMP; JC-1), DNA integrity (AO), and acrosome status (PSA) were evaluated. For cryopreservation, semen was frozen with: empty ZL (EL), EL + free CGA (CGA + EL), CGA-loaded ZL (CGA), or control medium (CTR). ZL were best tolerated and chosen for freezing. All supplemented groups outperformed CTR ($p < 0.001$). Notably, CGA and CGA + EL samples showed higher motility, DNA integrity, and acrosome preservation vs. CTR and EL ($p < 0.001$; motility EL vs. CGA + EL $p < 0.05$). ZL and CGA improve post-thaw sperm quality by reducing cold shock and oxidative stress, offering new insights for reproductive medicine.

Results

This study explored the effects of different types of liposomes (cationic, anionic, and zwitterionic) on human sperm. In the first phase, empty liposomes were tested to assess their impact on sperm motility, mitochondrial membrane potential (MMP), DNA integrity, and acrosome status. Zwitterionic liposomes, made of phospholipids similar to those in sperm membranes, were the most biocompatible and non-toxic. In contrast, cationic liposomes caused hyperactivated motility, increased MMP, and DNA damage indications of early sperm capacitation, a process needed for fertilization. However, due to their genotoxic potential and inflammatory effects, cationic liposomes were excluded from further use.

Chlorogenic acid (CGA) has a protective effect on human sperm during cryopreservation. Based on this, the study incorporated CGA into zwitterionic liposomes to enhance sperm protection during freezing. In the second phase, zwitterionic liposomes were loaded with CGA and used as cryopreservation

supplements for human sperm. These liposomes, previously shown to be safe in other cell types, were chosen for their high compatibility and non-toxic profile.



Cryopreservation, essential in reproductive medicine and fertility preservation, often leads to cellular damage due to factors such as ice crystal formation, oxidative stress from reactive oxygen species (ROS), and membrane disruption. Although sperm cells are structurally favorable for freezing, they remain highly vulnerable to cryoinjuries that compromise motility, DNA integrity, mitochondrial function, and overall viability. In this study, adding liposomes, whether empty, loaded with CGA, or combined with free CGA, to cryopreservation media improved sperm cryostability and functionality. The liposomes likely aided membrane repair by restoring phospholipids lost during freezing, while CGA contributed antioxidant protection. The best results were observed when CGA was both encapsulated in liposomes and present freely in the medium, leading to higher sperm motility, DNA integrity, mitochondrial activity, and acrosome stability.

The improvement observed in samples supplemented with empty liposomes could be explained by the fact that the liposomes can act as excellent reservoirs of phospholipids and help in replenishing those lipids that are lost from the sperm membrane damaged by cold shock during the freezing process.

In addition, our data indicate that the concomitant use of CGA, both loaded in the liposomes and free in the media, resulted in a significant increase in the sperm's progressive motility, DNA integrity, mitochondrial.

In conclusion, zwitterionic DOPC/DOPE liposomes can represent an excellent drug delivery system for a water-soluble drug. In addition, they are compatible with human spermatozoa, and, when used in combination with CGA, can improve the post-thaw sperm quality, acting both on the management of cold shock effects and on ROS generation. These findings can open a new field of studies with a large number of perspectives on human and animal reproduction.

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1B – Kolbe electroorganic synthesis of hydrocarbons from carboxylic acids derived from vegetable oils

F. Fontana , I. Natali Sora , R. Pelosato, H. Ahmad
(Department of Engineering and Applied Sciences, University of Bergamo, Dalmine (Bg), Italy)

Aims

Valorization of renewable materials such as biomass is raising increasing attention in order to reduce the use of fossil raw materials. This project aims to use electrochemical processes, such as the Kolbe reaction, to transform raw materials such as vegetable oils into long chain hydrocarbons or other organic intermediates, for the formulation of fully green bio-lubricants.

Results

After a study concerning the transformation of pure fatty acids, namely lauric and palmitic acids, into long-chain hydrocarbons by electrochemical decarboxylation followed by radical coupling, in which conditions were optimized and byproducts identified, the procedure was extended to raw materials such as coconut oil. The impact of operating parameters such as current intensity (10 mA–100 mA), amount of KOH (0.4–1.7 eq), electrolysis time (2–18 h), and different solvent environments on the process performance were investigated in terms of chemicals production, especially focusing on the dimers yield.
Future prospects aim to tune the reaction conditions to obtain different products, such as alkenes, and to use different raw materials, possibly focusing on wastes from agriculture.

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1B – Lipid-based nanoformulations for treatment of eye pathologies

I. Clemente[1], L. Talarico[1], I. Mavromatidou[1], G. Gabbricci[1], S. Pepi[1], G. Vigni[1], S. Cataldini[1], C. Migone[3], L. Vicarelli[3], G.M. Fortunato[4], A. Esposito[4], C. Bonechi[1], G. Leone[1], M. Andreassi[1], A. Cappelli[1], F. Rossi[2], J.L.Y. Chen[1], A.M. Piras[3], V. Calderone[3], G. Vozzi[4], A. Magnani[1]

[1]Department of Biotechnology, Chemistry and Pharmacy, University of Siena;
[2]Dipartimento di Scienze Fisiche, della Terra e dell'Ambiente, University of Siena
[3]Dipartimento di Farmacia, University of Pisa
[4]Dipartimento di Ingegneria dell'Informazione, University of Pisa)

Aims

Lipid-based nanocarriers represent the emergent technology for drug delivery, owing to the capability to protect the bioactive cargo and improve intracellular transport and release. Since their approval for clinical use as vectors for anticancer drugs and gene therapy, several lipid nanocarrier formulations were investigated to obtain optimal physicochemical properties and enhanced therapeutic efficacy. They possess optimal characteristics as carriers for topical treatment of eye pathologies e.g. high surface contact with ocular membranes, enhanced retention and permeation capability, ability to cross physiological barriers, biocompatibility, and proven clinical efficacy.

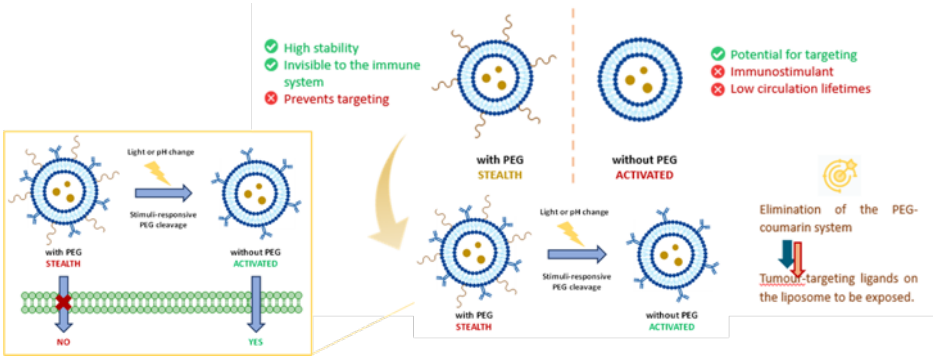
Results

The design, synthesis and characterization of lipid-based nanoformulations namely Lipid Nanoparticles (LNPs), Solid Lipid Nanoparticles (SLNs) and TransEthosomes (TEs), as stimuli-responsive carriers for treatment of inflammatory/infectious and degenerative eye pathologies with good encapsulation efficiency of drugs, enhanced stability and switchable stealth/active properties, efficient and controlled cell-targeting to achieve good cell internalization and drug release were successfully obtained.

Natamycin (NAT), an antifungal polyene and the only currently FDA-approved drug for topical treatment of fungal keratitis, and Triamcinolone Acetonide (TA), an angiostatic steroid effective against intraocular inflammations and Age-Related Macular Degeneration (AMD), were here chosen as model drugs. Nanosystems optimization and synthetic process scale up were obtained by robust statistically-driven methods (precise microfluidic assisted preparation driven by experimental design approaches) to the final prototypes.

The optimized smart nanosystems loaded with model drugs were characterized in terms of both dimensions, colloidal stability and supramolecular structure. In vitro testing with cell lines for the foreseen applications and 3D biomimetic models of eye were used to evaluate their therapeutic efficacy [1-4].

PEG dilemma (a) and self-assembly for the formation of the stimuli-responsive stealth/active LNPs (b).



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1B – Lipid nanoparticles (LNPs) for gene delivery: synchrotron measurements correlate bulk phase structure and mRNA transfection efficiency

C. Carucci[1], J. Philipp[2], J.A. Müller[2], A. Sudarsan[3], E. Kostyurina[2], C.E. Blanchet[4], N. Schwierz[3], D.F. Parsons[1], A. Salis[1], J.O. Rädler[2]

[1]*Department of Chemical and Geological Sciences, University of Cagliari & CSGI, Italy*

[2]*Faculty of Physics, Ludwig-Maximilians University, Munich, Germany*

[3]*Institute of Physics, University of Augsburg, Germany*

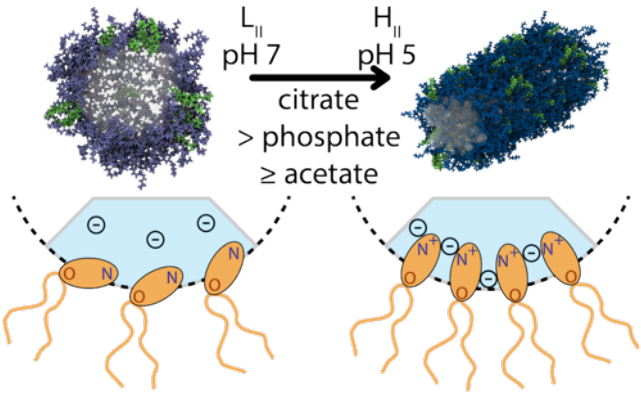
[4]*European Molecular Biology Laboratory Hamburg Outstation c/o Deutsches Elektronen-Synchrotron, Hamburg, Germany*

Aims

After Covid-19 outbreak gene delivery for vaccine therapy has rapidly gained interest. Lipid nanoparticles (LNPs) technology has been chosen, thanks to properties such as low cytotoxicity, high colloidal stability and pH dependent behavior.[1] LNPs are composed of an outer shell of zwitterionic lipid and a pegylated moiety while into the core an ionizable lipid and cholesterol self-assemble to create inverse micellar structures where the mRNA is encapsulated. During endocytosis, LNPs face a change of pH going from pH 7.2-7.4 up to slightly acidic pH 6.0-5.5 to reach the target of delivery. The core LNPs structure, due to the protonation of ionizable lipids, undergoes to a change into interface curvature that results in a phase transition from inverse micellar (L_{II}) to inverse hexagonal (H_{II}) phase. The internal core phase structures change due to pH, have been followed by means of synchrotron Small Angle X Ray Scattering (SAXS) measurements. The L_{II}-H_{II} transition has been demonstrated to influence the mRNA transfection efficiency thus showing a primary role in gene delivery. [2] Since decades, buffers to set and to maintain the pH, have been demonstrated to influence biological systems in a specific manner. [3] However, while the pH effect has been demonstrated to affect the phase transition and the biological efficiency, the preparation buffer influence on LNPs core phase has not been considered. The aim of the present work, is to study the internal phase structure as function of pH and buffer type.

Results

The internal LNPs phase formulated with 1) DLin-MC3-DMA 2) SM-102 and 3) ALC-315 have been studied as a function of pH and buffer type by means of synchrotron SAXS measurements. The transition of the LNPs core phase, from L_{II} to H_{II} phase is found to be buffer specific, occurring at a pH decreasing along the series citrate > acetate > phosphate. Moreover, a correlation of the transfection efficiency, depending on the buffer, and bulk phase transition has been demonstrated for the analyzed ionizable lipids. A mechanism based on the buffer specific phase transition L_{II} to H_{II} has been proposed; the change in structure is due to different headgroup areas due to specific buffer adsorption on the ionizable lipid moieties. The hypothesis of the buffer specific structural changes was also confirmed by DLin-MC3-DMA MD simulations. [4]



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1B – Liposomal formulation of Citicoline for Ocular Drug Delivery

C. Bonechi, F.F. Mahdizadeh, L. Talarico, S. Pepi, S. Costantini, M. Andreassi, G. Tamasi, G. Leone, M. Consumi, A. Donati, C. Rossi, A. Magnani
(Department of Biotechnology, Chemistry and Pharmacy, University of Siena, Siena)

Aims

Glaucoma represents a group of neurodegenerative diseases characterized by optic nerve damage and the slowly progressive death of retinal ganglion cells. Pharmaceutical treatment of glaucoma is critical because of the properties of the ocular barrier that limit the penetration of drugs, resulting in lower systemic bioavailability. This behavior causes the need of frequent drug administration, which leads to deposition of concentrated solutions on the eye, causing toxic effects and cellular damage to the eye. To overcome these drawbacks, novel drug-delivery systems, such as liposomes, can play an important role in improving the therapeutic efficacy of antiglaucomatous drugs. Liposomes were synthesized to improve various aspects, such as ocular barrier penetration, bioavailability, sustained release of the drug, targeting of the tissue, and reduction in intraocular pressure. Citicoline (cytidine 50-diphosphocholine) is an important intermediate in the biosynthesis of cell membrane phospholipids, with neuroprotective and neuroenhancement properties, and it was used in the treatment on retinal function and neural conduction in the visual pathways of glaucoma patients. Citicoline was loaded into the 1,2-dioleoyl-sn-glycerol-3-phosphocholine and cholesterol liposomal carrier to enhance its therapeutic effect. The encapsulation efficiency, drug release, and size analysis of the different liposome systems were investigated using dynamic light scattering, nuclear magnetic resonance, infrared spectroscopy, and ToF-SIMS experiments.

Results

The physicochemical properties of liposomes were studied to evaluate the behaviour of citicoline in the presence of bilayers and to highlight its ability to deliver drugs. Conformational properties were determined by nuclear magnetic resonance (NMR), attenuated total reflection Fourier transform infrared spectroscopy (ATR-FTIR), and time-of-flight secondary ion mass spectrometry (ToF-SIMS) experiments. Stability studies were also performed on all liposomal preparations to evaluate their storability as a pharmaceutical form.

The dynamic light scattering results showed that the mean particle size of plain liposomes, DOPC:Chol (1:1) and DOPC:Chol (2:1), were 118 ± 4 and 105 ± 3 nm, respectively. The binding of citicoline to liposomes as well as their nanoencapsulation increased the particle sizes, indicating an increase in the hydrodynamic diameter of liposomes due to the presence of a hydrophilic molecule in the system. Moreover, the size of liposomes did not vary as a function of lipid composition (or molar ratio between lipids), and the different amount of cholesterol affected only the

fluidity/permeability and the organization (phase and domain formation) of phospholipid bilayers.

Figure 1 shows the comparison between loaded and plain liposomes DOPC:Chol (2:1) and the NMR spectrum of pure citicoline in solution. This approach allows us to highlight the presence of the active compound in the liposomes. In the spectrum of liposomes loaded with the drug, low-field proton signals attributable to citicoline protons can be seen after dialysis. In particular, the aromatic signals indicate the insertion of citicoline into the hydrophilic head of the phospholipid bilayer and confirm the successful encapsulation of citicoline in the vesicles. The broadening of the NMR signals of citicoline directly indicates the correct incorporation of the drug into the liposome.

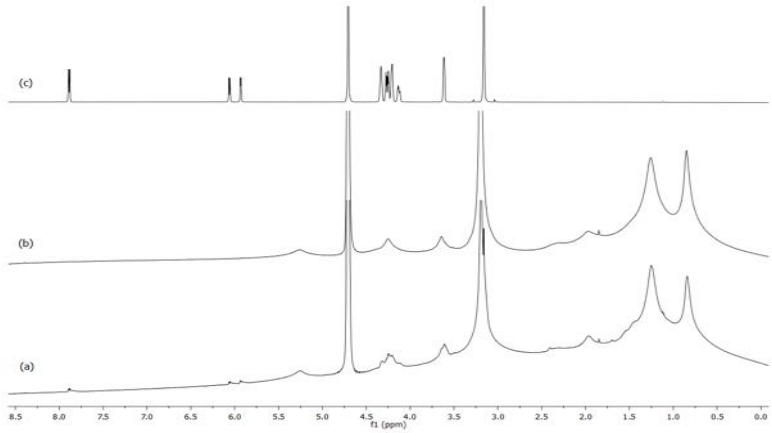

Figure 1: 1H-NMR spectra of liposomes: (a) DOPC: Chol, Cit (2:1),1; (b) DOPC:Chol (2:1) and (c) citicoline 10-2 M in D2O

The NMR, ATR-FTIR, and ToF-SIMS experiments indicated that the citicoline was loaded correctly into the vesicles and that no differences between the two formulations were apparent. Cholesterol concentration affects the release of the drug in the ophthalmic fluid: a high concentration accelerates the release of the drug. The slower release of citicoline in the liposome, with the low amount of cholesterol, allows the drug to act more effectively to protect the optic nerve over time and reduce the administration of eye drops.

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1B – Long-term Water Management Model in the Presence of Extraordinary Events

A. De Vincenzo , B. Molino, A. De Nigris , L. Ambrosone

Aims

In order to make the “Sediment Disposal, Recovery, and Reuse” supply chain efficient in a reservoir management project, sediment storage methods are fundamental. The project's objectives include studying the recovered submerged sediments present in a reservoir, their storage in geotubes, and the possibility of their environmental reuse.

Results

The stretched exponential model describing the sedimentation process of a reservoir was extended to appropriately encompass extraordinary events. These were divided into rapid and sudden events and programmatic events. Among the uncontrollable events, we analysed landslides or extreme weather events. Scheduled events included the construction of satellite dams upstream of the reserve. In addition, a continuous process that reaches a stationary condition is analysed. Finally, it was indicated how to become aware of non-routine events by having a limited number of bathymetric surveys available. The management plot in the presence of two sudden events, which take place at two different times in the life of the dam, was illustrated and discussed

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1B – Membrane binding of charged compounds and ion transport by P-type ATPases investigated on solid supported membranes

F. Tadini-Buoninsegni, P.S. Sfragano, I. Palchetti (Department of Chemistry "Ugo Schiff", University of Florence), R.J. Clarke (School of Chemistry, University of Sydney, Australia)

Aims

Solid-supported-membranes (SSM) represent a convenient model system of a biological membrane, with the advantage of being mechanically so stable that solutions can be rapidly exchanged at the surface. The SSM consists of a hybrid alkanethiol-phospholipid bilayer supported by a gold electrode. In the present research we used the SSM method to analyze the membrane binding of the hydrophobic ions tetraphenylborate (TPB-) and tetraphenylarsonium (TPA+) [1]. We determined the dissociation constant (Kd) for interaction of the ions with the membrane. Our measurements also provided kinetic information on the ion-membrane binding process. Notably, the SSM method is potentially applicable to studying the membrane interaction of any charged compounds, such as charged drug molecules. Besides the sensitive detection of membrane binding, we employed the SSM technique to characterize the interaction of various compounds, e.g. natural products or compounds of synthetic origin [2,3], with the sarcoplasmic reticulum Ca2+-ATPase (SERCA), which belongs to a superfamily of membrane transporters known as P-type ATPases. SSM measurements were performed to characterize the effects of such compounds on the Ca2+ transport activity of SERCA. The reported data qualify the SSM method as a reliable and simple assay that can be conveniently employed to evaluate pharmacological agents that affect membrane transporter function.

Results

The SSM can be considered as an electrical capacitor within the electrical circuit. When ions are introduced into the system above the SSM surface, this is equivalent to switching on a DC power supply, providing ions to charge up the SSM capacitor. This causes a transient capacitive current to be induced in the circuit, with the time integral of the current corresponding to the amount of charge binding to the SSM membrane. In our measurements TPB- produced significantly larger capacitive currents than TPA+, suggesting that TPB- binds more deeply within the membrane than TPA+ (Fig. 1). To gain information on the binding strength of the two ions to the SSM, the charges obtained by integrating the current signals were analyzed as a function of the hydrophobic ion concentration. We determined Kd values of 10±2 µM for TPB- and 180±60 µM for TPA+. The Kd of TPA+ is much higher than that of TPB-, indicating a weaker binding of TPA+ to the membrane than TPB-.

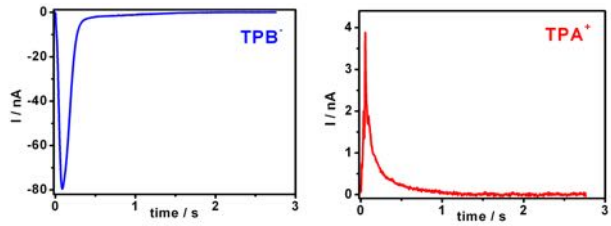

Figure 1: Current signals induced by a 100 µM TPB- (left panel) or a 200 µM TPA+ (right panel) concentration jump on the SSM surface.

The SSM method was also used to study the effects of various pharmacologically relevant compounds on the SERCA transport activity [2,3]. SERCA, which is found in the sarcoplasmic reticulum (SR) of muscle cells, hydrolyzes one ATP molecule to transport two Ca2+ ions against their electrochemical potential gradient from the cytoplasm to the SR lumen, thus inducing muscle cell relaxation. SR vesicles containing SERCA were adsorbed to the SSM and the ATPase was then activated by an ATP concentration jump (Fig. 2, left panel). Following protein activation, an electrical current was detected which was attributed to translocation of Ca2+ ions within SERCA due to the capacitive coupling between the SSM and the SR vesicle adsorbed on it.
We investigated the effect of the natural product 6-gingerol, that is known for its antioxidant, anti-inflammatory and anticancer properties [2]. The SSM measurements indicated that 6-gingerol is able to stimulate SERCA by enhancing ATP-dependent Ca2+ translocation (Fig. 2, right panel). We found that 6-gingerol has a rather high affinity for SERCA (EC50 of 1.8±0.3 µM) and SERCA activation by 6-gingerol is reversible.

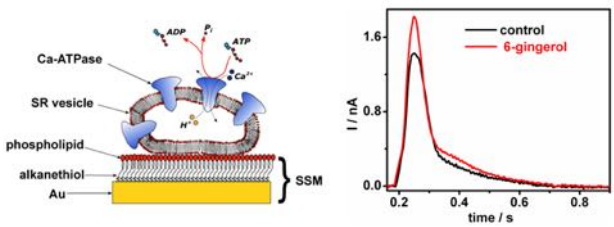

Figure 2: Schematic diagram of a SSM with an adsorbed SR vesicle containing SERCA (left panel). Current signals induced by 100 µM ATP concentration jumps on SR vesicles in the absence (initial control, black line) and in the presence (red line) of 10 µM 6-gingerol (right panel).

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1B – Non lamellar lipid nanoparticles for RNA delivery

C. Montis, L. Caselli, J. Cardellini, L. Conti, D. Bonavolontà, D. Berti

Aims

Lipid nanoparticles (LNPs), recently used in mRNA vaccines against SARS-CoV-2, are the most promising vectors for nucleic acids (NA). To escape endosomes and release NA into the cytosol, they leverage ionizable lipids, whose charge become positive at the acidic pH of endosomes, destabilizing the endosomal membrane. However, growing evidence suggests that also the structure of LNPs may play a key role in endosomal destabilization. Non-lamellar lipid nanoparticles (NLLNPs), such as cubosomes and hexosomes, may possess intrinsic fusogenicity due to their highly curved bilayer structure. While far from understood, these effects could boost endosomal escape, overcoming current limitations in NA delivery efficiency (1-2%). This project aims at developing innovative NLLNPs, as nanocarriers for the delivery of nucleic acids. The key objective is to establish guidelines for the rational design of NLLNPs capable of effectively destabilizing the endosomal membrane or bypassing endosomal route, thus increasing the efficiency of NA release.

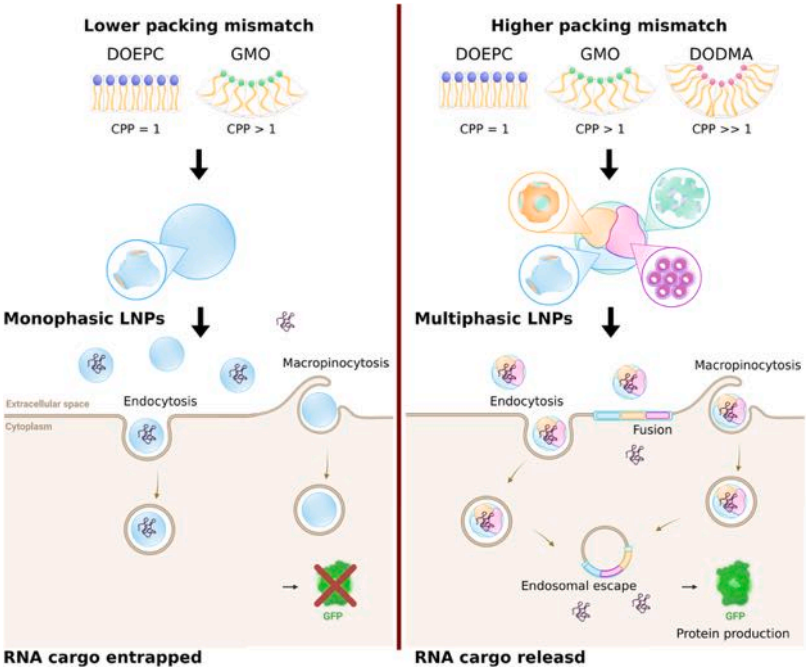
Results

Incorporation of functional lipid additives into glyceryl monooleate (GMO)-based lipid nanoparticles (LNPs) induced pronounced changes in internal organization, generating structural heterogeneity through phase separation. The nature of this heterogeneity strongly depended on additive lipid geometry and charge. The cationic lipid DOEPC, which favors lamellar packing, introduced a strong topological mismatch within the inverse-curvature GMO matrix, leading to coexistence of structurally distinct domains driven by both geometric frustration and electrostatic interactions. In contrast, incorporation of the ionizable lipid DODMA promoted highly curved inverse structures, consistent with its preference for negatively curved assemblies over a wide pH range. Its pH-dependent charge further contributed to dynamic rearrangements of the internal nanostructure.

The combination of DOEPC and DODMA produced the highest degree of internal structural complexity, reflecting synergistic effects arising from opposing molecular shapes and distinct charge profiles. These structural differences persisted across both acidic and neutral pH conditions, although the extent of phase separation and curvature frustration was modulated by pH. Efficient encapsulation of nucleic acids was observed for all formulations, indicating that increased structural heterogeneity did not compromise loading capacity.

Importantly, variations in internal nanostructure translated directly into biological performance. LNPs exhibiting greater internal heterogeneity showed enhanced cellular uptake and RNA transfection efficiency, establishing a clear structure–function relationship. These results demonstrate that controlled manipulation of lipid curvature and electrostatics enables tuning of LNP internal architecture, and that such nanostructural features play a decisive role in nucleic acid delivery efficacy. Overall, the findings highlight internal structural heterogeneity as a key physical–chemical

determinant of biological function and provide design principles for next-generation LNPs.



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1B – Non-linear viscoelastic Extracellular Matrix (ECM)-mimics (hydrogels) mechanics in cell culture and transduction

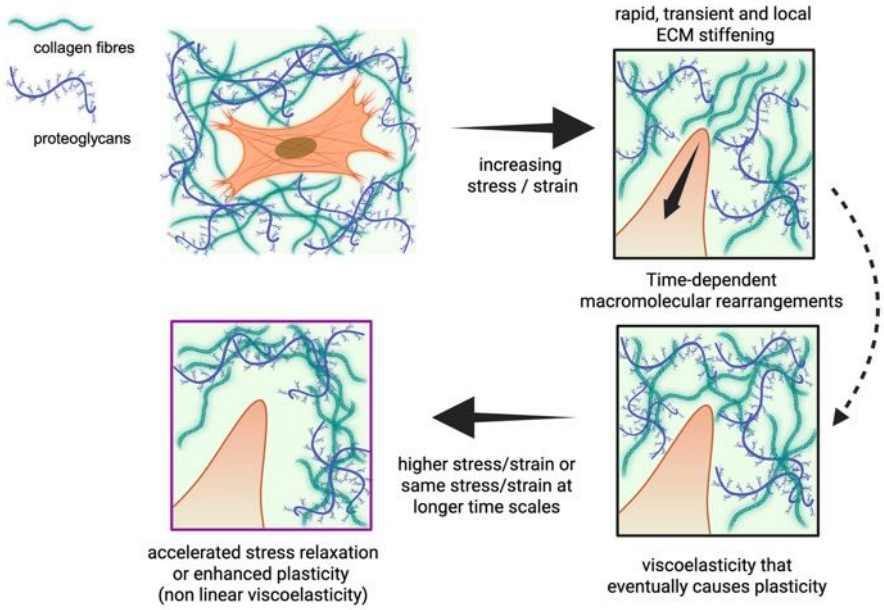
F. Piazza , P. Bertsch , I. Donati , P. Sacco

Aims

The mechanical complexity of the extracellular matrix (ECM) is central to how cells sense and respond to their environment, yet hydrogel design has often focused narrowly on stiffness. Emerging evidence highlights the importance of viscoelastic stress relaxation and plasticity in cell mechanotransduction. However, a key aspect remains underexplored: non-linear viscoelasticity, where stress relaxation and plasticity depend on the magnitude of applied stress or strain and on the time-scales of their application.

Results

In living tissues, cells are embedded in a 3D microenvironments consisting of an intricate hydrogel network of structural proteins such as collagen and proteoglycans that form the extracellular matrix (ECM). Cells interact closely with the ECM and sense its biophysical properties while generating stress/strain cycles through polymerization/depolymerization of cytoskeletal components or volume expansion. At low stress, cells sense the immediate resistance of the ECM, i.e., linear elasticity or stiffness. The cells can produce an almost immediate, but transient, local non-linear stiffening due to the alignment of the ECM fibers. However, when the stress persists the ECM responds in a time-dependent manner (viscoelasticity). The ECM can eventually undergo plastic deformation when weak bonds in the ECM unbind, allowing the cells to remodel, or when ECM proteins molecularly slide, leading to an arrangement of the ECM by cell contraction. This results in a non-linear softening that causes a diffuse change in the ECM network. We propose that repeated cycles of polymerization/depolymerization of cytoskeletal components generating the same stress/strain on different time scales or gradually increasing their magnitude may lead to non-linear viscoelasticity effects, with enhanced stress relaxation and increased plasticity of the ECM.



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1B – Out-of-Equilibrium bio-based polymeric complex fluids (OutBioPoly)

L. Gentile

Aims

Complex fluids play an emerging role in fundamental research and have wide-ranging medical and industrial uses, ranging from biological fluids and drug delivery to food, textile, and personal care products. Complex fluids manifest non-Newtonian rheological behavior, changing their structures and properties due to shearinduced supramolecular transitions, leading to large changes (shear-thinning or shear-thickening) in bulk viscosity. This project focus on an innovative high-throughput thermomechanical approach to induce supramolecular transitions in polymeric bio-based complex fluids, specifically, biopolymers in natural solvents. High shear rates will promote the formation of out-of-equilibrium structures. The aims are to understand the supramolecular transition mechanism, improve thermomechanical processes for regenerating materials, and ultimately produce materials with interesting properties for future applications. These materials may have novel applications ranging from shear-thickening bulletproof jackets or heat-resistant materials for aerospace to self-healing membranes.

Results

The OutBioPoly project (FIS 1) has yielded significant results on cellulose-based thin films produced by dissolving cellulose in out-of-equilibrium solvents, achieving semi-transparent adsorbent materials with exceptional mechanical properties, including robust torsional and tensile strength evaluated *via* rheometry. These films demonstrate high adsorption capacity for sustainable applications, as published in Carbohydrate Polymers, advancing the high-throughput thermomechanical processing of biopolymers in natural solvents to induce shear-driven supramolecular transitions and out-of-equilibrium structures. Complementary dissemination through the ECIS2024 talk on "Cellulose-based active materials: from semidilute unentangled solutions to films" underscores the project's progress toward multifunctional materials like self-healing membranes and shear-thickening composites. Peptides have also demonstrated sensitivity to external stimuli, particularly in response to the presence of buffers and mechanical forces. These factors induce conformational changes and supramolecular transitions, influencing self-assembly and rheological properties in bio-based complex fluids. Such responsiveness enhances the potential for developing adaptive materials, aligning with ongoing advancements in shear-induced processing for OutBioPoly applications.

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1B – Oxidation state and chelating agent affect iron bio-accessibility

S. Pepi, L. Talarico, G. Leone, C. Bonechi, G. Tamasi, I. Clemente, M. Consumi, F. Bisozzi, G. Gabbricci, F. Ietta, C. Rossi, A. Magnani (Department of Biotechnology, Chemistry and Pharmacy, University of Siena)

Aims

Iron deficiency anemia (IDA) is a pathological state characterized by reduced oxygen delivery that provokes generalized weakness and, as a consequence, low productivity. The most diffused treatment to reduce iron deficiency is oral iron supplementation. Nevertheless, the absorption of iron in subjects is very low, ranging from 5% to 28% and the unabsorbed percentage is responsible for the most common observed side effects, i.e. gastrointestinal alterations [1]. The effect of iron oxidation state, complexing agent, and particle dimension on the iron release and bioavailability was studied.

Results

Seven different formulations based on five different chelating agents [i.e. lipidic Fe (III)-pyrophosphate, Fe (III)-pyrophosphate, lipidic Fe (II)-sulphate, Fe (III)-saccharate and Fe (III)-EDTA] were analyzed (Table 1).

Table 1. Composition of analyzed formulations.

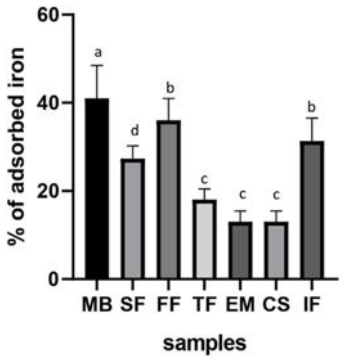
Sample	Iron-complex
CS	Lipidic Pyrophosphate-Fe(III)
SF	Lipidic Pyrophosphate-Fe(III)
TF	Pyrophosphate-Fe(III)
MB	Lipidic Sulphate-Fe(II)
IF	Lipidic Sulphate-Fe(II)
EM	Saccharate-Fe(III)
FF	EDTA-Fe(III)

Infrared and thermal analyses highlighted that ferrous ions complexes were able to strictly interact with ascorbic acid thus forming stable soluble systems. Dynamic light scattering (DLS) analysis pointed out that lipidic Fe (II)- sulphate formulation showed the largest particle size (i.e. 184 nm against 120 nm found for lipidic Fe (III)-py rophosphate based formulations) but showed the lowest PDI (0.25 against 0.30) that was not subjected to change after 7 days (Table 2).

Particle size of selected formulations after 2 h and 7 days.

Sample	2 h		7 days	
	Z-average (nm)	PDI	Z-average (nm)	PDI
CS	115 ± 4	0.29 ± 0.01	87 ± 4	0.38 ± 0.01
SF	126 ± 3	0.30 ± 0.01	136 ± 4	0.34 ± 0.05
MB	184 ± 6	0.25 ± 0.01	214 ± 9	0.25 ± 0.01
IF	14±1[b]	0.32 ± 0.03	–	–

Moreover, lipidic Fe (II)-sulphate formulation guaranteed a better bioavailability of iron using Caco-2 Cell model, permitting the absorption of more than 40% of administered iron against 20–30% found for formulations containing Fe (III) ions [2].



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1B – Phenolic polymers at bio-interfaces: self-assembled functional nano-vectors with controlled colloidal properties and enhanced antioxidant activity (PhenoVectors)

L. Gentile, G. D'Errico (Università di Napoli Federico II), C. Montis (Università di Firenze)

Aims

The rational design of functional self-assembled nanostructures for biomedical applications relies on the intricate interplay by which molecular structures and physicochemical constraints determine the supramolecular aggregation and the interactions with biological interfaces. With this perspective, the aim of the project is to design a new-concept bioactive nano-vector endowed with potent antioxidant activity.

Results

The UNIBA coordinates the 3 units of the PhenoVectors project (PRIN 2022 a scorrimento). Experiments remain ongoing to rationally design bioactive nano-vectors with antioxidant activity through self-assembled nanostructures that integrate molecular structure, aggregation dynamics, and biological interface interactions. Preliminary insights from related surfactant-fatty alcohol formulations, shared via conference posters, continue to support these investigations by elucidating structural impacts and physicochemical properties.

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1B – Photophysical and Photochemical Features of Lysine Derivatives Bearing Two Triphenylaminocinamic-Based Fluorophores

M. Saletti, M. Paolino, J. Venditti, G. Giorgi, C. Bonechi, A. Donati, C. Rossi, S. Costantini, G. Fattori, G. Giuliani, A.C. Coccia, C. Botta, L. Blancfort, A. Cappelli

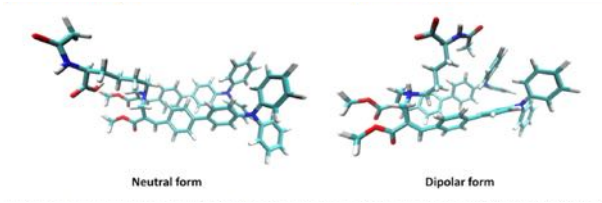
(Department of Biotechnology, Chemistry and Pharmacy, University of Siena, Siena; Istituto di Scienze e Tecnologie Chimiche G. Natta Milano; Institute of Computational Chemistry and Catalysis and Department of Chemistry, University of Girona, Spain)

Aims

A Morita−Baylis−Hillman adduct (MBHA) derivative bearing a triphenylamine (TPA) moiety was previously found to react with Nα-acetyl-L-lysine methyl ester with the formation of the corresponding diadduct derivative as the major reaction product and a monoadduct as the minor one. The characterization of photochemical features of the diadduct bearing two triphenylaminocinnamic (TPAC) fluorophores suggested that this compound shows the tendency to undergo the [2 + 2] photocycloaddition reaction. This hypothesis was evaluated in the present study in both the diadduct derivatives obtained with Nα-acetyl-L-lysine methyl ester and Nα-acetyl-L-lysine. The hypothesis was confirmed in the case of the diadduct derivative obtained from Nα-acetyl-L-lysine methyl ester, whereas the UV-A irradiation of the diadduct derivative obtained from Nα-acetyl-L-lysine led to the formation of a strongly emissive (QY = 69 %, λ_{em} = 460 nm) symmetric dimer.

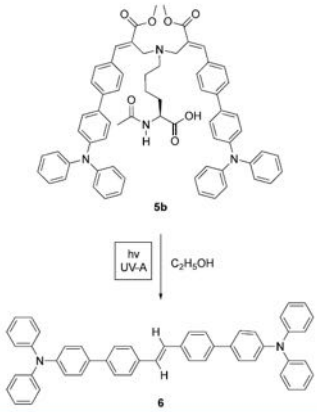
Results

The peculiar reactivity shown by MBHA derivative 3 with Nα- acetyl-L-lysine derivatives led to focusing our attention on diadduct 5b (figure) as the most important reaction product that contains two triphenylaminocinnamic (TPAC) chromophores in its structure. The structure of 5b was investigated by ^{1}HNMR spectroscopy and molecular modeling.

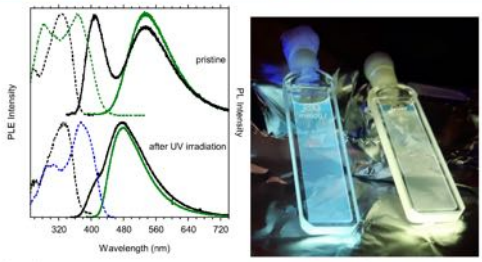


The evaluation of the photophysical features of 5b in the solid state showed that the presence of two TPAC chromophores in the same molecule of 5b appeared to redshift

the emission and decreased the PL QY as it usually occurs in aggregation quenching phenomena. On the other hand, diadduct 5b showed in solution a very complex photophysical profile with higher PL QY values, suggesting a possible susceptibility toward the [2 + 2] photocycloaddition reaction.



Thus, this liability was evaluated systematically in photolysis experiments monitored by absorption/emission and ^{1}H NMR spectroscopy experiments. These experiments revealed the occurrence of a rather complex pathway of the photolytic reactions but allowed us to isolate (although in low yield) very emissive compound 6.



(Left panel) PL (λex = 335 nm; black solid lines; λex = 390 nm, green solid lines) and PLE (black dashed lines, λem = 410 nm; green dashed lines λem = 535 nm; blue dashed line, λem = 480 nm) spectra of diadduct 5b in DCM before (top spectra) and after (bottom spectra) UV-A irradiation for 480 min. Solution concentration, 0.7 mg/mL. (Right panel) Picture of the solutions under UV lamp exposure, before (right) and after 480 min of UV-A irradiation (left).

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1B – Physico-chemical insights into stimuli-responsive and complex aqueous surfaces

G. Li Destri, N. Tuccitto, P. Tomasella, R. Ruffino

Aims

Aqueous surfaces are easy and versatile systems to drive the spontaneous assembly of soft matter into quasi bi-dimensional structures having well defined and controlled properties. This allows preparing monolayers acting as model systems to gain fundamental insight into the behaviour of molecules and soft matter under extreme confinement.

In this framework we have investigated the physico-chemical properties of monolayers formed by a photosensitive surfactant, whose conformation can be modulated by irradiation with the proper wavelength, with high control of the surfactant's conformational composition. Our approach allowed us discriminating the behaviour of the two conformers and to extract semi-quantitative physico-chemical details on the surfactant desorption kinetics.

Furthermore, we developed a novel methodology to investigate in real time with nanoscale resolution the irreversible adsorption of nanoparticles at the air/water interface. The analysis of the evolution of the surface excess with time permitted the determination of both kinetic and thermodynamic parameters shedding new light into the physico-chemical fundamentals of the adsorption process.

Results

Figure 1A shows the conformational cis/trans percentage, determined spectroscopically, of the triethylene glycol mono(4-butylazobenzene) ether surfactant as a function of the irradiation time at 340 nm. Mixtures with different trans/cis ratios were spread at the air/water interface and then let dissolving at a constant surface pressure as reported in Fig. 1B. The desorption curves were fitted with the following equation:

$$\frac{A(t)}{A_0} = \frac{A_\infty}{A_0} + \frac{A_1}{A_0} e^{t/t_1} + \frac{A_2}{A_0} e^{t/t_2}$$

The fitting results are reported in Fig.1C. The desorption kinetics of the monolayers is described by two regimes, having two different characteristic times. The fast regime, with a characteristic time within $\sim 10^2$ s, mainly accounts for the desorption of cis molecules while the desorption of trans molecules predominantly occurs with longer characteristic times of $\sim 10^3$ s.

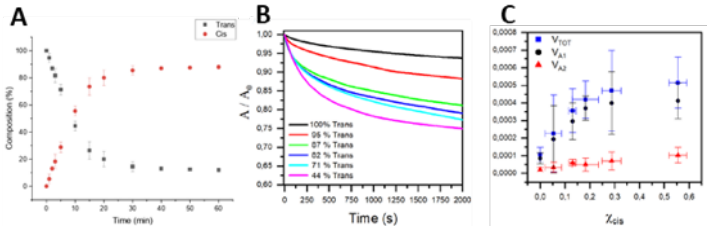

Figure 1

The surfactant-induced adsorption of nanoparticle at the air/water interface was followed in real time with synchrotron radiation grazing incidence small angle X-ray scattering (GISAXS). In order to overcome experimental limitations related to both the alignment procedure and safety requirements, we developed a novel methodology consisting of spreading the surfactant solution on the pre-aligned nanoparticle-containing dispersion. This allowed us to follow the very first minutes of adsorption. Exemplificative results are reported in Figure 2 were the nanoparticle surface excess (Γ(t)) is plotted as a function of the time. The first part of the time-dependent adsorption curve agrees well with a surfactant diffusion-driven adsorption process. The second part of the curve was fitted with the following exponential equation

$$\Gamma(t) = y_0 + A(1 - e^{-kt})$$

allowing us to determine, for the first time, both the first order kinetic constant *k* and the non-equilibrium surface excess at infinite time (Γ_∞) as

$$\Gamma_\infty = y_0 + A$$

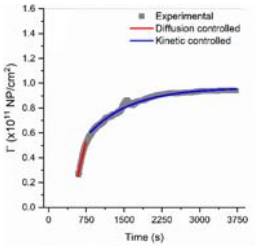

Figure 2

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1B – Physico-chemical properties of vital dyes in the form of solutions or dispersions for use in medicine

A. Mino' , G. Cinelli , F. Lopez , L. Ambrosone

Aims

The research aim is to study the nature of the self-association of dyes in aqueous solutions in order to understand and interpretation the tissue staining in biology and microsurgery.

Results

Although the applications of vital dyes are numerous, some problems such as the questions of how the chemical structure of dye and its tendency to associate in solution are related to the toxic effects observed in-vivo, are still unsolved. Another interesting aspect is the sensitivity of vital dyes to different chemical environments. In this respect Nile Red (NR) has been advantageously applied to probe the local polarity in the study of various heterogeneous systems, including micelles, reverse micelles, dendrimers, liposomes, proteins, and ionic liquids. Furthermore, NR in solution self-associates owing to strong intermolecular van der Waals attractive forces between molecules. It was recently demonstrated that alkan-1ols solvents are significantly more polar than expected based on the measured H-bonding properties of "monomer" alkan-1ols in dilute solution. By varying the length of *n*-alkanols differently hydrophilic environments have been created, where the NR dye is soluble. The NR dimerization equilibrium constant, *K*, in the first eight n-alkanols was calculated: the hydrophobicity of alkanol significantly reduces the red shift of the NR absorption band. The role of the medium hydrophilicity on the NR spectroscopic response was further investigated. The introduction of water to the binary system NR-alkanol causes a decrease in fluorescence

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1B – Post-Synthetic Degradation of Toxic Quantum Dots via Oleic Acid Complexation

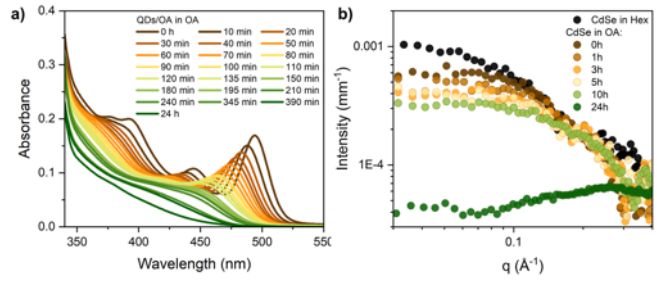
E. Cambiotti, E. Fratini, L. Latterini

Aims

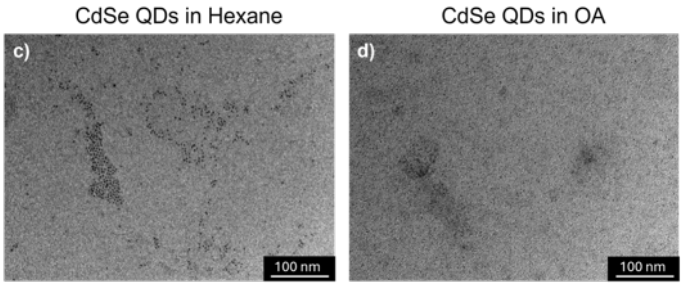
Quantum-confined semiconductor nanocrystals (NCs) are widely used in optoelectronic technologies, but their integration into devices raises environmental and health concerns due to the presence of toxic heavy metals. Here, we present a post-synthetic degradation approach for quantum dots (QDs) based on oleic acid (OA), a long-chain fatty acid with strong metal-binding capability. The degradation process is monitored by UV–Vis spectroscopy, small-angle X-ray scattering (SAXS), and transmission electron microscopy (TEM). Our results show that OA induces gradual nanocrystal degradation, leading to continuous size reduction and complete dissolution of QDs within 24 hours. This approach provides a scalable and environmentally sustainable strategy to mitigate risks associated with NC disposal.

Results

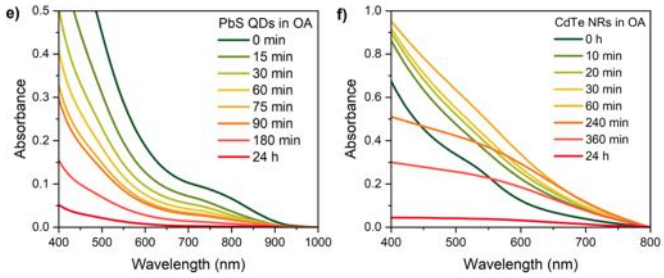
CdSe QDs capped with oleic acid were synthesized via hot-injection method and subsequently transferred from hexane to excess OA by solvent exchange. UV–Vis spectra collected over 24 h at room temperature show a progressive blue shift of the excitonic peak and a continuous decrease in absorbance, indicating QD size reduction followed by complete loss of band-edge features (Figure a). SAXS measurements of QDs in OA show a shift toward higher *q* values and a decrease in scattering intensity compared to the hexane sample, consistent with an initial QD size reduction. Over time, the continued decrease in intensity and further shift to higher q indicate progressive dissolution. After 24 hours, no detectable SAXS signal remains, confirming complete QD dissolution via OA complexation (Figure b). Along with second-order kinetic model derived from UV-Vis data, these results support a bimolecular dissolution mechanism in which two OA molecules coordinate the CdSe surface, promoting extraction of Cd^{2+} and Se^{2-} ions.



A morphological analysis was performed on QDs dispersed in hexane and in OA. TEM images of QDs in hexane shows an average diameter of approximately 2.5 nm (Figure c). However, when OA is used as solvent, a noticeable decrease in the QD size is evident (Figure d), consistent with previous results. This study confirms that excess OA irreversibly alters QD dimension.



The impact of OA was further evaluated in nanocrystals with different compositions (PbS QDs) and morphologies (CdTe nanorods, NRs) using UV–Vis spectroscopy. NCs were exposed to excess OA and monitored in real time. As shown in Figure e, PbS QDs exhibit a blue shift of the excitonic peak, indicating progressive size reduction. For CdTe NRs (Figure f), an initial increase in absorbance is observed within the first hour, followed by the disappearance of the excitonic feature upon prolonged OA exposure. In both systems, extended treatment results in complete loss of quantum-confined signatures. These findings demonstrate that OA acts as a versatile and sustainable agent for post-synthetic modification and dissolution of NCs, offering a strategy to reduce the environmental impact of heavy-metal based nanomaterials.



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1B – Potential utilization of olive-oil mill by-products for food applications: the 'olive vinegar' case study

A. De Leonardis , F. Lopez , V. Macciola

Aims

Both the cultivation of olive trees and the process of industrial production of olive oil generate enormous quantities of solid wastes and dark liquid effluents, most of them with no practical applications and environmental problems. Conversely, these wastes, thanks to their abundance in nutrients, value-added additives and bioactive compounds, could be viewed as “raw materials” for the recovery of high value-added compounds. Nowadays, there is an evident growing interest in obtaining new vinegar variety from alternative substrates, especially from by-products of food industry. Aim of the developed research has been that to realize vinegar from olive-oil mill by-products, specifically from olive-mill wastewater (OMW) and olive leaves (OL).

Results

Olive vinegar obtained from OMW appeared permanently clear, vinous-red colored and without any abnormal smell. Acetic acid level up to 4% is performed by applying both the alcoholic-acetous double fermentation with addition of Saccharomyces cerevisiae starter and the spontaneous acetification without addition of any other starter. OMW vinegar was characterized by huge presence of mineral compounds (ash 2%) and phenol substances (total phenols higher than 4 g/L as GAE), especially hydroxytyrosol. Olive leaf (OL) vinegar was obtained by maceration of dried olive leaves (at a 10:90 w/v leaves/vinegar ratio) in wine vinegar (OL-Wv) and alcoholic 18% vinegar (OL-Alc18). Total phenols of OL-Alc18 was about 5 g/L as GAE, while those of OL-Ww was about 3 g/L evidencing a phenol solving power acetic-acid-concentration-dependent. Oleuropein was found to be the most abundant phenol compounds in the OL vinegar. Both OMW and OL vinegar had shown an excellent antioxidant activity in food.

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1B – PVA-Based Theta Gel for diseased cartilage treatment

S. Pepi, L. Talarico, G. Gabbricci, G. Leone, C. Bonechi, M. Consumi, A. Boldrini, A. Lauro, A. Magnani, C. Rossi (Department of Biotechnology, Chemistry and Pharmacy, University of Siena)

Aims

In the last 20 years the use of Polyvinyl alcohol (PVA) for altered cartilage treatment has gained enormous attention [1]. Several approaches have been explored to increase the mechanical resistance of PVA hydrogels. Starting with the work of Ruberti and Braithwaite [2] the use of theta gel method has been applied to improve the crystallinity and mechanical properties of physically crosslinked PVA hydrogels. The theta gel formation mechanism consists of physical phase separation of a high-molecular-weight polymer solution (e.g., PVA) using a gelling agent (e.g., low-molecular-weight poly(ethylene glycol) (PEG)) that is able to reduce the quality of the solvent, forcing the high-molecular-weight polymer to phase separate and crystallize, forming a physically crosslinked hydrogel network. In this scenario, 42 different physical PVA-PEG-based theta gels were prepared with the aim of evaluating, using a statistical approach, the effect of PEG molecular weight, PVA molecular weight and alkaline pH values on water content and mechanical performance, exploiting the possibility of obtaining theta gels working at room temperature in a water environment and testing the crystallization occurrence at basic pH (10 or 12).

Results

PVA belonging to three molecular weight classes (low MW: 25–35 kDa; medium: 40–85 kDa; high: 120–220 kDa) and two hydrolysis degree classes (high: 98–99%; low: 87–89%) was used to prepare hydrogels. An identical concentration of both polymers was selected to evaluate only the effect of the polymers' molecular weight and basic pH values. A concentration of 10% w/w (molar ratio 1:1) was chosen to ensure a homogeneous aqueous solution while promoting adequate phase separation .

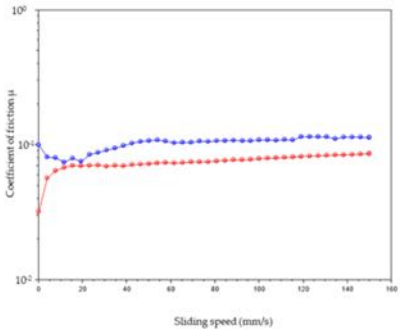
Our findings indicated that the degree of hydrolysis of native PVA significantly influenced the formation of stable 3D matrices. Specifically, a low hydrolysis degree (87%) inhibited the PVA chains approaching, preventing the establishment of stable frameworks. We also investigated the effects of PVA and PEG molecular weights, as well as pH values, on the water interaction, thermal properties and rheological behavior of the theta gels using a statistical approach. The statistical analysis highlighted that pH values had no significant impact on swelling, thermal and rheological behavior.

The molecular weight of PEG primarily influenced the hydrophilic properties of the materials in their swollen state, whereas the thermal properties measured on dried samples were predominantly affected by PVA MW. Both polymer molecular weights impacted the shear and compression mechanical behavior of the gels. The sample prepared with PVA 125 kDa and PEG 20 kDa as a porogen emerged as the most suitable

for cartilage disease treatment, exhibiting an equilibrium shear modulus in the range of 50–250 kPa, similar to that of native articular cartilage.

Sample ID	G* (Pa)	tan δ (-)
274	3243 ± 3508	$6.7 \times 10^{-2} \pm 4.4 \times 10^{-3}$
278	$16{,}452 \pm 5589$	$9.8 \times 10^{-2} \pm 4.4 \times 10^{-2}$
2720	$29{,}869 \pm 3962$	$7.6 \times 10^{-2} \pm 1.7 \times 10^{-2}$
474	5383 ± 482	$6.9 \times 10^{-2} \pm 7.0 \times 10^{-3}$
478	$15{,}677 \pm 4793$	$6.2 \times 10^{-2} \pm 1.5 \times 10^{-2}$
4720	$21{,}588 \pm 2915$	$7.8 \times 10^{-2} \pm 1.5 \times 10^{-2}$
614	7227 ± 3899	$5.7 \times 10^{-2} \pm 1.4 \times 10^{-3}$
618	$22{,}221 \pm 10{,}124$	$6.5 \times 10^{-2} \pm 1.1 \times 10^{-2}$
6120	$53{,}202 \pm 3817$	$8.8 \times 10^{-2} \pm 1.2 \times 10^{-2}$
1254	$23{,}079 \pm 7747$	$4.8 \times 10^{-2} \pm 4.4 \times 10^{-3}$
1258	$27{,}394 \pm 5473$	$8.4 \times 10^{-2} \pm 5.3 \times 10^{-3}$
12520	$44{,}305 \pm 1932$	$9.5 \times 10^{-2} \pm 6.1 \times 10^{-3}$
1954	$35{,}314 \pm 12{,}235$	$8.1 \times 10^{-2} \pm 2.6 \times 10^{-3}$
1958	$27{,}432 \pm 2341$	$8.6 \times 10^{-2} \pm 2.0 \times 10^{-2}$
19520	$36{,}906 \pm 3142$	$8.5 \times 10^{-2} \pm 1.7 \times 10^{-2}$

Additionally, it demonstrated an optimal mechanical response under compression across the entire frequency range analyzed, with a mean value of 0.12 MPa. The coefficient of friction (COF) under a 4.5 N load remained below 0.10 for all tested sliding speeds [3].



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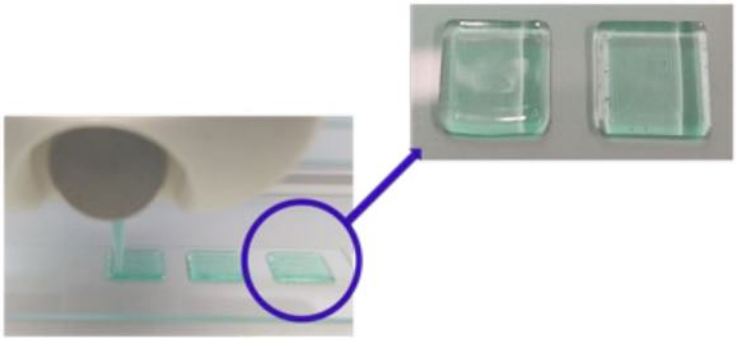
1B – Quasi-static and dynamic nanoindentation for mechano-chemical analysis on biodegradable polymeric nanocomposites for regenerative medicine

A. De Nigris, D. Gentile, G.P. Vanoli, L. Ambrosone

Aims

The objectives of this project are to gather a large amount of information straightforwardly from the load–displacement response of a coated system when plotted for comparison with that of the substrate alone at the same load. This mechanical fingerprint immediately reveals the differences in response conferred by the coating as the load is increased to the maximum used for any given test.



Results

Four different biomedical patches were bioprinted using nanocomposite hydrogels of sodium alginate/gelatin, sodium alginate/gelatin/indocyanine green freely dispersed, sodium alginate/gelatin/empty liposomes and sodium alginate/gelatin/indocyanine green loaded liposomes. Quasi-static and dynamic nanoindentations of the patch surfaces were performed to examine the effect of the single component on the mechanical response. The combination of results suggests that the mechanical structure of the gels is strongly influenced by crosslinking and the liposomes incorporating dye. Indeed, the non-crosslinked samples exhibit lower G′ and G′′ values, with more viscoelastic behavior. The absence of a marked increase in G′ after crosslinking, both in samples with free dye and those with dye encapsulated in liposomes, indicates that strong interactions between dye, liposomes, and ionic calcium exist. Indeed, phosphatidylcholine and indocyanine green react electrostatically with calcium cations, sequestering crosslinkers. Crosslinking with Ca+2 improves matrix stiffness, but its effectiveness depends on the composition of the system. All results were validated with comprehensive statistical analysis among the different patches and their crosslinked counterpars.

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1B – Recovery, Storage and Recycling of Lacual Sediments

B. Molino, A. Minò, L. Ambrosone

Aims

The research aims at the recovery of submerged silt-clayey sediments and their reuse, in order to reduce the movement, through the combination of plant schemes with a high level of technology.

Results

A mathematical model for determining the sediment volume profile in a reservoir is proposed. The resulting equation is similar to a first-order kinetics with lifetime varying with time. Such model was applied to a large number of dams whose bathymetric reliefs were drawn from the literature. For reservoirs, where the number of bathymetric reliefs is high the model is directly applied and the parameters extracted from a non-linear fitting. Where the number of bathymetric data does not allow a non-linear regression, a straightness test is performed first, then, the parameters computed by the regression line of log Z vs. log t. Finally, for dams where only two bathymetric surveys are available, equations have been provided to estimate the model parameters. These equations have been applied to Altinapa dam (Turkey) and Chimhanda dam (Zimbabwe). Furthermore, a good agreement was verified between the sedimentation profiles obtained by the model and the results estimated by the satellite surveys. The model provides a framework which enables us to correlate data in sensible manner, it tells us what to plot against what, the coordinates we must use to get a smooth line. For engineering work such a framework is extremely useful because it enables to interpolate and extrapolate limited bathimetric reliefs and to manage long-term water of reservoirs. Looking ahead, if one can relate the model parameters to the chemical properties of solids it will become highly predictive for the management of a reservoir and its sediment.

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1B – Sol-gel phase transitions in a Pluronic F127/carboxymethyl cellulose aqueous system.

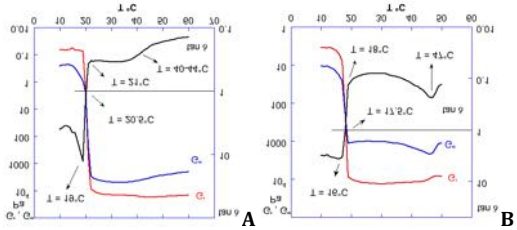
M. Monduzzi, G. Musu, M. Grosso, C. Carucci, A. Salis, B. Lindman, O. Söderman (Chemical Centre, Lund, Sweden)

Aims

Thermoresponsive copolymers are a class of "intelligent" materials that have the property of responding to stimuli due to changes in temperature, and can be functionalized to include other stimuli dependence such as pH, ionic strength, electric and/or magnetic fields and light. These polymers have a wide range of applications including sensors, drug delivery or gene delivery systems and tissue engineering.
Pluronic F-127 is a non-ionic three-block copolymer, namely EO97PO68EO97 (EO = oxyethylene, PO = oxypropylene), with relatively high molecular weight MW ≈ 12.5 kDa. The phase diagram, shows that a clear solution of unimers and micelles exists at low temperature and concentration. At higher temperatures, phase transitions occur leading to the formation of liquid crystalline gels (fcc structures) having different viscoelastic behaviour in response to changes either in temperature or in concentration. Sodium carboxymethylcellulose (NaCMC) is another widely investigated polymeric hydrocolloid, obtained from cellulose treatment. NaCMC is a water-soluble anionic polyelectrolyte, often used as a modifier of the rheological properties, binding and thickening agent. In this study we consider a mixed system of Pluronic F 127, and NaCMC. In such a system, interactions with ions will be crucial but the two components will respond very differently. Stability and dynamic behaviour of these macromolecules in aqueous solution can be modified by adding different salts, through electrostatic and dispersive interactions. Dispersive interactions are often referred as “Hofmeister effect”. The solubility of macromolecules in water may decrease on adding anions in the order HPO42- > SO42- > F- > Cl- > Br- > I- > NO3- > ClO4- > SCN-, or cations in the order Cs+ > NH4+ > Rb+ > K+ > Na+ > Li+ > Mg2+ > Ca2+. Investigation is performed through rheological measurements, NMR self-diffusion and SAXS.
The main aim is to obtain tunable phase transition temperatures through Sodium salt addition (concentration 0.05 and 0.07 mol/kg) for a thermosensitive formulation platform potentially useful for specific nanomedicine applications.

Results

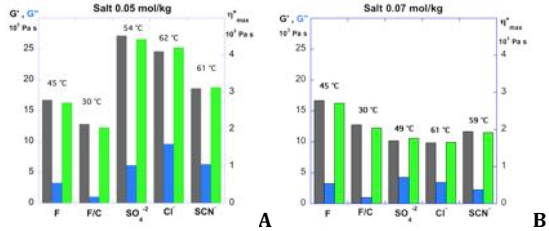
Figure 1 shows the Rheology parameters Storage Modulus (G’), and Loss Modulus (G”) on left axis (log scale) and Loss Factor (tan δ = G”/G’) on right axis (log scale) vs. T (°C) for the samples Pluronic F127 20 wt% (Fig. 1A) and Pluronic F127 20 wt% + NaCMC 4 wt% (Fig. 1B). Both cmt (critical temperature of micelle formation) and T_{hg} temperatures decrease in the presence of NaCMC, that suggests a crowding effect on F127 exerted by NaCMC which leads to a lowering of the temperature for micelle and cubic liquid crystal formation.



A B

Figure 1

Figure 2 shows the effect of salts on the rheological parameters G' (dark grey bars), G" (blue bars), and η* (green bars), in the absence and in the presence of different sodium salts 0.05 mol/kg (A) and 0.07 mol/kg (B). Data for samples F and F/C without salts are given for comparison.



A B

Figure 2

The formation of a cubic liquid crystalline (fcc Fm3m and simple cubic SC) phases at temperatures higher than 37 °C was confirmed in all systems through SAXS measurements.

1H NMR self-diffusion experiments display a non-mono-exponential decay of the echo signals of Pluronic F127. Thus the echo decay (I) can approximately be described through a biexponential function charcterized by a fast DPfast and a slow DPslow component. The slow component DPslow does not decreases with increasing T, as a result of the polydispersity of commercial Pluronic F127.

Taken together, the findings of this study indicate that a mixture of Pluronic F127/NaCMC (20/4 weight ratio), in the presence of NaCl at 0.07 mol/kg, is a suitable formulation platform for developing a potential thermosensitive drug delivery system, being the increase of the sol-(hard gel) transition temperature the main effect of the salt.

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1B – Structural characterization of chia mucilage for food processing applications

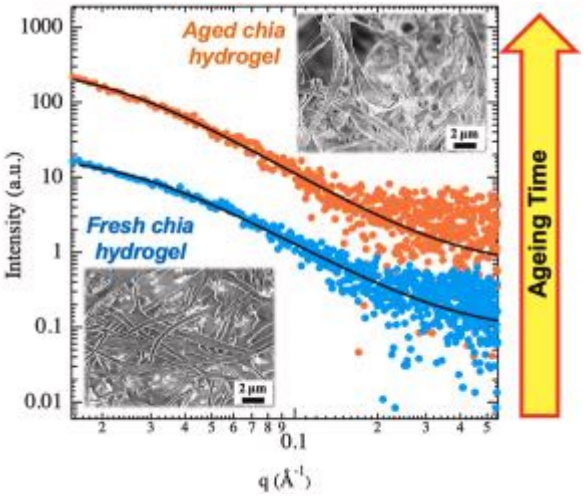
G. Ferraro , F. Cuomo, E Fratini, S. Iacovino , F. Lopez

Aims

Considering the interest in chia mucilage for various applications, it seems to be of key importance to provide experimental evidence for the change in the microstructure of the biomacromolecule over time and to link the structural changes to the amount of water adsorption observed at the macroscopic level. Therefore, a structural study performed by FTIR spectroscopy, small angle X-ray scattering (SAXS), rheology and microscopy on CM hydrogels was undertaken.

Results

We investigated on the effect of polymer concentration and ageing on the mechanical properties of chia mucilage hydrogels. Rheological characterization highlighted that ageing destabilizes the hydrogel network. Indeed, the hydrogel elastic modules (G') decreases and the linear viscoelastic range is reduced, as well as the viscosity shows a decrease of the resistance to flow of the viscoelastic fluid. This behavior can be correlated with a structural change observed by microscopy, in particular the formation of less entangled and packed structures. This was further confirmed by SAXS analysis, which helped us to find that the correlation length (i.e., mesh size) of the hydrogel network increases with the ageing of the samples. In view of the wide range of chia mucilage potential applications in food industry, considering the variability of the mucilage composition depending on its origin and on the production procedure, the crucial role of ageing could represent a significant information for food processing involving chia polymer.



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1B – Structural organization and molecular interactions at lipid/LPS nano-biointerfaces by Neutron Scattering

G. Vitiello, A. Cangiano, N. Gallucci, A. Luchini (University of Perugia), L. Clifton (ISIS, UK) G. Fragneto (ESS, SE), L. Paduano (U.O. of Naples, University of Naples Federico II)

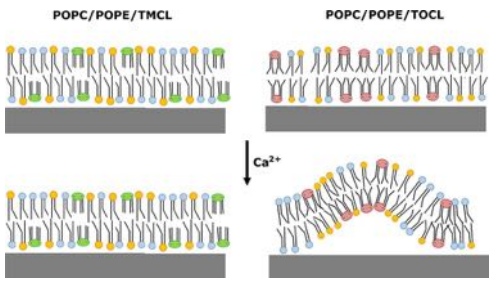
Aims

Nano-biointerfaces are being mimicked by various models which allow studying important components of cell-life, hence permitting to reproduce various structural conditions, such as the architecture of plasma or bacterial membranes to monitor their interactions with guest molecules and the vesicle fusion intermediates. The type of nano-biointerfaces, such as lipid vesicles or Supported Lipid Bilayers (SLBs), and the nature of lipids, such as zwitterionic or anionic bi- or multi-chained phospholipids, sterols/hopanoids and lipopolysaccharides (LPS), drive the structural organization and the interactions with bioactive molecules, like antimicrobial peptides, nanoparticles, antibodies and/or oligonucleotides. Neutron Scattering techniques represent powerful tools to shed light onto molecular features of functional nano-biointerfaces and their function with guest molecules involved into many molecular recognition processes.

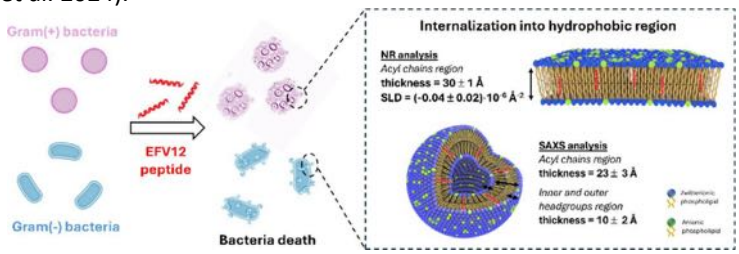
Results

Small-Angle Neutron Scattering (SANS) and Neutron Reflectometry (NR) were used to describe the structural organization of lipid nano-biointerfaces biomimicking plasma or outer membranes of Gram (-) bacteria.

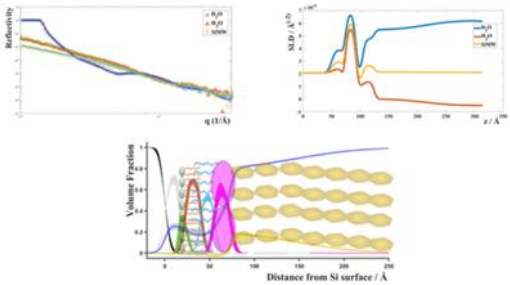
SLBs of cardiolipin (CL), phosphatidylcholine (PC) and phosphatidylethanolamine (PE) were studied as model systems mimicking the inner membrane of mitochondria (IMM). Tetra-oleyl cardiolipin (TOCL) with four C18 acyl chains and tetra-myristoyl cardiolipin (TMCL) exhibiting shorter C14 acyl chains were considered. NR results indicated that samples with TMCL were organized as a regular SLB with a small impact of TMCL on the bilayer structure. Instead, a large structural rearrangement occurred at a TOCL concentration > 10% mol and upon injection of Ca^{2+}, compatible with the formation of curved bilayer regions that protrude towards the bulk solvent (Luchini et al. 2024).



Similarly, SLBs and liposomes composed of 1,2-oleoyl-*sn*-glycero-3-phosphocholine (PC) and 1,2-oleoyl-*sn*-glycero-3-*rac*-phosphoglycerol (PG), both in the absence and presence of cardiolipin and lipopolysaccharides (LPSs), were selected to investigate the interaction with the small EFV12 peptide, deriving from the bacterium *Lactobacillus gasseri* SF1109 regularly placed in the human intestine, which showed a significant antimicrobial activity. The obtained results indicated association of EFV12 peptide with the hydrophobic region of lipid bilayers, which caused their destabilization, and is thus driving the antimicrobial activity against bacterial cells (Vitiello et al. 2024).



Recently, a structural characterization of aggregates and asymmetric SLBs containing LPS from Gram-negative bacterium *Paenalcaligenes hominis* was realized by DLS, SANS and NR. This last indicated the lipid bilayers 20.3 Å thick and 4 Å rough, with 16% hydration, indicating a high level of packing among the PC and P. hominis LPS lipid A chains. Additionally, the core region was characterized by a thickness of approximately 20 Å and a hydration level of about 26%. The O-Antigen region showed a thickness of 90 Å, a roughness of 42 Å and an 81% hydration level, indicating significant water penetration (Nieto-Fabregat et al. 2025). The role of LPS portions in modulating the biorecognition mechanism by the endotoxin-specific LA27 aptamer is now in progress.



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1B – Structure and flow dynamics of Concentrated AMphiphilic BIOmolecules (CAmBio): driving the change to eco-sustainable surfactant formulations (PRIN2022 PNRR - P202229ME2)

G. D'Errico[a], M. Tancredi[a], D. Parsons[b], L. Gentile[c]

[a] *University of Naples Federico II, CSGI U.O. Naples*

[b] *University of Cagliari, CSGI U.O. Cagliari*

[c] *University of Bari "A. Moro", CSGI U.O. Bari*

Aims

Developing eco-sustainable surfactant-based formulations is increasingly urgent, given the projected growth in their industrial production. The research project CAmBio envisions a shift from traditional formulations to innovative ones based on bio-based surfactants and biosurfactants. Biosurfactants are naturally produced by plants, yeasts, and bacteria and include a range of amphiphilic biomolecules.

CAmBio aims to enhance our fundamental understanding of the structure and dynamics of concentrated bio-based surfactant self-assemblies through a physicochemical approach. Among the leading biosurfactants are rhamnolipids, which are commercially available in various forms. These surfactants typically include one or two rhamnose sugars, a carboxylic group, and one or two acyl chains, presenting a complex molecular structure that makes understanding their self-aggregation behavior a challenging yet important task. The final goal is to demonstrate that the acquired scientific knowledge fosters the applications of the investigated system, their functional properties will be tested in model formulations such as water-poor detergents, which minimize the environmental impact of packaging and transport, and contaminant absorbents for pollutant removal from wastewater.

Results

The UNIBA unit of the CAmBio project (PRIN PNRR 2022) has investigated alkyl polyglucoside (APG) surfactants, such as C8-10 variants like Triton CG-110, in combination with fatty alcohols like 1-dodecanol, revealing salt-induced modulation of self-assembly that shifts rheological properties from viscous to viscoelastic and yield-pseudoplastic behaviors. These formulations exhibit enhanced interparticle correlations in bicellar nanostructures under elevated salinity, boosting viscoelasticity, stability, and oil-uptake efficiency up to 82%, which supports greener industrial applications. Complementary studies on rhamnolipids have informed biosurfactant strategies, with conference posters detailing surfactant-fatty alcohol interactions, structural impacts, and characterizations aligned with APG-focused formulations for eco-sustainable detergents and wastewater absorbents.

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1B – Structure-Function Relationships in Thermoresponsive Soft Colloids

J. Vialetto, M. Laurati, G. Bassu, E. Zaccarelli[1], L. Isa[2]

[1] *CNR-ISC, Dipartimento di Fisica, Sapienza Università di Roma, 00185 Roma, Italy.*
[2] *Department of Materials, ETH Zürich, 8093 Zürich, Switzerland.*

Aims

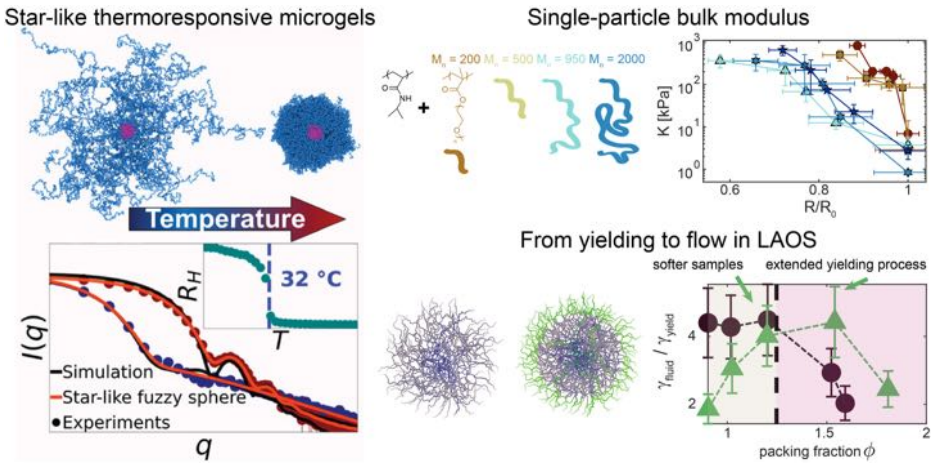
Particle compressibility plays a key role in governing the structural and mechanical properties of concentrated suspensions of synthetic and natural soft colloids, as well as their interaction with other objects and interfaces, being thus an important parameter for the design of functional materials and complex fluids. The aim of this research project is the design of novel thermoresponsive microgels (i.e. crosslinked networks of polymers partially soluble in the solvent in which they are dispersed) with the goal of establishing direct, quantitative links between single-particle structure, softness, and surface properties, with their collective behavior in dense suspensions. By combining advanced synthesis routes, multiscale scattering techniques, numerical simulations and rheological measurements, the project seeks to provide design rules for novel soft colloids whose macroscopic mechanical response can be predictably tuned for potential applications in functional materials, biomedicine, and soft-matter processing.

Results

A first objective is to expand the family of thermoresponsive microgels beyond conventional architectures.[1] This is achieved by using ethyleneglycol dimethylacrylate as crosslinker in poly(N-isopropylacrylamide) (PNIPAM) polymerization. Its fast reactivity leads to a highly crosslinked core surrounded by long, crosslinker-free arms. Experimental scattering data and monomer-resolved simulations provide clear evidence of a star-like internal density profile resembling that of star polymers. Despite their unconventional architecture, these microgels fully retain PNIPAM's thermoresponsivity and display a remarkably sharp volume phase transition ~ 32 °C, largely independent of crosslinker concentration. This establishes star-like PNIPAM microgels as a new, versatile platform for soft matter research, combining polymer-star conformations with microgel responsiveness.

A second aim is to finely tune particle softness and thermal response through copolymerization strategies [2,3]. By incorporating oligo(ethylene-glycol) methacrylates (OEGMA) with different chain lengths, we systematically modified the network conformation. Light and neutron scattering allowed us to quantify the single-particle bulk modulus and link it to temperature-induced deswelling. The results reveal a non-trivial dependence on comonomer chain length: short OEGMA chains smooth the core–shell contrast yielding more homogeneous particles, while longer chains produce extremely compliant star-like morphologies that resist collapse even at high temperature. These findings show that microgel softness can be modulated not only by crosslink density, but also by tuning architecture in copolymer networks.

The project further addresses how internal architecture, softness, and surface chemistry determine the structure and mechanical response in dense states.[4,5] Ultrasoft PNIPAM–OEGMA microgels with star-like profiles display strong deswelling and a sharp increase in bulk modulus upon compression at moderate packing fractions, followed, at higher densities, by a crossover from dispersion-like to hydrogel-like behavior, accompanied by two-step yielding in rheology. Additionally, by independently tuning crosslinking and PEG-based surface modification, we disentangle the roles of softness, adhesion, friction, and surface fuzziness. Large-amplitude oscillatory shear rheology and colloidal-probe AFM measurements show that surface properties control yielding and fluidization at lower packing fractions, whereas particle softness and fuzziness dominate the response at very high densities, enabling better stress accommodation and extended fluidization. Together, these findings clarify how single-particle parameters determine structure, yielding and flow in dense soft colloidal materials.



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1B – Textile Sol-Gel Hybrid Coating for Real-Time Sweat pH Detection

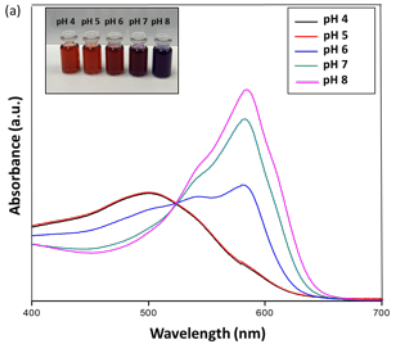
A. D'Agostino, M. Hadhri, R. Palucci Rosa, G. Rosace, A. Safarshargh, V. Trovato
(Department of Engineering and Applied Sciences, University of Bergamo, Dalmine (Bg), Italy)

Aims

Recent advances in nanotechnology for textiles have enabled the development of wearable chemical sensors for continuous physiological monitoring. Sweat, mainly composed of water, electrolytes, and metabolites, is a valuable biofluid for noninvasive health assessment. Among its measurable factors, sweat pH is a key indicator of hydration status and electrolyte balance. In this work, the halochromic dye litmus (LTM) was covalently attached to the silica precursor 3-glycidoxypropyltrimethoxysilane (GPTMS) through a sol-gel method. This functionalization improved surface polarity, mechanical stability, and porosity, thereby enhancing sensing performance. The treated fabrics exhibited reversible and reproducible pH responsiveness within the physiological range (pH 4.0-8.0). Their optical behavior was validated by diffuse reflectance spectroscopy and CIELAB color analysis. The system showed an estimation error of ±0.5 pH, highlighting its potential for wearable diagnostic technologies.

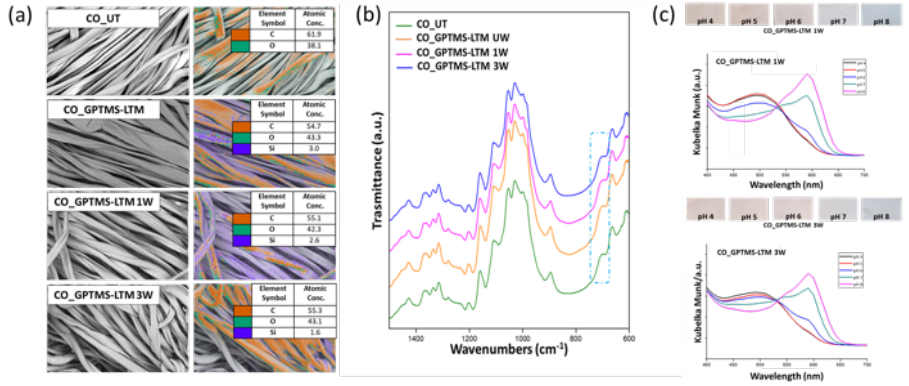
Results

The halochromic properties of GPTMS-LTM solutions were examined across pH 4-8 using visible absorption spectroscopy. Clear pH-dependent shifts in absorbance intensity and wavelength reflect the acid-base equilibrium of the phenoxazone chromophore (LTM) (a). At pH ≈ 4, a 515 nm band indicates the protonated quinonoid form, while deprotonation of the phenolic -OH group at higher pH induces a hypsochromic shift to 490-500 nm. GPTMS modification preserves the native π→π* transitions of litmus, confirming retention of the intrinsic electronic configuration within the sol-gel matrix and enabling covalent immobilization.



SEM micrographs showed a continuous, granular xerogel layer uniformly covering the cellulose substrate, in contrast to the smooth, untreated samples, confirming the

deposition of hybrid coatings. Energy-dispersive X-ray spectroscopy revealed a homogeneous silicon signal along the coated fibers, verifying the incorporation of the organosilicon network and the absence of extraneous elements (a). ATR-FTIR spectra corroborated these findings: new bands at approximately 1100 cm^{-1} and 775 cm^{-1} correspond to Si-O-Si stretching, while a band at 1270 cm^{-1} indicates Si-C linkages from GPTMS-LTM covalent bonding (b). Importantly, these silicon-associated features persisted after laundering cycles, demonstrating strong interfacial adhesion, and the hydrolytic stability needed for long-term wearable pH-sensing performance.



Colorimetric analyses confirmed that GPTMS-LTM fabrics maintain reversible pH responsiveness under mechanical and aqueous stress. Samples showed distinct visual transitions between pH 4 and pH 8 even after three washes, with ΔE values well above the perceptual threshold for clear color change. This stability is attributed to covalent immobilization of the LTM within the siloxane matrix, which prevents dye leaching and protects the π-conjugated system from degradation (c). The retained halochromic performance and wash durability match or surpass those reported for other high-performance pH-responsive coatings, validating the GPTMS-LTM platform for scalable production of wearable diagnostics and environmentally responsive smart textiles. This work was funded by the National Plan for Complementary Investments project n. PNC0000003 - AdvaNced Technologies for Human-centrEd Medicine (ANTHEM).

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1B – The effect of 2D substrate mechanics and specific peptide sequences on cell response

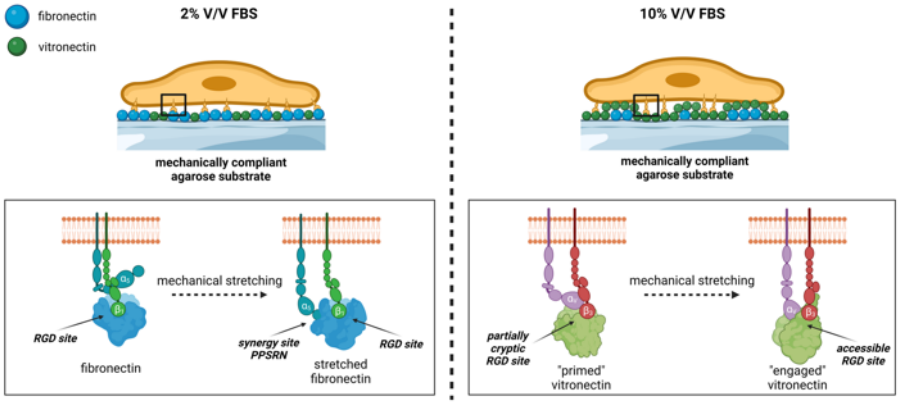
F. Piazza , S. Lipari, , I. Donati , P. Sacco

Aims

2D hydrogel-based substrates with adjustable mechanics are routinely used in cell mechanobiology studies as a simplified model of the extracellular matrix (ECM). Cells plated atop these materials initially recognize adhesive peptide sequences and then respond to the underlying mechanics of the substrate, thereby regulating their functions and fate. Recently, we have investigated the possibility of correlating the link between peptide sequences physically adsorbed to the substrate and the mechanics of the biomaterial in terms of cell response. For this purpose, we are currently using two types of substrates consisting of gelatin-methacryloyl or agarose.

Results

With regard to agarose substrates, we elucidated how the cells exhibit two anchoring mechanisms depending on the amount of proteins in the serum (FBS) used for cell culturing process. Under low FBS conditions, the cells recognize the surface-coupled adhesive sequences of fibronectin via the binding of the heterodimer $\alpha_5\beta_1$ integrin. Functionality of the actomyosin axis and mechanoactivation of focal adhesion kinase (FAK) are essential for the stretching of the protein, thereby accessing the “synergy” PPSRN site and enhancing cell adhesion in combination with the downstream RGD motif. Under high FBS conditions, the specific peptide sequences are much less relevant as the adsorbed serum proteins conceal the coupled fibronectin and the cells recognize the adhesive protein vitronectin, which is constitutively present in FBS, via the binding of the heterodimer $\alpha V\beta 3$ integrin. Similarly, the intracellular tension and FAK activity are decisive, which collectively indicate that the cells stretch the partially cryptic RGD site of vitronectin and thus make it more accessible for integrin binding. Both anchoring mechanisms only work properly if the agarose substrate is mechanically compliant in terms of linear stress-strain response, unravelling a critical balance between the mechanics of the agarose substrate and the presentation of the adhesive peptides.



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1B – Tuning Pluronic F127 phase transitions by adding physiological amounts of salts

G. Russo, G.R. Delpiano, C. Carucci, M. Grosso, C. Dessì, M. Monduzzi, A. Salis, B. Lindman, O. Söderman (Chemical Centre, Lund, Sweden)

Aims

The aim of the work is to obtain a drug delivery platform based on the thermosensitive Pluronic F127 where the transition temperatures can easily be tuned adding physiological concentration (0.05-0.15 mol/kg) of salts, depending on the type of administration route. Detailed information on the changes in cmt, and sol-gel transition temperatures in the presence of salts are obtained through rheology, using temperature ramps, at constant oscillation frequency. To clarify the effects of salts on Pluronic F127 self-assembly and phase behavior, SAXS experiments were performed at 40 °C to ascertain the occurrence of cubic LC gel phases. Additional information related to the molecular motions was obtained from NMR self-diffusion experiments at different temperatures. Relatively low salt concentrations from 0.075 to 0.15 mol/kg were considered for NaCl, KCl, $MgCl_2$, Na_2SO_4 and NaSCN. In the case of NaCl and NaSCN rheological measurements were also performed using a salt concentration 1 mol/kg.

Results

Figure 1 summarizes the main transition temperatures obtained analysing rheology parameters. The trends of Storage Modulus G', Loss Modulus G" and tan δ vs. T (10-85 °C) for salt free F127 (20wt%) sample is reported in Fig. 1A. The sol-hard gel transition T_{hg} and the hard-soft gel transition T_{sg} are shown in Fig. 1B and 1C respectively.

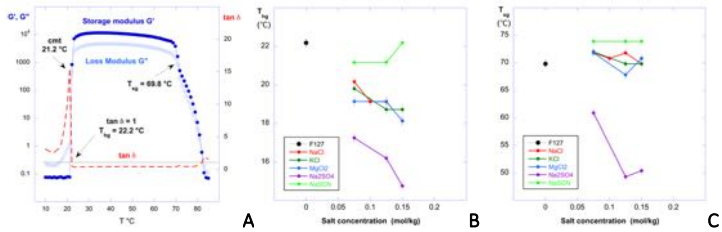
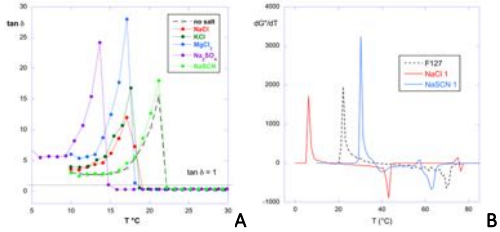


Figure 1

The transition temperatures of F127 are not significantly affected by the nature of the cations (Na^+, K^+ and Mg^{2+}) of the three chlorides while, the role of the anions can clearly be seen also at the relatively low concentrations of added salts. Both transition temperatures T_{hg} and T_{sg} follow the Hofmeister series in the increasing order SO_4^{2-} < Cl^- < SCN^-. This can clearly be seen in Figure 2A where the trend of tan d vs T in the presence of all salts (conc. 0.15 mol/kg). Figure 2B shows the effect of NaCl and NaSCN on dG"/dT vs. T trend where the maximum corresponds to T_{hg} (hard-soft gel transition)

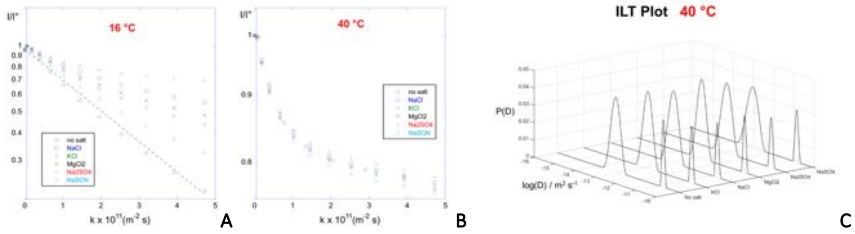
temperatures, while the minimum can be associated to the decrease of viscosity due to the hard-soft gel transition occurring at T_{sg}.



A B

Figure 2

SAXS data obtained at 40 °C using the q_{ob} ($Å^{-1}$) values that could clearly be assigned according to Miller indexes allowed to confirm the occurrence of cubic LC having Fm3m and SC lattice cells. Added salts 0.15 mol/kg caused a decrease of the interfacial area A_P per EO block, and an increase of the aggregation number N_{ag} of F127 micelles. Figure 3 shows ^1H NMR echo-decays of the CH_2 group with and without salts at 16°C and 40°C. At 16 °C (Fig. 3A) the effects of the addition of salts results in changes in the appearance of the echo decay with the magnitude of changes in the following order: (no salt) < NaSCN < KCl ≈ $MgCl_2$ ≤ NaCl < Na_2SO_4, which corresponds to a Hofmeister series. At 40 °C there are only minimal effects due to salts as reported in Figure 3B. The trend is more clearly highlighted by an inverse Laplace transformation of the CH_2 echo-decay shown in Figure 3C.



A B C

Figure 3

As suggest by Fig. 3B and 3C, at 40 °C the salt addition appears to have little effect on the aggregation process in the sense that the distribution among unimers and aggregated F127 molecules is not significantly affected. These findings prove the high stability of the cubic LC above 35°C and in the investigated range of ionic strength: this is of great interest in view of the potential applications of the formulations in diverse biomedical contexts. F127-based formulations, in the presence of physiological amounts of biocompatible salts such as NaCl or $MgCl_2$, give a tunable thermosensitive drug delivery platform, characterized by high stiffness and suitable transition temperatures. Particularly the high stiffness may assure a sustained drug release and provide prolonged resistance to dilution due to contact with body fluids, in the range of temperature, 30-45 °C, where cubic liquid crystals are thermodynamically stable.

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1C – An in-silico model of Bacteriorhodopsin/TiO2 hybrid system: toward the understanding of molecular factors influencing the performance of bio-inspired solar energy conversion devices

C. Coppola, A. d'Ettorre, M.L. Parisi, A. Sinicropi
(R2ES laboratory, Dept. of Biotechnology, Chemistry and Pharmacy, University of Siena)

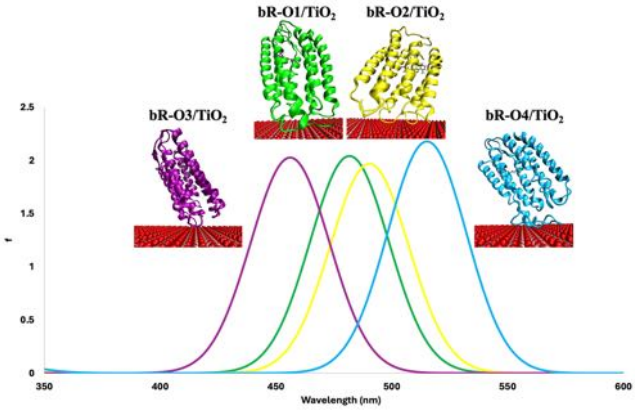
Aims

The use of bio-inspired hybrid materials in solar energy conversion devices has gained significant research interest. Due to its advantageous chemical and photochemical properties, bacteriorhodopsin (bR) from *Halobacterium salinarum* is a light-harvesting membrane protein that can serve as a sensitizer for TiO_2 in photovoltaic (PV) and photoelectrochemical cells (PEC), converting solar energy into electricity or chemical fuels. Extensive research has been conducted to experimentally study the bR/TiO_2 hybrid system in such devices; however, a thorough understanding at the molecular level is still lacking. In this context, we report for the first time the construction and characterization of an atomistic model of the bR/TiO_2 hybrid system, which could serve as a basis for future studies on the electron transfer mechanism in bR-based solar energy conversion devices. To achieve this, steered molecular dynamics-molecular dynamics (SMD-MD) and quantum mechanics/molecular mechanics (QM/MM) simulations have been combined to explore four different bR orientations on the anatase TiO_2 surface, with their absorption maxima computed and compared to that of isolated bR. This approach enables us to unveil the main protein−surface interactions and describe how the spectral properties of bR change upon contact with the surface.

Results

To simulate the adsorption mechanism of bR on TiO_2, a gas-phase, and globally uncharged QM/MM model of bR was fully relaxed at a QM/MM level and placed on the anatase TiO_2 surface in four different orientations (bR-O1/TiO_2, bR-O2/TiO_2, bR-O3/TiO_2, and bR-O4/TiO_2) corresponding to the most representative of the physisorption mode at the C-terminus of bR. SMD-MD simulations were carried out to drive the peptides toward the surface while applying a constant force to them. On the other hand, harmonic restraints were applied to preserve the geometry of the retinal chromophore. After SMD-MD simulations, all four bR/TiO_2 hybrid systems exhibit favorable (negative) interaction energies, with the main contribution represented by the electrostatic component. This result suggests that, during the adsorption process, the electrostatic interactions among the charged residues (Lys, Arg, Glu, and Asp) and the TiO_2 atoms predominate. Meanwhile, the number of contacts between the protein and the surface, which accounts for the van der Waals energy, similarly increases among the bR/TiO_2 systems. The structural stability of the bR/TiO_2 hybrid systems was confirmed by analyzing the backbone RMSD during 7.5 ns of the MD adsorption

process, showing that the secondary structure of all the bR/TiO_2 hybrid systems is marginally affected during the interaction with the surface. Hence, the four bR/TiO_2 hybrid systems were subjected to a QM/MM optimization and the analysis of the relevant parameters, such as deviation of C−α coordinates, bond length distances, bond length alternation (BLA), positive charge distribution, and dihedral angle values, revealed that the structure of the protein was not affected during the optimization process and the retinal chromophore can retain its functions after the adsorption. To investigate the possible differences in the UV−Vis absorption maxima of isolated bR and bR/TiO_2 systems, we calculated their absorption maxima at the TD-DFT level, using the ONIOM-EE (electrostatic embedding) method and employing a two-layer (QM:MM) calculation scheme. In agreement with experimental findings, we computed blue-shifted absorption maxima for the bR/TiO_2 hybrid systems to that of the isolated bR, which, consistently with previous findings in the literature, also reflect the lower delocalization of the positive charge through the polyene chain and higher BLA values that we found for the hybrid systems compared to those of the isolated bR. Additionally, to investigate the possible influence of the protein environment on the chromophore spectroscopic properties, we computed the absorption maxima of the bare chromophore extracted from the optimized hybrid systems. Still in good agreement with literature data, our results show that the interaction between the chromophore and the protein environment account for 0.07 eV toward the blue region, which is part of the protein-induced spectral shift of the retinal absorption, known as the opsin shift. The outcomes of this study allowed us to unravel fundamental effects that characterize the more complex interactions measured in real systems and validate the TiO_2-induced geometrical and electronic modifications of the chromophore moiety. The constructed models for the bR/TiO_2 hybrid system are a valuable basis for future studies focusing on the electron transfer mechanism in bR-based solar energy conversion devices, which are ongoing in our laboratories.



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1C – Ion specificity and Steric Forces at the Electrode-Electrolyte Interface

D. Parsons, M. Farci, C. Carucci, D. Tadesse (Murdoch University, Australia)

Aims

The influence of specific ion (Hofmeister) effects is well known in physiological and colloidal solutions, with zeta potentials of protein molecules and other particle varying greatly depending on the specific electrolyte, even resulting in charge reversal. Past projects have found that Hofmeister series can typically be interpreted theoretically through nonelectrostatic adsorption of ions driven by ion dispersion forces, although chemisorption also be considered in some cases. But the theoretical developments of these nonelectrostatic enhancements to DLVO theory have not previously been applied to electrochemical systems. A core challenge is managing the high potentials involved in electrochemistry. Typically, colloidal zeta potentials vary from 5-50 mV, that is less than 0.05 V. Electrochemical systems, by contrast, typically involve electrode potentials of 0.5-2 V or, of the order of 1000 mV. Point charge Poisson-Boltzmann models break down at such high potentials, and steric models accounting for finite ion size are needed. This project explores the application of such models.

Results

The general impact of steric forces, arising from finite ion sizes, is to introduce a concentration cap (cicap ≈1/Vi where Vi is the ion volume). The consequence is a peak capacitance at an electrode potential around 0.2V (relative to bulk solution), see Fig.1 [1]. Above 0.2V steric forces dominate over ion dispersion forces. The Bikerman model, an excluded volume model derived from the ideal entropy of water in the solution, offers a deceptively simple description of the steric force but results in electrode capacitances far in excess of values measured experimentally. The Carnahan-Starling model, derived from a nonideal equation of state for the osmotic pressure, provides a steric force able to reproduce experimental measurements sufficiently accurately. Adding steric and other nonelectrostatic interactions to Poisson-Boltzmann models is facilitated by analysis of the underlying thermodynamic potential.

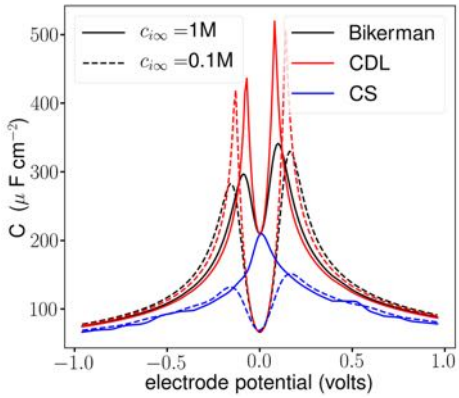

Figure 1: Single electrode differential capacitance of LiPF6 in propylene carbonate. CDL = composite diffuse layer (concentration capped). CS = Carnaham-Starling. Fig.1 from Ref.[1].

We note that conditions involving a bulk electrolyte imply a fixed chemical potential controlled by bulk ion concentrations. It is important to bear in mind this is the thermodynamics of the grand potentials, not free energy (which is controlled by a fixed number of ions, not the chemical potential) [2]. Numerical calculations of Carnahan-Starling models are challenging due to the transcendental nonlinear nature of the model, rendering computations of 1000 mV potentials difficult to obtain numerically. We derived a semianalytical approximation useful for steric modelling of ionic liquids as well as conventional electrolytes [3]. We have refined a throtting algorithm enabling numerical computation of electrochemical systems at potentials as high as 1000 V [4].

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1C – Life Cycle Assessment of Green Hydrogen Production: Analysing Energy Scenarios of the Italian grid

M.A. Gonzalez Monroy, A. Sinicropi, M.L. Parisi
(R2ES laboratory, Dept. of Biotechnology, Chemistry and Pharmacy, University of Siena, Italy)

Aims

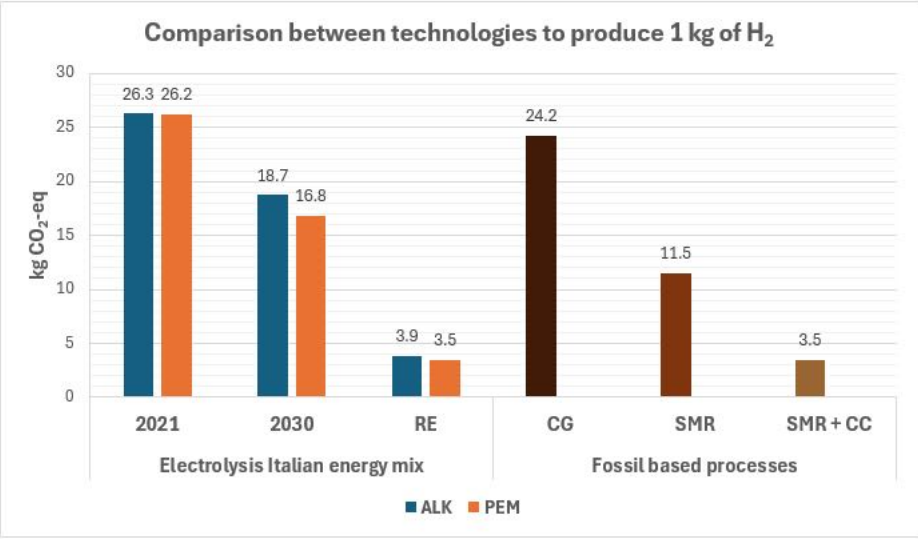
Hydrogen (H_2) stands out as a versatile and clean energy carrier with the potential to play a pivotal role in the transition to a sustainable energy future. However, H_2 production is still strictly tied to fossil fuels. In 2022, almost 95 Mton of H_2 was produced globally, with 62% derived from natural gas without carbon capture, and 21% from coal. Less than 1% came from low-emission sources, with 0.7% coming from fossil resources combined with carbon capture, usage and storage [1]. H_2 production from renewable sources via water electrolysis remains marginal. To assess the potential of low-emission hydrogen, environmental accounting methods such as Life Cycle Assessment (LCA) provide a robust framework to evaluate the environmental performance of these systems. This study presents a cradle-to-gate LCA of hydrogen production via water electrolysis. Two electrolysis technologies were evaluated: Alkaline (ALK) and Polymeric Electrolyte Membrane (PEM). The main input: electricity, comes from the Italian electricity grid. Three grid scenarios were evaluated: the current mix ("2021 scenario"), a second scenario ("2030 scenario") based on the PNIEC 2030 objectives [2], and a fully renewable scenario ("RE scenario").

Results

The first results focus on the electrolyser unit, comparing ALK and PEM technologies. ALK shows higher impacts in most categories, except for Particulate Matter, Land Use, and Ozone Depletion. For ALK electrolyser, the main contributors are nickel, steel, and copper, while PEM impacts are primarily linked to titanium, iridium, and platinum. These findings reflect key trade-offs: ALK avoids the use of Platinum Group Metals, but PEM achieves a more compact design and therefore, uses less amount of materials.

The environmental hotspots for H_2 production via ALK and PEM delivered at 350 bar with the 2021 energy mix were analysed. For both technologies, the electrolysis unit dominated the contribution to CO_2-eq emissions, accounting for 85% (ALK) and 89% (PEM) of the total. The Balance of Plant (BoP), including gas separators, pumps and dryers, contributed 11% for the ALK and 4.6% for PEM. Compression and construction materials for the electrolyser and storage tanks accounted approximately 4% and 1%, respectively, in both cases. The 2030 and RE scenarios followed the same pattern, confirming that electrolysis remains as the primary contributor to environmental impacts, highlighting that it is an energy-intensive process.

The Climate Change Impact category results for the three Italian energy scenarios are shown in the figure. The “2021 scenario” presents 62% of fossil share (oil 4%, coal 8%, natural gas 51%) and a renewable share of 38% (geothermal 2%, biomass 7%, wind 9%, hydro 20%); The “2030 scenario” shifts to 63% renewables (geothermal 2%, biomass 3%, hydro 13%, wind 18%, photovoltaic 27%), and 37% from fossil fuels (oil 2%, coal 5%, natural gas 30%). The “RE scenario” is fully renewable, with wind 25%, photovoltaic 45%, biomass 4%, hydro 21%, and geothermal 5%. As expected, an energy mix with a higher share of renewables resulted in a lower environmental impact. In ALK electrolysis, CO_2-eq emissions decreased by 85.2% when moving from the 2021 energy mix to the RE scenario. For PEM electrolysis, the reduction was 86.6%. When compared to fossil-based hydrogen production, both the 2030 and RE scenarios outperform Coal Gasification (CG: 24.2 kg CO_2-eq/kg H_2). However in comparison to Steam Methane Reforming (SMR: 11.5 kg CO_2-eq/kg H_2), only the RE scenario presents lower emissions. The results for SMR coupled with Carbon Capture (SMR + CC: 3.5 kg CO_2-eq/kg H_2) are comparable to the RE scenario.
The results of this study support the idea that when electrolysis is connected to the grid, its environmental impact depends entirely on the grid's composition—if the grid relies on fossil fuels, electrolysis can produce even higher emissions than fossil-based processes.



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1C – Novel organic dyes for indoor dye-sensitized solar cells: a machine learning and density functional theory study

C. Coppola, M.L. Parisi, A. Sinicropi (R2ES laboratory, Dept. of Biotechnology, Chemistry and Pharmacy, University of Siena)

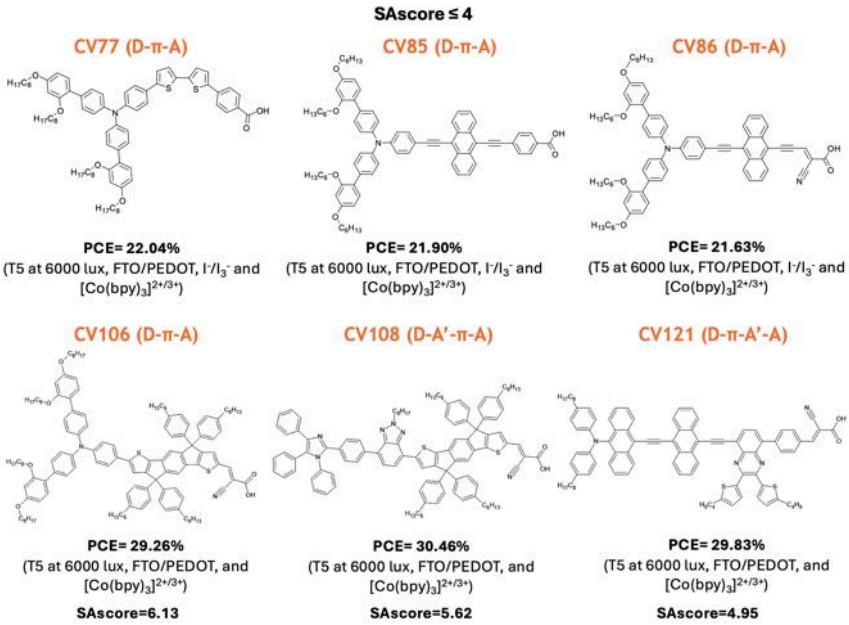
Aims

In recent years, dye-sensitized solar cells (DSSCs) have become a popular choice for indoor applications and to power Internet of Things (IoT) devices due to their ability to capture ambient light and convert it into electricity. In this context, the traditional research process for developing new sensitizers is often costly and time-consuming. To address these challenges, this study introduces a combined Machine Learning (ML) and Density Functional Theory (DFT) protocol to accelerate the discovery of novel and synthetically accessible organic dyes with D-π-A, D-π-A'-A, and D-A'-π-A architectures for indoor DSSCs applications. By predicting the power conversion efficiency (PCE) of the dye candidates under various indoor light sources and intensities, the developed protocol enabled the identification of three promising dyes with PCEs exceeding 29% under different artificial lighting conditions.

Results

To develop a reliable ML-DFT protocol, data from the literature published until the end of 2023 and related to 61 dyes previously tested under indoor conditions with PCE > 3% were collected in the training dataset. Then, 2.000 D-π-A, 240.000 D-π-A'-A, and 240.000 D-A'-π-A novel dye candidates were automatically designed by applying a fragmentation-recombination technique. To identify the candidates with the highest PCE values under artificial lighting conditions, a two-stage ML approach was developed and implemented (Model A and Model B). Specifically, Model A utilizes 1442 molecular descriptors and 2 experimental descriptors (light intensity and light source) for preliminary screening. To improve the predictions of the PCE, DFT calculations were performed by benchmarking various levels of theory, resulting in 24 new DFT descriptors. These descriptors were incorporated into Model B, which also relies on 1442 molecular descriptors and 4 experimental descriptors (light intensity, light source, counter electrode, and electrolyte composition). The performance of Model B was evaluated by comparing the performances of six regressors: XGBoost, Random Forest, Ridge regression, Elastic Net, K-nearest neighbors, and Decision Tree. In particular, the XGBoost model was the most accurate in predicting most of the PCE values (MAE: 1.19, RMSE: 2.88, STD: 0.17, R2: 0.94) and its performance was also improved compared to that of Model A (MAE: 1.45, RMSE: 4.31, STD: 0.23, R2: 0.90), suggesting that the implementation of DFT descriptors is a key point in the PCE prediction. Hence, Model B was applied to four independent datasets (D1, D2, D3, and D4), associating each dye candidate with all the possible combinations of the experimental descriptors. Additionally, the synthetic accessibility of the dye candidates was assessed by using the SAscore method, which considers the overall molecule complexity and the contribution of each fragment. The developed approach

led to the identification of three D-π-A dye candidates (CV77, CV85, and CV86) with predicted PCE > 21.5% and SAscore ≤ 4 under different artificial lighting conditions, as well as three dye candidates (CV106, CV108, and CV121 for D-π-A, D-A'-π-A, and D-π-A'-A architectures, respectively) with PCE > 29% under the emissions of fluorescent lamps at intensities higher than 3500 lux, regardless of the counter electrode and electrolyte composition. By comparing these data with the experimental PCE values under indoor conditions of the most performant dyes from the training dataset, we could assume that CV106, CV108, and CV121 could yield experimental PCE values comparable to or even exceeding current literature findings. Furthermore, all the predicted dye candidates exhibit SAscore values that align perfectly with those of the dyes in the training dataset, and their synthetic accessibility was further validated through detailed retrosynthetic analysis. The results of this study demonstrated that the presented ML-DFT protocol has the potential to successfully accelerate the procedures routinely employed for developing organic light-harvesting materials.



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1C – Sustainability Analysis of Indoor Photovoltaics (IPVs) for Smart Buildings and IoT Applications in MENTOR project

R. El Kouissi, M.L. Parisi, A. Sinicropi (R2ES laboratory, Dept. of Biotechnology, Chemistry and Pharmacy, University of Siena)

Aims

Indoor Photovoltaics (IPVs) represent a pivotal technological advancement that converts artificial indoor lighting into electrical energy to power electronics, particularly Internet of Things (IoT) devices within smart buildings. This technology is essential for reducing the dependency on batteries and external power sources, which are typically environmentally unfriendly and costly to maintain. However, the development and deployment of IPVs must also be scrutinized for their environmental sustainability to ensure that the solution itself does not contribute significantly to global resource depletion and greenhouse gas (GHG) emissions throughout its life cycle. Sustainability analysis, particularly through Life Cycle Assessment (LCA), is critical to evaluate the full environmental impact of IPVs. Without such assessments, there is a risk of inadvertently introducing new forms of pollution or resource exhaustion while trying to solve energy challenges in smart building ecosystems. The MENTOR project research aims to create a comprehensive technology platform for the sustainable development of next-generation IPVs. Sustainability considerations are embedded across the entire value chain: from material synthesis and device fabrication to performance optimization and recycling strategies. The initiative focuses on enabling sustainable IoT energy autonomy, contributing to the broader goal of achieving climate-neutrality by 2050.

Results

IPVs devices have been commercialized since the 1970s, but in the last two decades, the market for IPV has seen unprecedented expansion, driven by the development, commercialisation, and cost reduction of low-power electronic devices for the IoT[1]. This expansion is aligned with the rise of low-power electronics and the increasing demand for self-sufficient, portable power sources[1]. As the power requirements of these devices continue to decrease, the number and types of nodes that can be persistently powered by indoor photovoltaic cells are rapidly growing[3]. Among the various photovoltaic materials being explored for indoor applications, metal-halide perovskites (LHPs), organic photovoltaics (OPVs), dye-sensitized solar cells (DSSCs), and perovskite-inspired materials have emerged as promising candidates[2]. However, these technologies are not always intrinsically sustainable. Life cycle assessment is a valuable tool that provides a methodological framework to calculate their eco-profiles.

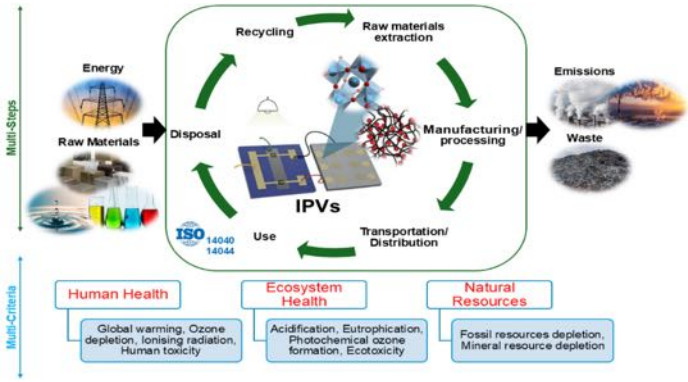

Figure1: Sustainability analysis for IPVs devices

LCA can help model reliable, innovative technological value chains that are scalable, reproducible, and aligned with circular economy principles. The flexibility of the LCA methodological framework enables inclusion of discriminating aspects such as hazardous and critical materials, in alignment with international regulations and voluntary approaches to guide chemical and materials innovation[2]. Among emerging IPV technologies, LHPs have demonstrated remarkable PCE in indoor environments[2]. However, lead-containing compositions pose environmental and health risks through energy-intensive processing, greenhouse gas emissions, and potential contamination from device disposal, necessitating careful end-of-life management[4]. Lead-free alternatives with bismuth or antimony offer reduced toxicity and sustainability[1], though comprehensive evaluation of material sourcing, manufacturing, and longevity remains essential. OPVs, on the other hand, offer the advantage of carbon-based materials, which are generally more abundant and less toxic than inorganic counterparts. The indoor environment presents less demanding conditions than outdoor applications due to minimal ultraviolet radiation, lower light intensities, and stable humidity and temperature[2]. However, OPV manufacturing may involve organic solvents and energy-intensive processes that contribute to global warming potential. DSSCs represent another emerging IPV technology class. While DSSCs avoid toxic solid-state absorbers, the solvents used in their fabrication may still pose environmental and health risks[4]. Overall, LCA evaluation of these IPV technologies is crucial for identifying sustainable pathways balancing performance, environmental impact, and health considerations.

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1C – Sustainability assessment of photovoltaic devices based on halide perovskites: A Life Cycle Assessment approach to innovative photovoltaic technology development

M.J. Kipyator, F. Rossi, M.L. Parisi, A. Sinicropi (R2ES laboratory, Dept. of Biotechnology, Chemistry and Pharmacy, University of Siena)

Aims

Perovskite solar cell (PSC) technology is emerging as a promising alternative to traditional photovoltaic (PV) systems due to its excellent optoelectronic properties, high power conversion efficiency, cost-effective manufacturing, and versatility in design. As PSC technology advances, it is crucial to conduct sustainability assessments to ensure eco-efficiency. This project presents a multidisciplinary sustainability assessment of PSC-based devices, integrating environmental and techno-economic evaluations through a life cycle perspective. The assessment begins with a harmonized, comparative scenario-based life cycle analysis (LCA) focused on recycling as the end-of-life strategy for different PSC/silicon (PSC/c-Si) tandem configurations. This analysis provides a comprehensive understanding of the environmental implications associated with the production and use of PSC/c-Si tandem at laboratory scale, as well as quantifying the environmental effects of various recycling strategies. Furthermore, the environmental impacts of scaling up operations of PSC-based PV systems from the laboratory to industrial levels are also considered through an integrated prospective LCA approach, combining environmental and economic analysis to explore the future use of single junction PSC PV systems in building-integrated PV (BIPV) application.

Results

The first analysis assessed the environmental impact of five tandem solar cells (TSCs) across their lifecycle, focusing on different end-of-life recycling strategies. Four scenarios were developed to determine the most sustainable approach and address the lifetime gap between c-Si and PSC. The scenarios include: S1, recycling both cells; S2, recycling only the Perovskite cell; S3, retaining the degraded perovskite cell; and S4, removing the degraded perovskite cell and the silicon cell operates alone. Overall, the results highlight that the environmental impacts of the PSC/c-Si TSCs are dependent on the materials used within the configuration, the lifetime and the PCE of the devices. The work also emphasizes that in addition to designing the PSC-based modules to achieve stability and high PCE, it is crucial to design the devices with recyclability in mind since it is shown that if the PSC are not able to achieve high stability, they may find long- term application if periodic module recycling and refurbishment is implemented (S4). This will, therefore, require that the modules are

designed in a way that will facilitate easier dismantling and recycling. Overall, a trade-off between scalability and the PCE of the device should be analyzed when choosing the materials to be employed in the PSC-based devices to ensure that they can be recycled effectively and in a cost-effective manner.

From the second analysis, it is shown that from a long-term perspective, the economic gap between the single junction PSC devices and the c-Si is expected to decrease, with the PSC expected to outperform traditional c-Si PV devices in terms of environmental impacts in future. However, this will depend on the extent of the development of the PSC technology. If their development is high and they are able to achieve a high PCE of 25%, a lower degradation rate of less than 0.9% and a lifetime of 25 years, their implementation will provide economic and environmental benefits as early as 2029. Nevertheless, if the development process is low, the economic and environmental advantages of PSC will be realized only in 2045.

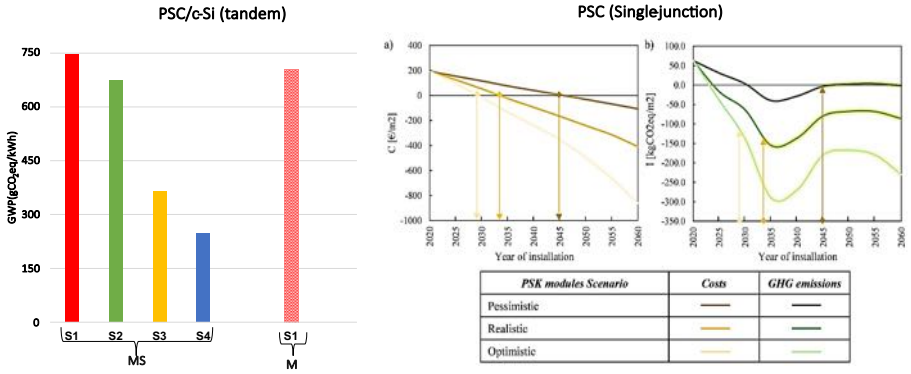

Figure 1: Results of the analysed PSC-based devices with the figure on the left showing the global warming potential (GWP) of the harmonised analysis of a PSC-Si as function of the end-of-life scenario (S1,S2,S3,S4) and the figure on the right shows the Pessimistic, Realistic, and Optimistic scenarios for the future a) net costs and b) GWP profiles of the BIPV system equipped with PSC modules

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1C – The effects of saline water on the recovery of sulfide minerals during froth flotation

D. Parsons, A. Nowosielska (Murdoch University, Australia)

Aims

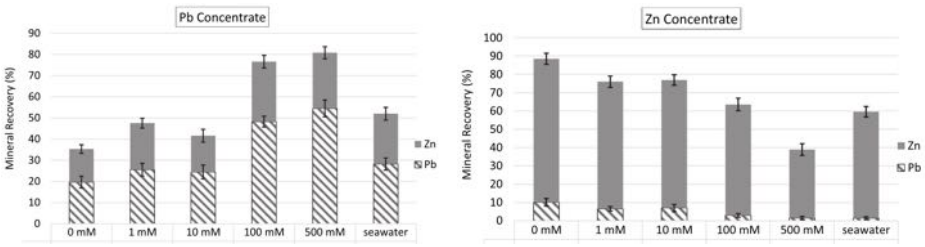
With freshwater becoming a scarce resource in metallurgical operations, the use of seawater or recycled water is being increasingly recognised in areas with limited resources of freshwater. It is known that the use of saline water enhances mineral flotation, nonetheless, to date there is no single mechanism to explain the increased flotation efficiency using saline water. Proposed mechanisms include (a) destabilisation of the hydration layers around the particle, (b) inhibition of bubble coalescence, and (c) the compression of the electric double layer around the particle and bubble. Limited studies have been conducted to examine the role of inorganic electrolytes on the recovery of sulfide minerals as well as the recovery of gangue minerals using flotation. This research project applied expeirmental testwork and theoretical analysis to answer the question:

What are the main effects of saltwater on the fundamental particle-particle and particle-bubble interactions during sulfide mineral flotation?

Results

Experimental flotation testwork showed that the recovery of pure galena and pure sphalerite improved with NaCl addition. This was attributed to the lower zeta potentials due to the compression of the ionic diffuse layers, creation of smaller-sized bubbles and the inhibition of bubble coalescence. In the case of seawater, the overall galena and sphalerite recoveries decreased, attributed to the negative effects of different additional ions (eg. Ca2+, Mg2+, SO42-) present in seawater.

Electrokinetic measurements were conducted on galena, sphalerite, and quartz. Measured zeta potential values were used to optimise parameters in pH-dependent chemisorption (charge regulation) models. Our chemisorption model representing ion competition at the galena and sphalerite surface sites is the “two site/not amphoteric” surface model; our quartz and air bubble chemisorption model, representing competitive ion binding at the surface sites is the “one-site/two pK” model.



Modified charge-regulated DLVO-like calculations of particle-particle and particle-bubble interactions found attractive PbS-bubble interactions, while the ZnS-bubble interactions were always repulsive, despite an

increase in ionic strength. These ZnS-bubble repulsions were attributed to the repulsive nature of the van der Waals forces, due to the negative Hamaker constant calculated for the ZnS-bubble interaction in water. Similarly, quartz-bubble interactions were always repulsive, irrespective of the NaCl concentration, also due to the repulsive nature of the van der Waals interactions. Based on these theoretical predictions, it was suggested that a stronger repulsion between sphalerite and quartz particles and air bubbles could be the driving force for higher galena recoveries, when present in the same ore body.

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1C – Trends, Potentials and Challenges of Innovative PV Technologies: Lessons Learned from the CANVAS Project

P. Fornarini, M.L. Parisi, A. Sinicropi (R2ES laboratory, Dept. of Biotechnology, Chemistry and Pharmacy, University of Siena, Italy), C. Polacchi, E. Veronese (Eurac Research, Bolzan, Italy)

Aims

The CANVAS project investigates emerging photovoltaic (PV) technologies with the goal of bridging the gap between laboratory-scale innovation and industrial-scale implementation. The project focuses on identifying strategies that balance technological innovation, economic viability, and environmental sustainability.

This study presents a comparative analysis of selected third-generation PV technologies, including perovskite solar cells (PSCs), dye-sensitized solar cells (DSSCs), and crystalline silicon (c-Si) modules integrated with luminescent solar concentrators (LSCs). For each technology, key performance indicators such as module efficiency, active area, production throughput, and material requirements were assessed.

Primary data were collected at both laboratory and pilot scale, enabling a preliminary evaluation of scalability and associated technical and economic barriers. Special attention was paid to throughput techniques such as spin coating, screen printing, and sputtering, which significantly affect industrial feasibility.

A life cycle cost (LCC) analysis was performed to evaluate the full economic footprint of each technology, including material and energy costs, equipment uses, labor, and process expenses. In parallel, an environmental life cycle assessment (E-LCA) quantified emissions and resource impacts across the production chain. The analysis highlights trade-offs between scalability, performance, cost, and environmental burden, offering insights for guiding future research and policy on low-TRL PV solutions.

Future steps involve scaling up the analysis, evaluating integration potential in Building Integrated Photovoltaics (BIPV), and developing simulation tools for techno-environmental optimization of next-generation solar technologies.

Results

The life cycle assessment of emerging photovoltaic technologies has revealed several key aspects across their value chains, offering insights into their potential for more sustainable energy generation in the near future.

The production phase remains one of the most impactful, largely due to the high energy demand of various laboratory-scale processes and the still non-optimized consumption of chemical reagents. Although many of these emerging technologies rely on small amounts of active materials and sometimes simplified synthesis pathways, overall process efficiency and resource utilization are not yet fully optimized. This suggests considerable potential for improvement in future industrial-scale production through process refinement and scale-up.

Despite their early-stage development, several technologies demonstrate promising scalability potential. The compatibility with cost-effective fabrication techniques, along with the prospects of increasing process efficiency, support the idea that emerging photovoltaics may become increasingly competitive as they move beyond the laboratory.

During the use phase, these technologies show encouraging initial performance. However, long-term durability remains a concern, with environmental exposure and material stability influencing operational reliability. Interestingly, instead of viewing the limited lifespan of panels as a drawback, some studies suggest that scheduled replacement of the entire photovoltaic module can be reframed as an opportunity. Planned replacement strategies, or repowering, may allow for the deployment of more efficient and environmentally friendly technologies over time, supporting sustained optimal performance and embracing technological progress.

Another issue relates to the use of critical or geopolitically sensitive materials. Although their presence is currently limited, research is ongoing into alternative materials and recycling strategies, both of which could mitigate future supply risks and improve the overall sustainability of these technologies.

Regarding the end-of-life phase, some complexity still exists due to the multilayered nature of the devices and the diversity of materials involved. Nonetheless, there is a growing emphasis on designing components that can be more easily dismantled and recycled, in line with the principles of a circular economy.

Finally, although still under investigation, the potential integration of these technologies into the built environment represents one of the most exciting prospects. While this phase of the research is still evolving, the flexibility, color tunability, and semi-transparency of certain emerging PV solutions could make them particularly suited to architectural integration. These features open new possibilities for aligning energy production with design and functionality, especially in the context of next-generation building applications.

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2A – Adsorbent materials and composites for the emerging contaminants removing in polluted waters

D. Capsoni, M. Sturini, C. Urru

Aims

Antibiotics and hormones are considered contaminants of emerging concern (CEC), as they are widely detected in wastewater, surface water, drinking water, and soils in many developed countries, even at trace levels (ng L-1); they easily re-enter the aquatic compartment, as the urban wastewater treatment plants cannot abate them. Adsorption is considered a consolidated technique for CEC water remediation. It is advantageous (low cost, high efficiency and easy conventional WWTPs integration), and efforts are being done to develop and test new adsorbent materials for pollutants removing from waters. The ideal adsorbent materials should display high surface area, high stability in aqueous media, and low toxicity. In the present research project, we synthesize and characterize clays and nanoclays as suitable adsorbents to remove antibiotics (fluoroquinolones) and hormones from environmental water. Secondly, we investigate Fe3O4-clays composites as magnetic adsorbents, to take advantage of the magnetic component to separate the adsorbent solid phase from the solution. Preliminary results were also obtained on clays loaded into polymeric membranes by electrospinning.

Results

The adsorption capability of commercial and etched halloysite nanotubes was preliminarily investigated (acidic and alkaline etching) to remove ofloxacin from polluted water. The characterization and absorption capability results demonstrate the strict relationship between the ofloxacin recovery and the morphology of HNTs, modulated by the etching process. The promising results of the ofloxacin-halloysite system suggest us to investigate the efficiency of HNTs decorated with magnetic Fe3O4 nanoparticles through different synthetic routes (co-precipitation, hydrothermal, and sol-gel) to remove Ofloxacin from water. Independently of the synthesis procedure, the magnetic composites display nanometric magnetite particles (about 10 nm) and the weight percentage of the magnetic component depends on the synthetic method used. The thermodynamic and kinetic experiments showed different adsorption capacities, but the kinetic process occurred within a few minutes, independently of the composite. Despite the good results obtained for all the composites, the sample by co-precipitation is the most performant and exhibits advantages: (i) easy magnetic separation from the media after the use; (ii) no degradation after three adsorption cycles; (iii) low-cost of the synthetic procedure.
More recently, the halloysite nanotubes were loaded onto polymeric membranes prepared by electrospinning a PAN solution containing HNTs particles. The membranes demonstrated to be efficient in the removal of both ofloxacin and hormones: their adsorption performance can be explained by the chemical and

physical features of the membranes, evaluated by applying several characterization techniques (XRPD, SEM, EDS, TEM, FT-IR, thermal analysis).
Finally, preliminary results were obtained by using smectite clays such as laponite and saponite. Again, the investigated minerals demonstrate to be effective in removing mixtures of fluoroquinolones in water, and their efficiency depends on the clays structural and microstructural features.

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2A – Amphiphile-based nanofluids for the removal of undesired organic matter from works of art

M. Baglioni, E. Carretti, L. Dei, D. Berti, E. Fratini, D. Chelazzi, T. Guaragnone, R. Mastrangelo, G. Poggi, R. Giorgi, P. Baglioni

Aims

Development of innovative, effective, safe and environmentally-friendly systems for the cleaning of painted surfaces – systems' characterization and cleaning assessment. Improvement of the available formulations with the inclusion of degradable (biodegradable, labile, cleavable) surfactants, which could solve the residues' issue, and/or with more efficient surfactants, having high solubilization power towards small hydrophobic molecules.

Results

The removal of undesired material from the surface of a work of art has always been one of the most important and delicate operations in the conservation of cultural heritage. Surfactant-based aqueous nanostructured fluids (NSFs), such as micellar solutions and microemulsions, represent the most effective, safe and selective cleaning media currently available for cleaning operations in conservation of cultural heritage. Due to their nature, these systems can be used to remove oily grime or hydrophobic substances from hydrophilic surfaces, as in the case of polymer removal from wall paintings and stones.

The nature and properties of surfactants are key to the effectiveness of NSFs, thus the search for highly-performing, environmentally-friendly, readily-degradable surfactants is one of the main aims of present studies. The research focus was recently moved from ionic surfactants to nonionic alcohol ethoxylates, which possess interesting (bio)degradability properties and excellent detergent power, and the

performances of new classes of surfactants were explored, such as cleavable pH-sensitive autodegradable surfactants. Interesting results were obtained using these innovative surfactants in new NSFs. As a result of these research efforts, nanofluids for the cleaning of cultural heritage have been made available to conservators and restorers as commercial products under the trademark of Nanorestore Cleaning®.
Recently, new surfactants, such as alkyl ester ethoxylates were considered, in view of their excellent solubilization properties, with respect to more common ether ethoxylates. It was shown that alkyl ester ethoxylates are more efficient than their homologue alcohol ether ethoxylates in removing both polymeric coatings and soil from artistic surfaces. This is due to their molecular structure, which includes an ester bond between the hydrocarbon tail and the polyoxyethylene chain, and a hydrophobic capping at the end of the polar head, and makes them more efficient in the solubilization of hydrophobic small compounds and in the interaction with hydrophobic polymers. The confinement of NSFs into retentive hydrogels, such as semi-Interpenetrated Polymer Networks (sIPNs) based on poly(hydroxyethyl methacrylate)/poly(vinyl pyrrolidone) or poly(vinyl alcohol)-based twin-chain polymer networks (TC-PNs) obtained as the result of freeze-thaw cycles, results in one of the most advanced solutions for the cleaning of works of art. NSF-loaded TC-PNs were recently and successfully used, within the frame of the EU-funded Nanorestart project, for the cleaning of masterpieces, such as “The Studio” by Pablo Picasso, or, for the first time, for the removal of aged detrimental polymeric coatings from the surface of Nuxalk painted wooden carvings conserved at the American Museum of Natural History.
The latest update involves the development of “green” nanostructured fluids in the HORIZON EUROPE GREENART (GREen ENdeavor in Art ResToration, https://cordis.europa.eu/project/id/101060941/it), where bio-derived non-ionic surfactants were employed in the fluids to remove soil and aged coatings from works of art.

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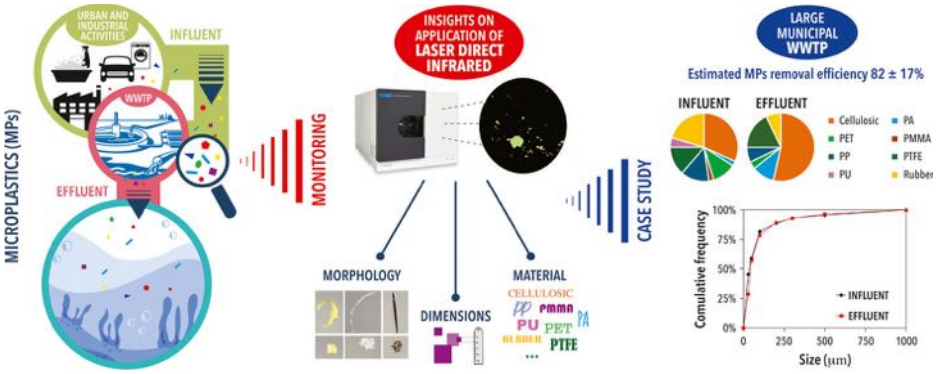
2A – An innovative method for the detection and characterization of microplastics in wastewaters based on Laser Direct InfraRed (LDIR)

E. Carretti

Aims

Wastewater treatment plants (WWTPs) are generally reported to be effective in removing microplastics (MPs). Nevertheless, the lack of standardized methodologies for their counting and characterization hinders direct comparison across literature reports, limiting the establishment of reliable benchmarks. In this perspective, this research aimed to provide methodological insights on a feasible approach for detecting and characterizing MPs in both raw and treated wastewater by exploiting the innovative Laser Direct InfraRed (LDIR) technique.



Results

MPs of various polymeric nature, size and shape were specially produced and used to fine-tune and validate a LDIR-based method for both their chemical identification and size/morphology description, while well-established techniques were employed to evaluate the reliability of collected data. The robustness of the tailored protocol was then assessed through a monitoring campaign conducted at a large municipal WWTP in Tuscany (Italy), for which an average MPs removal efficiency of 82 % was estimated. Various polymers were detected in the processed samples, with a high relative content of cellulose-based materials in both influent and effluent (32 % and 54 % of particles, respectively). Most MPs had a characteristic size lower than 100 µm, with particles <30 µm representing about 45 % and 29 % of MPs in the influent and effluent, respectively. MPs were in the form of fibers (25–39 %), fragments (32–43 %) and pellets (29–32 %). The consistency of the obtained results suggested the robustness and reliability of the proposed LDIR-based method, highlighting its potential for more in-depth monitoring of MPs in WWTPs.

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2A – Anti-counterfeiting photoluminescent nanomaterials to fight the illicit trafficking of artworks

R. Giorgi, T. Krasoudaki, F. Battaglia, A.L. Matulac

Aims

The rising incidents of illicit trafficking of cultural heritage objects highlight the need for advanced, cost-effective, and minimally invasive anti-counterfeiting solutions. This study, as part of the EU-funded AURORA project, introduces the development of novel invisible security inks designed to enhance the authentication processes of artworks. It leverages two types of fluorescent nanomaterials: Zinc Oxide quantum dots (ZnO QDs) and Carbon Dots (Cdots), both of which exhibit remarkable properties suitable for integration into advanced security systems.

Results

Silanised ZnO QDs, functionalised with (3-aminopropyl)triethoxysilane (APTES), were selected due to their enhanced water solubility, fluorescence stability under UV light and temperature fluctuations, and tunable emission. The nanoparticles were prepared using a straightforward, one-pot sol-gel method, and the final ink formulation was optimised with methyl hydroxyethyl cellulose (MHEC) to reduce feathering and improve fluorescence brightness across various substrates, including paper, stone, and glazed ceramic. Additionally, Cdots were developed via a green, cost-effective aqueous bottom-up synthesis route using urea and sodium citrate as precursors. The nanoparticles demonstrated excellent results in terms of fluorescence intensity, as well as pH and temperature stability. They were effectively dispersed in water-based conservation-grade binders, and their fluorescence, stability, workability and substrate-specific performance were assessed on various substrates.

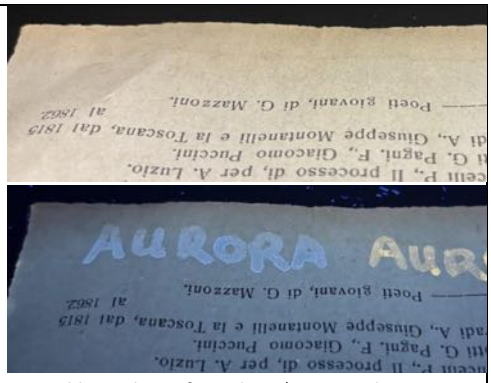
The study confirms the feasibility of formulating invisible, luminescent, anti-counterfeiting inks for the protection and authentication of cultural heritage using novel, easily synthesised, stable nanomaterials. These materials offer a promising strategy for the environmentally friendly and secure identification and traceability of artworks, contributing to the broader goal of combating art crime using nanotechnology.

The validation of the chemical markers on real cultural heritage objects demonstrates that the tagging process is inherently decision-driven and currently cannot be reduced to a single, universally applicable approach. The selection of an ink formulation must be based on its properties, requiring users to carefully consider the object type, its condition, and the storage or display environment in order to identify the most suitable solution.

The collaborative results further indicate that alternative binders are necessary for certain categories of objects, and that the use of preparatory and protective layers is, in some cases, essential to meet the established performance and conservation criteria. These factors directly influence the feasibility and acceptability of the chemical markers. Meanwhile, the size, shape, and overall form of the chemical

marker that can be produced are strongly influenced by the available application techniques.
A range of application techniques was evaluated during the validation phase. Among these, the use of felt-tip pens currently represents the most practical and readily implementable approach for routine applications.

Photoluminescence, under a 365 nm UV lamp, of invisible inks applied on stone samples



Invisible marking of a early 20th century document under normal light and 365 nm UV irradiation.

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2A – Biobased organogels for the cleaning of works of art

G. Poggi, D. Bandelli, D. Chelazzi, P. Baglioni

Aims

Gels are particularly useful for the cleaning of works of art as they allow the controlled delivery of cleaning fluids on solvent-sensitive substrates. Organogels, i.e., gels that can be loaded with organic solvents, are particularly useful for the cleaning of artistic surfaces that cannot withstand the application of water. Here we present several strategies for the synthesis of biobased organogels, developed within the European projects APACHE and GREENART.

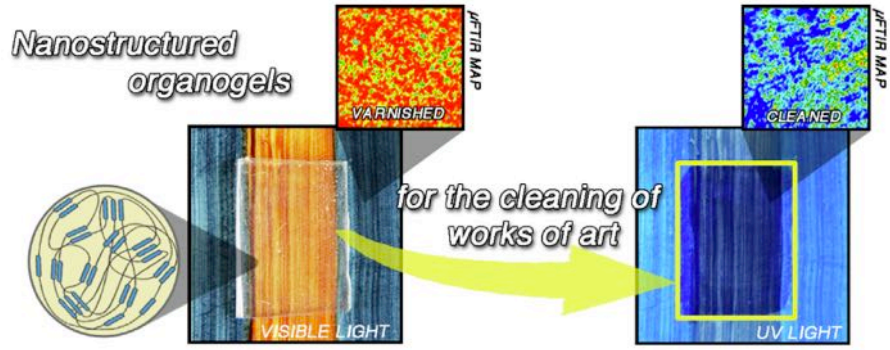
Results

Castor oil (CO)-based systems were specifically designed to address the challenge of cleaning artistic surfaces that cannot withstand the application of water. In such contexts, when conservators frequently opt for organic solvents over aqueous formulations, the new systems proved to be highly effective tools, complementary to the chemical hydrogel networks that we previously demonstrated as the most performing systems nowadays available.

In this regard, we have developed a solvent-free and cost-effective synthesis of a new class of gels derived from natural resources, based on castor oil and isocyanates mixtures. The gels are obtained as dry systems that can be loaded with organic solvents when needed, allowing for an easy storage (i.e. outside ventilated cabinets).

Changes in the composition of the pre-gel mixtures, e.g. tuning the CO-isocyanate ratio or partially substituting CO with polyethylene glycol, affects the overall number of crosslinking points between CO chains. This, in turn, results in differences in the mechanical behavior, as evidenced by rheological measurements, and in the nanostructure.

The different affinity between the gel network and solvents can be used to explain the difference between swollen systems in terms of elastic and loss moduli, of network organization at the nanoscale, and swelling degree. The swollen CO gels are transparent, which is advantageous to check their step-by-step cleaning action, and retain their good mechanical properties. Loading and confinement of the solvents in the nanosized polymeric mesh of the gels is likely key to explain their optimal cleaning effectiveness: the systems are highly retentive, allowing for the controlled release of solvents over delicate paint layers. This is a crucial feature, as modern and contemporary paintings frequently exhibit pronounced sensitiveness to solvents and cleaning fluids.



More recently, a series of new ‘‘green’’, sustainable poly(urethanes-co-oxazolidones) organogels, based on castor oil and its epoxidized derivative (EpCO), were prepared and characterized, with potential applications in the polyurethane chemistry research and industry. The effect of EpCO addition on some important physico-chemical properties was elucidated. During gel curing, the use of EpCO enabled to increase the speed of the polyurethane network formation, likely due to the capability of epoxides to react with isocyanates forming oxazolidinone linkages. Those materials show fast gelation, good mechanical properties in the solvent-less and swollen states, and interactions with solvents, together with high sustainability of the whole synthetic process. All these features make them good candidates for several application, potentially including also the cleaning of works of art. Research efforts are currently dedicated to the development of several new castor oil-based organogels formulation featuring specific green additives, such as oligoesters, with the aim of tailoring the final properties of the network to several real case studies in conservation.

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2A – Biowaste-derived carbon colloidal nanosensors for environmental pollutants detection

S. Russo, G. Vitiello
(U.O. Naples, University of Naples Federico II)

Aims

Colloidal carbon nanoparticles (CNPs) are fluorescent nanoparticles, composed mainly of carbon which are attracting great interest for various technological applications, as high-performance materials in biomedical, environmental and sensing fields. They exhibit unique properties including water solubility, low toxicity, and resistance to photobleaching and optimal optical properties (Li et al. 2012). Thanks to their peculiar fluorescent properties, they can be utilized as chemo-sensors, since CNPs exhibit excellent sensitivity and selectivity towards heavy metals, such as mercury, cadmium, and lead, as well as organic molecules with low detection limits (Sekar et al 2021).

Results

Here, we exploited a waste-to-wealth strategy to produce carbon nanoparticles (CNPs) with improved photoluminescent and pro/antioxidant properties through an eco-friendly approach based on a green hydrothermal synthesis in which bi-distilled water was used as solvent and humic acids (e.g., HASS) as molecular precursor. The CNPs obtained exhibited good colloidal stability over time, excellent optical properties and good selectivity towards specific heavy metals (Russo et al. 2025).
A comprehensive physicochemical analysis based on a combination of advanced analytical techniques, such microscopy, absorption and emission spectroscopies and scattering, was carried out. The production of small nanoparticles with an average diameter <10 nm was observed. However, they tend to form clusters in aqueous suspension which demonstrated interesting physicochemical properties (Figure 1).

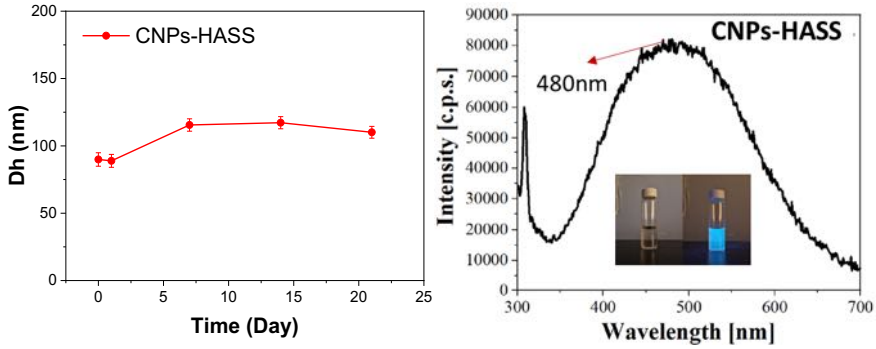

Figure 1: Physicochemical properties of synthetized CNPs: evolution of hydrodynamic diameter on time (*on the left*) and fluorescence spectrum (*on the right*).

In particular, a good colloidal stability over a period of three weeks was observed, which can be attributed to the presence of surface functional groups, specifically hydroxyl and carboxyl moieties. At the same time, upon excitation at 280 nm, CNPs exhibited a broad emission band centered around 470–500 nm.

These CNPs were tested as nano-sensors for the detection of environmental pollutants, such as metal cations and organic molecules. Among them, CNPs exhibited a good sensitivity towards copper ions present in water. Indeed, the limit of detection (LOD) was equal to 3.8 μM while the limit of quantification (LOQ) was equal to 12.7 μM (Figure 2), thus confirming the significant potentialities as innovative chemo-sensing platforms for the detection of metal cations in aqueous media. Indeed, these values were below the maximum permissible concentration established by current regulatory standards.

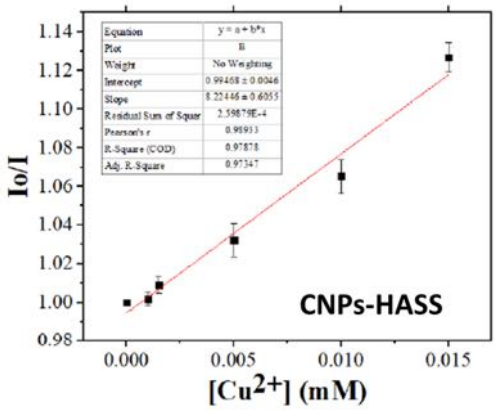

Figure 2: Calibration curve of I_o/I versus Cu^{2+} concentration.

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2A – Chemical mapping for insight into historical photographic films

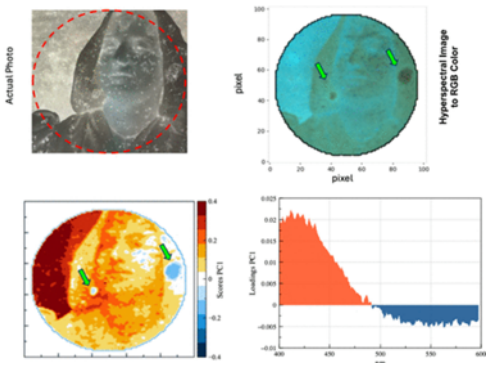
A. Licciardello, N. Tuccitto, V. Spampinato, A. Auditore

Aims

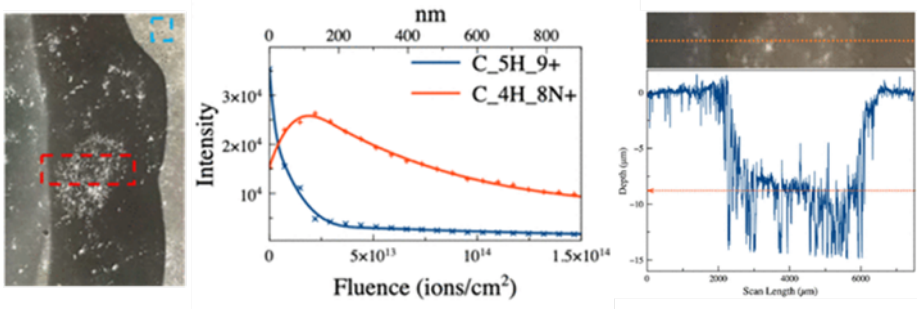
This study aims to investigate the chemical and structural degradation mechanisms of gelatin-based photographic films from the early 1900s, with the ultimate goal of informing conservation strategies for historically significant photographic materials. Given the widespread use of gelatin in early photographic emulsions and the observable deterioration phenomena—such as silver mirroring and protein matrix breakdown—the research pursues to provide a detailed molecular-level analysis of these degradation processes. The study employs a multiscale, integrated approach combining Hyperspectral Ultraviolet-induced Fluorescence Mapping (HUVFM), Principal Component Analysis (PCA), and Time-of-Flight Secondary Ion Mass Spectrometry (ToF-SIMS). These methods allow for the identification of localized degradation phenomena and their correlation with molecular changes across both spatial and depth dimensions of the samples. The aim is to develop a clearer understanding of how protective surface layers deteriorate and how gelatin degradation and silver migration manifest over time, thereby advancing the field of cultural heritage conservation.

Results

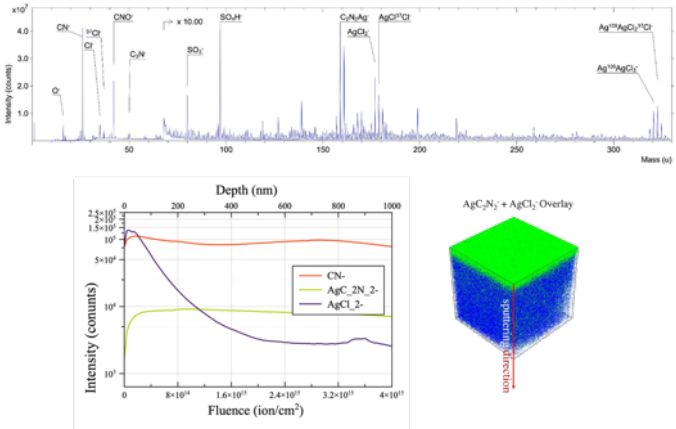
The integrated analytical approach revealed two principal degradation mechanisms in the studied photographic films. The first sample demonstrated localized quenching of fluorescence under UV light, which was mapped via HUVFM and analyzed through PCA. This analysis indicated significant degradation in the gelatin matrix, particularly affecting proteinaceous components like collagen.



These findings were corroborated by ToF-SIMS, which identified the absence of surface paraffin lacquer in degraded zones and the presence of protein fragments and oxidation products underneath. Depth profiling and profilometry confirmed that approximately 50% of the gelatin layer had eroded in these areas, exposing the underlying substrate and accelerating protein breakdown.



In the second sample, the study focused on areas affected by silver mirroring—a reflective surface phenomenon caused by silver ion migration. ToF-SIMS analysis identified silver compounds such as AgCl− and AgC_2N_2− and demonstrated their distinct spatial distribution. Depth profiling showed that silver mirror layers were concentrated near the surface, while gelatin-related components were more evenly dispersed through the film's depth. A three-dimensional reconstruction further confirmed the surface-localized nature of the silver degradation layer, aligning well with the oxidation−migration−reaggregation model of silver mirroring formation.



Together, these findings provide a detailed view of degradation pathways affecting early gelatin photographic films. The study highlights the synergistic use of hyperspectral imaging and mass spectrometry as an effective strategy to map chemical and structural changes, offering valuable insights for the development of targeted conservation treatments aimed at preserving fragile photographic heritage.

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2A – Diagnostic analyses supporting the restoration of Fonte Gaia in Piazza del Campo, Siena

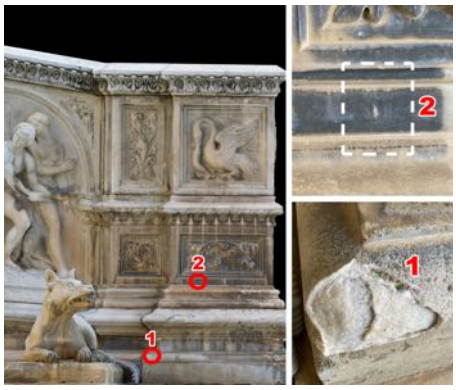
M. Baglioni, S. Landi, G. Tamasi, C. Rossi

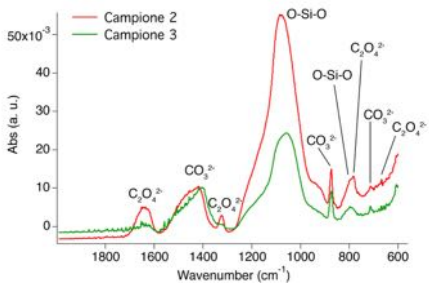
Aims

The restoration of the Fonte Gaia in Piazza del Campo, Siena (the 19th-century copy by Tito Sarrocchi of the original monument by Jacopo della Quercia, which is currently preserved at the Museo di Santa Maria della Scala, also in Siena) some diagnostic investigations aimed at characterizing the materials of the alteration patinas on the marble were carried out. For this purpose, small samples were collected and analyzed by X-ray fluorescence (XRF), both on the front (where the patina was present) and on the back (the marble matrix), to assess the elemental composition of the stone. Additional analyses included attenuated total reflectance Fourier-transform infrared spectroscopy (ATR-FTIR) and differential thermogravimetry, performed to reconstruct the chemical composition of the alteration patina in two different areas of the monument.

Results

Based on the assignment of IR absorption bands, the presence of three main classes of compounds was identified: carbonates, oxalates, and silicates. The occurrence of carbonates is rather obvious, given the marble substrate, as is that of oxalates, which are typically found on calcareous monuments as a result of alteration processes, very often mediated by microorganisms capable of producing oxalic acid, which in turn leads to the formation of calcium oxalate in mono- or di-hydrated form. The detection of silicates in the alteration patina is less obvious, but it can be explained by the use of fluosilicate-based consolidants during conservation treatments carried out in the 1970s.





The XRF analyses added some interesting details to the already well-defined picture of the patina composition: small amounts of sulfur were detected, attributable to sulfation processes; traces of phosphorus, most likely related to biogenic degradation (e.g., animal droppings); and iron, which could derive from the action of water on metal clamps within the structure, or more simply from atmospheric particulate deposition.

2A – Environmentally friendly ZnO/Castor oil polyurethane composites for the gas-phase adsorption of acetic acid

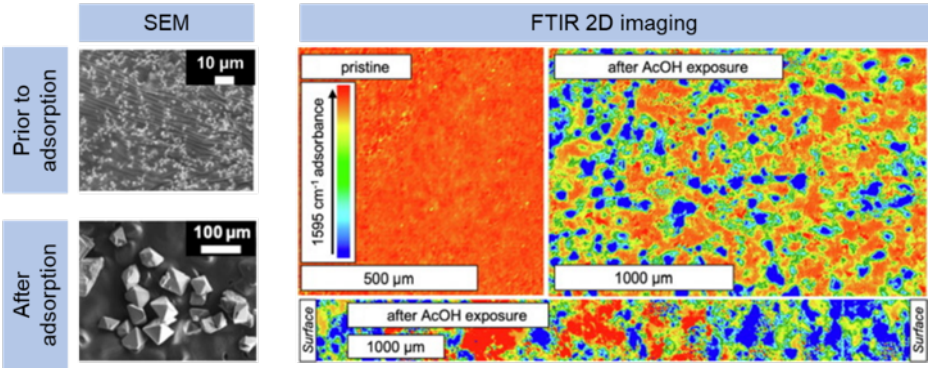
A. Zuliani, D. Bandelli, D. Chelazzi, R. Giorgi, P. Baglioni

Aims

Simple volatile organic acids are common pollutants in museums and art galleries, produced from the degradation of artifacts (*e.g.* paintings) or emitted from wooden frames/boxes and adhesives. As a result, compounds such as acetic acid (AA) can irreversibly damage works of art, making the development of preventive restorative strategies a central aspect in Cultural Heritage science. To this aim, novel adsorbers capable to irreversibly bound pollutants represent the cutting-edge materials to minimize degradative processes in preventive conservation. Herein, a sustainable and scalable synthesis of zinc oxide-castor oil polyurethane hybrids (ZnO/COPs), to be used as AA scavenger, is reported. The final material performances were evaluated in saturated and low concentrations (ppbv-scale) of AA by gravimetry. In addition, structural insights on the materials features prior and after adsorption were accessed by Thermogravimetric analysis (DTG), Infrared spectroscopy (FTIR-ATR), X-Ray diffraction (XRD) and imaging approaches (SEM and FTIR 2D).

Results

Castor oil-polyurethane composites were prepared employing commercially available ZnO particles with varied diameters from 20 nm to 44 μm, and ZnO content from 10 to 60 w%. The resulting materials featured comparable thermal stability, suggesting that the use of ZnO did not alter the three-dimensional structure of the composite. In contrast, adsorption experiments in saturated atmosphere of AA revealed the formation of Zn acetate species (XRD patterns) after 2 weeks of adsorption. In addition, SEM (and SEM-EDX) analysis revealed a variation in the morphology of ZnO particles, resulting in tetragonal pyramid structures with larger size (up to 100 μm) in comparison to the starting particles. Similar results were obtained by FTIR 2D imaging of the composite surface, while the analysis of the composite cross-section also revealed the homogeneous distribution of Zinc acetate, proving the efficient transport of AA in the COP matrix.



Gravimetric analysis during adsorption tests revealed higher AA retention for increasing weight% of ZnO and particle surface area (decreasing particle size); the composites exceeded the adsorption capability of activated charcoal that is commonly employed by conservators for similar applications.
Lower AA concentration (≈ 6000 ppbv) was also tested, with an adsorption capability of 97% after 150 h of exposure. As final test, ZnO/COPs were used for the adsorption of AA in a wooden crate, mimicking the typical storage conditions of piece of arts in both museums and storage facilities, and resulted in the decrease of AA below 250 ppbv already after the first week of usage, far below the 400 ppbv typically suggested for the preventive conservation of Cultural Heritage objects in museums and display cases. Having established a new class of materials able to absorb efficiently AA, our current focus is on the in-depth characterization of the process of diffusion and adsorption through the composite material, as well as the test of additional inorganic adsorbers in order to further extend the range of applicability.

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2A – EU HORIZON EUROPE Project "Bio-based sustainable SURFactants TO foster GREEN industry" - SurfToGreen (ID 101157688). 1/10/2024-30/09/2029

C. Adamo, P. Baglioni, R. Camerini, D. Chelazzi, G. Poggi
(University of Florence and CSGI, Italy)

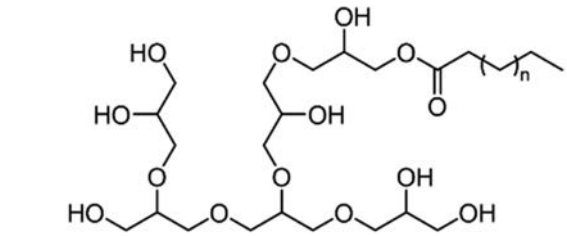
Aims

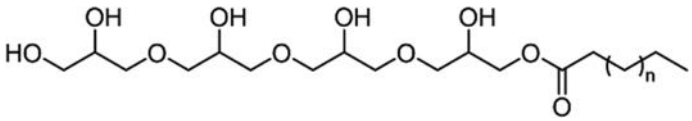
Formulations in industrial applications primarily rely on fossil-based surfactants/polymers significantly contributing to environmental pollution (CO_2 increase, microplastics) and are scarcely sustainable. The EU Green Deal demands for new chemistries based on sustainable and natural compounds. Effective bio-based surfactants are poorly integrated in industry and in their infancy in research. SurfToGreen will fill this gap with a completely new surfactants platform covering diverse industrial applications to replace current surfactant benchmarks. SurfToGreen gathers a unique partnership of major industrial actors and excellence research centers, with the advanced knowledge on soft matter and industrial processes fundamental to achieve this challenging goal.

Results

Biomass derived building blocks are being obtained from EU territorial value chains, including forests and agriculture waste/side streams to diversify biomass origin, and used to synthesize novel biobased surfactants. The new products will cover anionic, nonionic, cationic, zwitterionic surfactant families, and biopolymers-oligomers from renewable sources with no impact on the food chain. The platform will be validated in industrial demonstrators among the most fast-growing crucial sectors, e.g. home/personal care and textile. The compounds' surface properties are being assessed against detergency, interfacial, and rheological behaviour. Polymers/oligomers, hydrotropes and surfactants will be used for encapsulation to protect and control the delivery of actives (perfumes, and compounds for plant protection). Digital technologies and safe-and-sustainable by design methodologies will assess the functionality, safety, and sustainability of the biobased formulations within a circular value chain framework. Finally, extensive exploitation and communication will be carried out to promote the SurfToGreen advancements as a pilot to drive a paradigm shift in EU and global industry.

Figure below shows fatty acid ester of oligomeric glycerol. For the surfactant used in the food industry the value of n is typically around 3 but the oligoglycerol chain has a broad homologue distribution. The polyglycerol moiety can exhibit different degrees of branching [1].





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2A – EU HORIZON EUROPE Project "GREen ENdeavor in Art ResToration" - GREENART (ID 101060941). 1/10/2022-30/09/2025

P. Baglioni, A. Casini, D. Chelazzi, S. Lob, G. Poggi, V. Rosciardi
(University of Florence and CSGI, Italy)

Aims

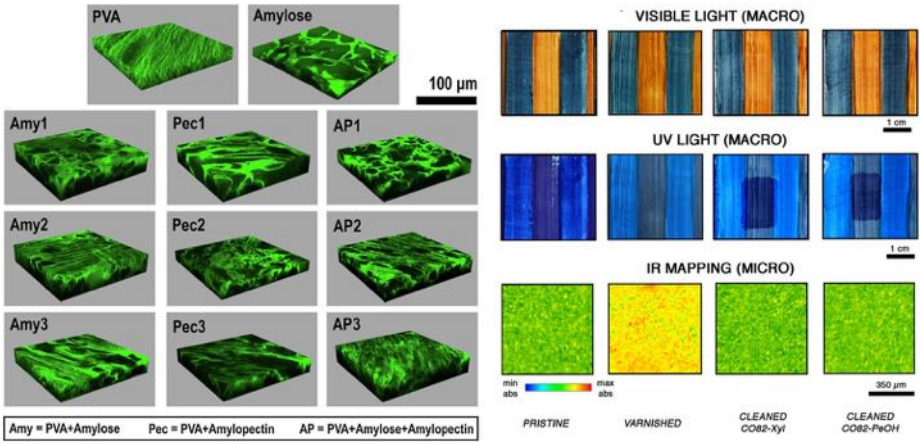
European Cultural Heritage (CH) is a crucial resource that must be maintained, preserved and accessible, to counteract degradation enhanced by unfavorable environmental conditions and climate changes. Conservation methodologies lack durability, sustainability and cost-effectiveness, and are typically based on energy-consuming processes or non-environmentally friendly materials. Coping with these issues, GREENART proposes new solutions based on green and sustainable materials and methods, to preserve, conserve and restore CH, spanning from gels, coatings, nanoparticles, sensors, all developed through a Safe and Sustainable by Design approach, and validated on actual masterpieces. Such holistic approach is granted in GREENART by a multidisciplinary partnership that gathers hard and soft sciences and engineering, including academic centers, innovative industries and SMEs, conservation institutions and professionals, museums whose collections hold absolute masterpieces in need of conservation, public entities and policy makers. The latter has favored extensive training and dissemination activities to make stakeholders familiar with the new methods.

Results

The following classes of advanced materials were produced: 1) Protective coatings based on green materials from waste and plant proteins, with self-healing and reversibility character, functionalized with organic/inorganic nanoparticles to impart VOC capture, anti-corrosion and barrier behaviors. 2) Foams and packaging materials made by biodegradable/compostable polymers from renewable sources (polyurethanes and natural fibers) to control T/RH. 3) Consolidants based on natural polymers from renewable sources, to mechanically strengthen weak artifacts. 4) Gels and cleaning fluids inspired by the most advanced systems currently available to conservators, improving them according to green and circular economy. 5) Green tech solutions for monitoring CH assets non-invasively against pollutants and environmental oscillations.

Life cycle Assessment and modeling has favored the “safe-by-design” creation of affordable solutions safe to craftspeople, operators and the environment, and minimize energy-consumption in monitoring museum environments. Extensive training to professionals worldwide and industrial cooperations completed the achieved results.

Examples are shown below, illustrating respectively: “green” gels of polyvinyl alcohol and starch components (left); painted layers where aged varnishes were removed using castor oil-based organogels (right) (from Chelazzi, D., Poggi, G., Baglioni, P. Studies in Conservation, 2024, 69(sup1), 25–34).



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2A – Fibroin and nanocellulose composite films as new adhesives for aged textiles

C. Adamo, D. Chelazzi, G. Poggi, R. Giorgi, M. Laurati

Aims

While historical and aged textiles (canvas, silk) constitute a relevant portion of our Cultural Heritage, there is a lack of physico-chemically compatible solutions to provide re-adhesion to the damaged fibers at the micro-scale without introducing potentially harmful adhesives such as those based on synthetic polymers.

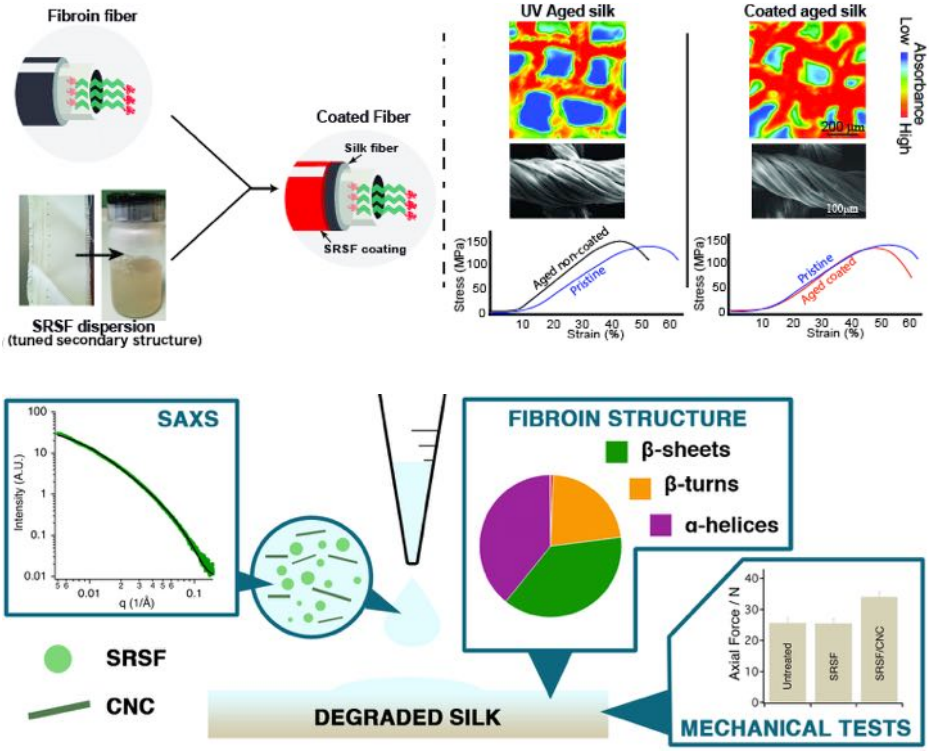
Colloidal systems and advanced functional materials based on biopolymers are optimal candidates to fill this gap. We recently investigated composite dispersions of self-regenerated silk fibroin (SRSF) or SRF and cellulose nanocrystals (CNC), to cast adhesive films able to recover the mechanical properties of aged silk fibers. Recently, we have tested some additives to hamper the self-assembly of fibroin with the aim of increasing the gelation time of fibroin dispersions.

Results

SRSF produce films with controlled crystalline/amorphous content depending on the protein concentration in the dispersion; however, there is a limit to the concentration for the sole SRSF dispersions, as crystalline SRSF phases (with scarce chain mobility) cast over aged silk fibers produce brittle films that worsen the fibers' mechanical behavior. Amorphous SRSF films instead improve the flexibility of the aged textiles. Adding CNC to the dispersions speeds up the assembly of SRSF likely thanks to protein organization on the cellulose fibers, and composite films with partially crystalline fibroin (high α-helices content) can be cast even at low fibroin concentration. Noticeably, the composite films produce better improvement than the sole SRSF amorphous films or CNC films obtained from dispersions with the same concentration of consolidant.

The hybrid SRSF-CNC dispersions candidate thus as new promising adhesives for aged silk (and canvas) textiles; in addition, we provided for the first time a semi-quantitative evaluation of the structuring effect of CNC on SRSF assemblies, which can help the development of "green" chemistry solutions in different fields even beyond Cultural Heritage preservation, such as biomaterials and tissue engineering, and the preparation of composites with enhanced properties.

Regardless the composition, the self-assembly of fibroin, which leads to the gelation of systems, must be avoided or controlled, with the aim of improving the shelf life of dispersions that are designed to be applied at the liquid state. In the framework of the European project GREENART, we have studied the effect of a protein, i.e., sericin, which is produced by silkworms in the production of silk and removed during fibroin extraction, and an amino acid, L-arginine, present in both fibroin and sericin, for hampering the self-assembly of fibroin, also in presence of CNC.



Gelation times are significantly increased with increasing amount of both additives, together with a reduction of the formation of crystalline structures in dried films. Nonetheless, the consolidating effects of hybrid dispersions featuring sericin or arginine as stabilizing agents is retained, allowing for the application on aged and historical silk artifacts, such as a Japanese kimono belonging to the MET (Metropolitan Museum of Art) in New York.

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2A – "Green" Poly(vinyl alcohol)/Starch based cryogels for the cleaning of works of art: application, characterization and investigation of the Amylose/Amylopectin structural role

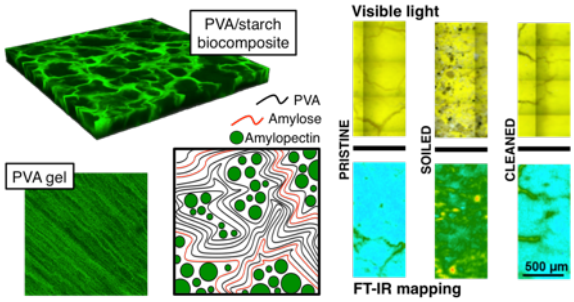
V. Rosciardi, D. Chelazzi, P. Baglioni

Aims

Gels made from synthetic polymers have improved the cleaning of artifacts, but there is the strong need to elaborate new systems through an all-green approach, developing materials with higher eco-compatibility while retaining optimal efficacy. In this perspective, we have developed and studied different biocomposite hydrogels based on poly(vinyl alcohol) (PVA) and rice starch (RS) obtained via freeze-thawing, with water as the only used solvent. Rice starch (RS) is a renewable biopolymer with a high potential for formulating sustainable gels from composites with synthetic polymers, but its interaction with the latter in composite structures is poorly understood.

Results

We characterized the effects of the freeze-thawing process on the gelation of PVA and native starch blends, tuning the starch content from 33 to 66% (w/w), and studying the gels' structure and structure-related properties. The obtained hydrogels showed a highly porous organization due to phase separation events occurring as a consequence of mixing different polymers in solution (i.e. PVA and starch's polymeric components, amylose and amylopectin). Such spongy porous arrangements have been previously reported to be key for dirt removal from painted surfaces and our systems have indeed proved effective when applied on artificially soiled painted mock-ups. Therefore, not only does the partial substitution of PVA with starch diminish the use of the synthetic polymer, with a straightforward advantage in terms of eco-sustainability, but mixing the different components together leads to the formation of a structure that promotes the hydrogels' cleaning effectiveness. The features of the synthesized PVA/starch hydrogels resulted to be broadly tunable in terms of viscoelastic behavior and water release, controllable by simply varying the PVA:starch mixing ratio. Nevertheless, all the considered formulations resulted in the formation of strong gels (i.e., chemical-like gels), despite the predominantly physical nature of the preparation method. As much as a good porosity ensures an efficient cleaning, a good cohesion of the gel grants a safe and residue-free application. Both the aspects have been confirmed through the application of two chosen hydrogels on two different artificially soiled painted surfaces: a poorly bound and water-sensitive tempera, and a highly irregular rough alkyd painting. The excellent outcome of the cleaning operations was assessed by means of micro-FTIR imaging, which also revealed the total absence of any gel residues.



Remarkably, the PVA/starch gels have proven to be as effective as their state-of-the-art commercially available synthetic counterparts, confirming the possibility to formulate greener products for the conservation of Cultural Heritage without compromises in terms of performances and safety. Indeed, these gels are among those assessed as new green gel systems in the HORIZON EUROPE GREENART (GREen ENdeavor in Art ResToration, https://cordis.europa.eu/project/id/101060941/it). In addition, given their biocompatibility and environmentally friendly character, these systems are easily transferable to transversal fields where "green" and biocompatible confining networks are needed, such as drug delivery, tissue engineering, topical treatments, cosmetics, and many others. However, to be able to finely tune the features of the PVA/starch systems in order to formulate materials that can respond to different applicative needs, a deeper insight into their formation mechanism is necessary. Starch contains two different polymers (amylose and amylopectin), and their behavior in solutions with PVA is still largely unexplored. To investigate the interaction at play between PVA and starch components, as well as their implications on determining the final features of biocomposite PVA/starch networks, we decomposed the real system in its simple components. Investigation on PVA/amylose, PVA/amylopectin, and PVA/amylose/amylopectin systems with variable PVA/polysaccharide ratios allowed a deeper understanding of the possible evolution of a real PVA/starch cryogel. Thanks to CLSM imaging of pre-gel solutions containing fluorescently labeled polymers, we determined the absence of miscibility between PVA and amylose, as well as PVA and amylopectin, in the considered temperature range (25-98°C). Comparing the morphology of PVA/amylopectin solutions and cryogels, the porogen role of amylopectin arises, suggesting that also in PVA/starch networks the observed spongy organization is ascribable to phase separation events specifically regarding amylopectin, rather than amylose. These observations are particularly relevant since they partially clarify the specific contribution of amylose and amylopectin in PVA/starch systems and can therefore help tuning the final properties of these gels.

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2A – Hybrid nanomaterials for the strengthening and deacidification of paper and canvases

G. Poggi, D. Bandelli, R. Giorgi, P. Baglioni

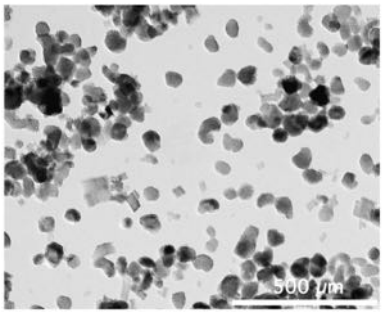
Aims

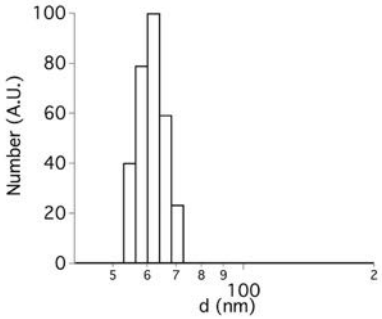
The acid-catalyzed hydrolysis of glycosidic bonds, that is the most important degradation pathway of paper and canvases, results in the decrease of cellulose DP and in the loss of the original mechanical properties. In the case of acidic and strongly mechanically-degraded artifacts, both a deacidification and a consolidation treatment are required.

Results

In the framework of the EU project NANORESTART, we have started working on the development of hybrid systems for the concomitant neutralization of acidity and the improvement of the mechanical resistance of cellulose-based materials. The advantages related to the use of a single-step treatment rely in the reduction of cost, treatment time, stress and risk for the artifact.

For what concerns paper, hybrid systems feature cellulose nanocrystals (CNCs) and alkaline nanoparticles, alternatively calcium hydroxide or calcium carbonate, both obtained via a solvothermal process. The innovative synthetic route of $CaCO_3$ nanoparticles, which is based on the usage of an alkyl carbonate for the conversion of the intermediate reaction products into carbonates, yielded small and highly crystalline nanoparticles already dispersed in an appropriate solvent for applicative purposes.





An improvement on the use of standard CNC was recently obtained by a surface modification of the nanocrystals using oleic acid, to favor the dispersion of CNC in pure ethanol. Modified CNC have been mixed with alkaline nanoparticles to have a blended system to be used for the consolidation of highly water-sensitive paper artworks. Nowadays, experiments are devoted to the synthesis of CNC modified with different carboxylic acid, with the aim of tuning the dispersibility of CNC in short-chain alcohols. For what concerns canvases, one of the most interesting strategy we designed is based on the use of calcium carbonate nanoparticles dispersed in water/ethanol mixtures.

The nanoparticles are intended to neutralize acidity. To stably disperse calcium carbonate nanoparticles in water/ethanol, we use a positively charged polyelectrolyte (PE), i.e. Polyethylenimine (PEI). A cellulose derivative, namely carboxyl methyl cellulose (CMC) is added to the system to induce a strengthening effect of nanocomposite on canvases. When the negatively-charged CMC is added, the presence of PE, prevents the flocculation and probably favors the interactions between nanoparticles and cellulose derivatives. All the systems are composed of small particles, whose size is around 200-300 nm (measured by DLS, analyzed using the cumulant fitting). The pH of systems is alkaline, as required by a deacidification treatment.

Ethanol can be added to the system featuring calcium carbonate nanoparticles and PEI up to a concentration of about 65%. It is worth noting that the addition of ethanol to the systems could ease their penetration inside canvas. On the contrary, CMC based systems are not stable after ethanol addition but could be diluted with water.

During preliminary tests, these systems were tested on two different types of aged cotton canvases: all the tested treatments increase the mechanical resistance of threads, up to 30%. It is also worth noting that all the treatments increased the pH of about 3 units, stabilizing the pH at about 7-8.

On the basis of these experimental tests, some of the most promising systems were tested on iron-tannate dyed cotton, also in combination with nanocellulose and other strengthening agents, such as silica nanoparticles. We show that conservation can only be addressed if the mechanical strengthening is preceded by a deacidification step. We used $CaCO_3$ nanoparticles to neutralize the acidity, while the stabilization was addressed by a combination of nanocellulose, and silica nanoparticles, to truly tackle the complexity of the hierarchical nature of cotton textiles. Silica nanoparticles enabled strengthening at the fiber scale by covering the fiber surface, while the nanocellulose acted at bigger length scales. The evaluation of the applied treatments, before and after an accelerated ageing, demonstrated the potential of using a combined deacidification-strengthening approach in the stabilization of degraded fibrous cellulosic materials.

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2A – Hybrid nanostructured systems for the consolidation and biocidal protection of outdoor cement-based artworks

R. Giorgi, R. Camerini, E. Gualini, S. Morrocchesi

Aims

This research focuses on the development of a hybrid nanostructured system conceived for the conservation of outdoor cement-based artworks, highly susceptible to weathering and biological degradation. The formulation combines silica and calcium hydroxide nanoparticles. To enhance this system, halloysite nanotubes are incorporated as carriers for a controlled and sustained release of a commercial biocidal agent, Biotin T. This dual-function approach intends to provide both mechanical stabilization and prolonged protection against biological colonization.

Results

This research originates from previous activity focused on the development of consolidants for silicate-based building materials also combined with nanocarriers. In this case, a ternary system based on halloysite nanotubes (HNTs) loaded with Biotin T (11.75% loading), hydroxypropyl cellulose (HPC), and nanolime was investigated following its application on microscope slides and cement-based mock-ups reproducing the characteristics of the real case study. Analytical investigations using FT-IR ATR and micro-Raman spectroscopy were carried out to identify the chemical phases formed within the films and to confirm the presence of the biocide within the applied coatings. To evaluate the effective biocide incorporation within the halloysite nanotubes, multiple characterization techniques were employed, including FT-IR spectroscopy, UV-Vis spectrometer analysis, gas-porosimetry, and thermogravimetric analysis. Mock-ups replicating the cementitious matrices of monuments have been prepared to test the efficacy of the treatment in terms of both consolidation and long-term biocidal activity.

Release tests were also performed to assess the diffusion of Biotin T from the ternary film into water. The presence of the active compounds in the release medium was confirmed by UV–Vis spectrophotometry, validating the system's controlled-release capability.

The investigated case studies include Burri's Cretto in Sicily, where extensive red-coloured biological patinas have compromised the visual aspect of the monument, and Sol LeWitt's "Cubo senza cubo" from the Gori Collection at Fattoria di Celle in Pistoia, whose aesthetic appearance has been similarly altered by biological growth.

A detached block from Cubo senza Cubo by Sol LeWitt was examined in collaboration with the Opificio delle Pietre Dure (OPD) and the Istituto di Scienze del Patrimonio Culturale (CNR–ISPC). Cleaning tests, accompanied by ATP measurements, demonstrated that Biotin T was the most effective biocide for the removal of biofilm. After biofilm removal, the block surface was divided into three zones: one treated with the ternary system loaded with Biotin T, one treated with the same ternary matrix but with unloaded HNTs, and one left untreated as a reference. The consolidation process

of the ternary system is currently ongoing. Once completed, hyperspectral and colorimetric measurements will be repeated, followed by inoculation with the microbial species previously identified on the block before cleaning. The sample will then be repositioned in situ to assess the long-term protective and biocidal effectiveness of the treatment under real environmental conditions.

Sol Lewitt, Cubo senza Cubo, 1988; Collezione Gori, Fattoria di Celle, Pistoia (Italy),

This innovative system represents a promising approach to enhance the durability and preservation of outdoor cement-based monuments by combining the benefits of nanostructured consolidation with sustained biocidal protection tailored to specific conservation challenges.

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2A – Hydrogel beads loaded with glucosinolates-rich Brassicaceae extracts as controlled-release alternative to biofumigation

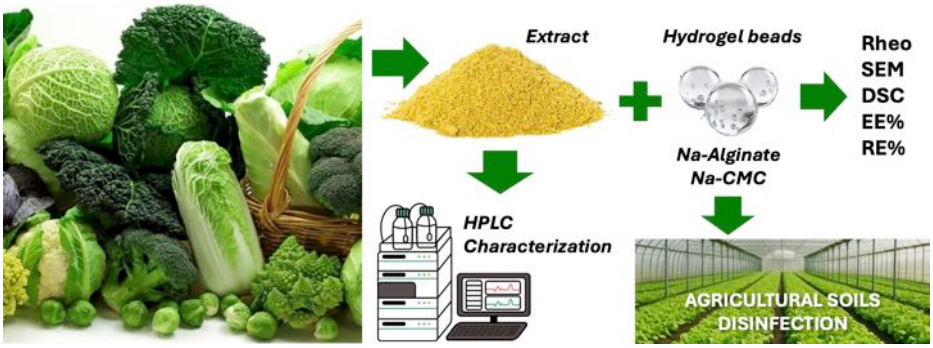
M. Baglioni, I. Clemente, R. Nardin, F. Bisozzi, S. Costantini, G. Fattori, G. Tamasi, C. Rossi

Aims

A renown and viable alternative to the use of chemical fumigants was the introduction of biofumigation [1], a method where fresh plants (mostly Brassicaceae) are cultivated, mown, and mixed into agricultural soils, due to their biocidal properties towards soilborne pathogens. Brassicaceae are characterized by a high content of glucosinolates, i.e. secondary metabolites produced by plants for defensive purposes, which can be hydrolyzed to isothiocyanates (ITCs) by the myrosinase enzyme. However, also biofumigation is affected by some limitations. It is a time-consuming practice, since fields need to be firstly cultivated with the plants that are later used as green manure. Then, the amount of glucosinolates/myrosinase delivered to the soil is hardly controllable, and this is reflected in the not-negligible frequency of ineffective outcomes of this agricultural practice. An advanced and viable alternative is represented by the use of controlled-release systems [2,3], i.e., porous carriers, mesoporous particles, or gelled polymer networks. In the present work we explore the use of biocompatible hydrogels, based on sodium alginate and sodium carboxymethylcellulose, conveniently loaded with Brassicaceae extracts for this purpose.

Results

The potential of Ca2+/alginate- (ALG) and Fe3+/carboxymethyl cellulose (CMC)-based hydrogel beads as a vehicle for the controlled-release of glucosinolates in agricultural soils was explored [4], with the aim of searching for improved and innovative treatments inspired by biofumigation.



A commercial Brassica oleracea extract was firstly characterized by means of HPLC-MS-DAD analyses and it was shown that total glucosinolates' content was around 28% m/m, with glucoraphanin being the most abundant one, while a 12% m/m of sinapine

was also determined, which can contribute to biocidal properties of the product. The extract was then loaded (exploring the 1-5% concentration range – this value representing the initial extract's concentration in the pre-crosslinking polymeric solution) into hydrogel beads, which were physico-chemically characterized by means of DSC, rheometry, and SEM, while encapsulation efficiency (EE%) and release efficiency (RE%) in water were investigated through HPLC-DAD analyses. ALG and CMC hydrogels share an equilibrium water content (EWC) of 93% and a high free water index (FWI), which has an opposite trend in the presence of increasing extract's concentration for the two polymeric networks. While FWI increases for ALG systems, indicating that glucosinolates likely replace water molecules in the interaction with alginate chains, it drops for CMC systems, possibly due to the formation of hydrated Fe3+/glucosinolates complexes. Rheological measurements confirmed what hypothesized looking at G' and G'', which show that CMC hydrogels possess higher mechanical properties than ALG. A slight difference between the two polymer networks was also observed relatively to the EE%, which resulted larger for CMC-based hydrogels. This can be due to a combination of factors, including the inner structure and the surface-to-volume (S/V) ratio of the beads. Indeed, SEM micrographs of CMC hydrogels show thicker and more robust gel's walls, which could better confine the active principles inside the bead. On the other hand, the lower viscosity of the alginate polymer solution is reflected in smaller hydrogel beads, which have a higher S/V ratio, accounting for a favored glucosinolates' migration from the gel to the surrounding aqueous environment. The RE% (measured in water), accordingly, is higher for ALG hydrogels, even if the release profiles, fitted using the Weibull model function, show a gradual and slow release for both systems, which tend to reach an asymptotic value after almost 3 hours of hydrogels immersion in water. This would grant a prolonged and controlled disinfection treatment for agricultural soils.

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2A – Isothiocyanate-Based Microemulsions Loaded into Biocompatible Hydrogels as Innovative Biofumigants for Agricultural Soils

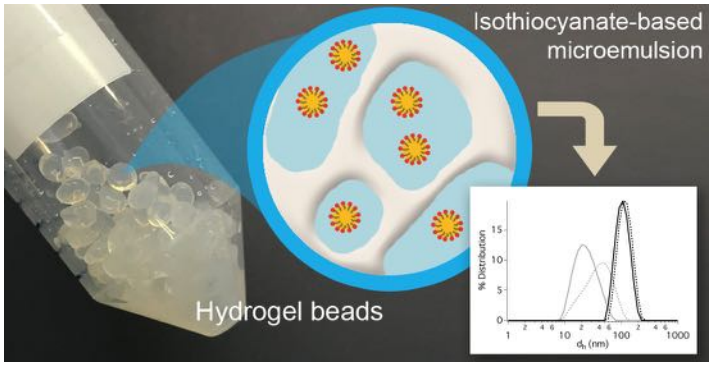
M. Baglioni, I. Clemente, G. Tamasi, F. Bisozzi, S. Costantini, G. Fattori, C. Rossi

Aims

Agricultural practices play a major role in ensuring global food availability and the need to boost crop productivity often involves the use of a number of chemicals, among which synthetic pesticides represent a serious concern, due to their detrimental impact on both human health and the environment. These chemicals, designed to combat pests and diseases, pose risks beyond their intended targets, contaminating soil, water, and food supplies. Biofumigation was proposed as an alternative to synthetic pesticides for the disinfection of agri-cultural soils, in view of the biocidal effect of isothiocyanates (ITCs) released by some vegetal species, like Brassicaceae. However, biofumigation also presents limitations. As a viable alternative to biofumigation, the possibility of building ITCs-based microemulsions was explored by studying the phase diagrams of nine different systems that combined three surfactants (SDS, Brij 35, and Tween 80), and three ITCs (Et-ITC, Ph-ITC, Al-ITC).

Results

The optimal formulation was found to be water, 85%; Tween 80, 9.4%; and Et-ITC, 5.6%, as it proved to be a stable microemulsion characterized by a good ITC/surfactant ratio. This microemulsion was characterized by means of DLS, which showed that micelles evolved from an average size of 34 nm to 100 nm while reaching their thermodynamic equilibrium. Then, the same microemulsion was loaded into presynthesized hydrogel beads made of ALG or CMC crosslinked by means, respectively, of Ca2+ or Fe3+ ions.



The loading efficiency and kinetics were studied via a spectrophotometric analysis, and it was found that both gels can be efficiently and quickly loaded with the microemulsion just by simple immersion of the gels in the nanofluid, in view of the

gels' large and interconnected pores, also evidenced by SEM micrographs, and due to particularly favored interactions between the polysaccharides polymers (ALG and CMC) and PEO chains of Tween 80, further confirmed by ATR-FTIR measurements. In more detail, CMC-based hydrogel beads can be loaded faster and with a higher LE%. It was then shown that loading the ITC-based microemulsion does not significantly affect the structure and properties of hydrogel beads, which maintain the same equilibrium water content (EWC) and free-water index (FWI). Finally, CMC hydrogel beads also showed a slightly more efficient profile of micelles' release in water. For this reason and due to the enhanced contributions of Fe(III) to the biocidal properties of the microemulsion-loaded gel beads, the CMC-based system seems to be the more promising for further testing. These will include comprehensive and systematic microbiological experiments, both in vitro and in situ, in agricultural soils, to assess the effectiveness of the developed systems on different pathogens for plants. Nevertheless, this work lays a solid basis for the development of hydrogel-mediated controlled release of microemulsions based on ITCs, which can find their main application in the advanced fumigation of agricultural soils, but also possess the potential to be candidates for use in other fields, from cultural heritage conservation to food science and nutraceutics, or biomedicine.

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2A – Jin Shofu Starch Nanoparticles for the Consolidation of Modern Paintings and Graphic arts

A. Casini, D. Chelazzi, R. Giorgi

Aims

Modern paintings and graphic documents frequently undergo severe degradation processes driven by both endogenous and exogenous factors, which promote chemical alteration and a consequent loss of mechanical integrity. In many cases, such degradation is further exacerbated by inappropriate conservation treatments carried out in the past. The preservation of these objects therefore represents a major challenge, demanding the continuous development of innovative conservation strategies that must simultaneously satisfy multiple constraints, including environmental sustainability, chemical compatibility with original materials, long-term stability, and cost-effectiveness. The consolidation of graphic media is among the most critical issues faced by conservators. Weakly bound dyes and inks, commonly encountered in works on paper and modern graphic art, pose particularly complex conservation problems. Conventional consolidation methods typically rely on natural or synthetic polymeric adhesives, which are often unsatisfactory due to their tendency to alter the optical properties of the treated surfaces. In this context, nanostructured starch-based systems have recently emerged as promising alternatives. In particular, a bottom-up approach was followed to obtain a gluten-removed Jin Shofu wheat starch that was gelatinized and then precipitated in a non-solvent to obtain a stable dispersion to be used by nebulization.

Results

Starch nanoparticles (SNPs) were obtained to boost their penetration into the porous painted layers; upon solvent evaporation, the particles were expected to adhere to the pigments thanks to their large surface area and abundant -OH groups. The SNPs were formulated through a bottom-up approach, where gluten-removed Jin Shofu wheat starch was gelatinized and then precipitated in a non-solvent. The low gelatinization temperature of wheat starch is likely key to favor disassembly in alkali and re-assembly in the non-solvent. The synthesis conditions can be tuned to obtain amorphous SNPs of ca. 50 nm with acceptable polydispersity. The particles swell in water to form nano-sized gel-like fractal domains (as observed with Cryogenic Electron Microscopy), formed by the organization of smaller units in polymer-rich and deficient regions. SNPs significantly strengthen weak, poorly bound paints. Consolidation efficacy was assessed using an in-house methodology for fragile painted surfaces. Pigment loss was evaluated semi-quantitatively via standardized micro-sampling, microphotography, and FTIR 2D imaging. Results showed minimal pigment removal in consolidated samples, compared to substantial loss in untreated layers. Both aqueous and hydroalcoholic dispersions were tested on artificially aged ultramarine blue mock-ups simulating degraded modern paints. A successful real-case application was carried out within a research collaboration with the Opificio delle Pietre Dure (OPD), focusing

on the re-cohesion of the paint layer on paper in Vase with Flowers by Edoardo Marchionni. The original painting technique was reproduced in the laboratory, and the SNPs formulation was applied to highly fragile paint layers. These samples were then subjected to mechanical testing, including the polyurethane sponge method and peeling tests. The experimental results indicate a marked enhancement in paint layer stability, thereby supporting the feasibility of SNPs application on the original artwork. In conclusion, the synthesis and application of Jin Shofu starch nanoparticles represent a significant advancement in the conservation of fragile painted surfaces, providing a chemically compatible, effective, and environmentally benign consolidant for modern paintings and graphic artworks, for which reliable and safe solutions are still critically needed.

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2A – Nanofluids and chemical hydrogels for the selective removal of overpaints and graffiti from murals

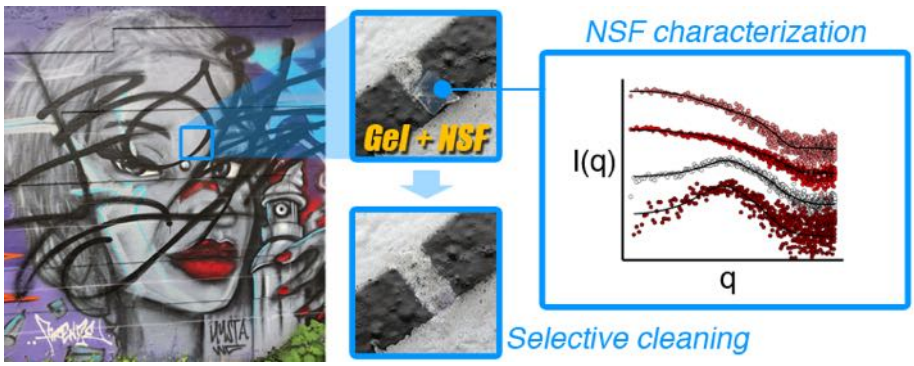
C. Suraci, R. Giorgi, M. Baglioni, G. Poggi, P. Baglioni

Aims

Graffiti removal from monuments, such as statues or architecture, is becoming a priority for conservators and restorers. This operation is further complicated when the vandalism is carried out on surfaces that should be preserved, as in the case of writings or tags on historical wall paintings, or even on modern or contemporary pieces of street art. The needed selectivity can then be achieved using nanostructured fluids loaded into highly retentive hydrogels.

Results

The removal of graffiti from paintings that must be preserved is a particularly challenging and relatively new issue in conservation of cultural heritage. This is the case of contemporary street art (by unconventional contemporary artists, such as Banksy or Blu) jeopardized by tags, signs and writings. In these conditions, the cleaning action must be extremely selective, as the binder of the undesired paint is likely to have a very similar chemical nature to the one of the underlying original painting.



Unfortunately, selective and controlled removal of graffiti and overpaints from Street Art is almost unachievable using traditional methodologies. To this aim, starting from the Horizon 2020 EU-funded project NANORESTART, the use of nanostructured fluids (NSFs), such as micelles and microemulsions, especially confined into highly retentive chemical hydrogels, was proposed as one of the most promising, selective and controllable cleaning systems for the removal of graffiti and overpaints from street art.

Semi-interpenetrated polymer networks (sIPNs) composed by a tridimensional network of poly(hydroxyehtyl methacrylate)/N,N'-Methylene bisacrylamide (pHEMA/MBA) or polyvinylalcohol (PVA), interpenetrated by a high molecular weight poly(vinyl pyrrolidone) (PVP), or poly(vinyl alcohol)-based twin-chain polymer

networks (TC-PNs), obtained as the result of freeze-thaw cycles, can be used as highly retentive hydrogels. These gels were shown to be particularly suited to limit the cleaning action to the surface layers of the treated area. It was recently shown that this methodological approach is effective for the selective removal of a set of modern paints, based on vinyl, acrylic and alkyd binders, laid on similar or the same paints. In particular, excellent cleaning results were obtained for the vinyl-on-vinyl and acrylic-on-acrylic samples, while alkyd-on-alkyd specimens were partly resistant to the removal. This represents a substantial improvement over previous formulations used for the same purpose, and a major advancement with respect to the existing methodologies available to conservators. FTIR measurements on the treated areas confirmed that the overlying paint was completely removed without altering the paint layer underneath. Finally, the proposed methodology and cleaning system were assessed in the selective removal of black tags from real pieces of street art, with excellent results.

More recently, to address this specific problem, research efforts have been dedicated to the use of linalool, which is the main compound in Lavandula essential oil, and other components of essential oil blends for the formulation of O/W nanostructured fluids. The aim of this research is to developed more sustainable and eco-friendly cleaning fluids, taking advantage of natural products having a limited impact on the safety of the operator and on the environment.

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2A – Nanostructured fluids for the conservation of cultural heritage – Understanding the mechanism of organic coatings removal

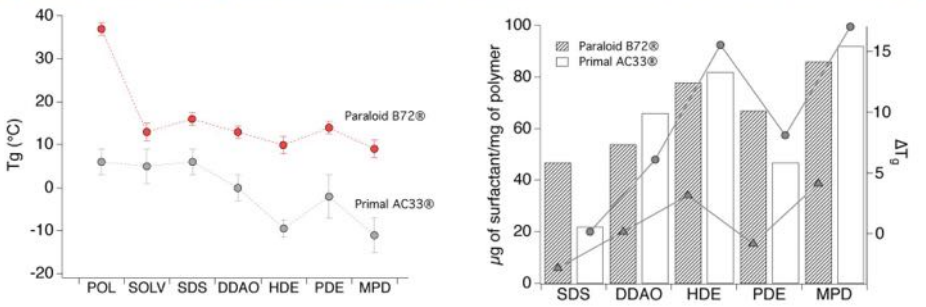
M. Baglioni, D. Berti, C. Montis, T. Guaragnone, M. Raudino, M. Bonini, R. Mastrangelo, D. Chelazzi, R. Giorgi, P. Baglioni

Aims

Understanding the mechanism of interaction between polymer coatings and nanostructured fluids (NSFs) will contribute to improve cleaning formulations in the field of conservation of cultural heritage, and, besides having some scientific relevance from fundamentals standpoint, it may open new perspectives on different applicative fields.

Results

Since the early 1990s, the moment of the very first application of NSFs to art conservation, their effectiveness in removing polymeric coatings from different surfaces was thoroughly demonstrated. Therefore, a major effort has lately been spent in order to investigate the mechanism of polymer removal through which these systems work.



Confocal laser scanning microscopy (CLSM) imaging was combined with differential scanning calorimetry (DSC), fluorescence correlation spectroscopy (FCS), SAXS, SANS, contact angle and surface tension measurements, in order to understand the role of each NSF component in the fluid/polymeric coating interaction. We found that this interaction usually involves dewetting processes, especially in the case of films formed from solvent solutions. Films formed from polymer latexes, on the other hand, are generally swollen even just by water, but they tend not to dewet, due to the presence of a significant amount of amphiphilic additives, which alter their interfacial behavior. It was shown that the nature of solvents in the NSFs plays a major role in the dewetting of polymer coatings, i.e., good solvents for the polymer are needed in order to swell the film and induce the mobility of polymer chains.

On the other hand, surfactant nature is crucial to kinetically favor this process. Surfactants, lowering both the liquid/polymer and liquid/solid interfacial tensions, energetically favor the detachment of the film from the surface, which represents the first step of dewetting processes. Therefore, amphiphile-based systems having very

low surface tension may be particularly effective in dewetting polymer films. Then, by means of FCS measurements, it was found that: i) the surfactant present in the NSFs is able to penetrate through the polymer film, that acts as a sort of "sieve" with respect to micelles' size, and reach the polymer/solid surface interface, where liquid-filled cavities are formed, where micelles are present; ii) during the penetration in the polymer film, part of the micelles is disrupted, with a release of surfactant molecules that promote polymer swelling and softening and further increase polymer chain mobility. Most recently, surfactants were shown to also act synergistically together with organic solvents in lowering the glass transition temperature of polymers below room temperature, which is the prerequisite to increase polymer chains' mobility, which is needed to kinetically undergo dewetting, even if thermodynamically favored. It was demonstrated that nonionic surfactants are more efficient than zwitterionic/ionic ones in the polymer swelling, and, overall, alkyl ester ethoxylates resulted the most effective among the investigated surfactants. Finally, the results of FTIR imaging on Paraloid B72®-coated mortar tiles provided an explanation for the observed effectiveness of NSFs in real case studies, highlighting the mechanism through which they act and remove aged polymer coatings (cast from solutions).
Recent updates involve the use of bio-derived nonionic surfactants in water-based nanofluids with "green" solvents, investigating the effect of the surfactant's structure on the dewetting of synthetic organic coatings. These developments were carried out in the HORIZON EUROPE GREENART project (GREen ENdeavor in Art ResToration, https://cordis.europa.eu/project/id/101060941/it).

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2A – Nanostructured hybrid composites for the consolidation and protection of street art

C. Cianci, E. Gualini, S. Morrocchesi, G. Poggi, R. Giorgi

Aims

This research focuses on the formulation of nanostructured hybrid composed of a macromolecular component, chitosan, and an inorganic component, silica, aimed at overcoming limitations of traditional protective materials used in conservation [1]. Chitosan (Chs) was selected as the organic component due to its good film-forming, optical, and antimicrobial properties [2], as well as for its sustainability and non-toxicity. The incorporation of silica into the Chs matrix contributes to improving the compatibility and adhesion of the coating towards mineral substrates. The durability of the hybrid system under outdoor aging conditions was also evaluated. The goal is to develop an eco-friendly, compatible coating that preserves the visual appearance of street murals.

Results

The hybrid formulation was characterized using ATR-FTIR spectroscopy, SEM, DLS, and zeta potential measurements. Applied to spray-painted concrete mock-ups, the coating underwent accelerated artificial aging tests to assess its performance in terms of durability, colour stability, water vapour permeability, hydrophobicity, and adhesion.

To assess coating stability of the coatings, colorimetric measurements were carried out on the mockups every 10 days. Compared to untreated mockups, the coated ones showed a lower ΔE value, indicating a higher stability and a protective action.

The treatment effect on the breathability and hydrophobicity of the mockups was also evaluated. The application of spray paint significantly reduces the breathability of the cement-based substrate; however, the subsequent application of the protective coatings does not cause further reductions, nor does it significantly affect capillary water absorption. In conclusion, experiments demonstrated that the coating provides effective protection while preserving the breathability and visual integrity of the artwork.

In addition, the project includes the results of a two-year monitoring campaign of a large-scale mural painted by Skim in 2023 on an ETICS (External Thermal Insulation Composite System) wall in Sesto Fiorentino, Italy. The conservation state of 26 different colors, systematically mapped across the mural surface, was periodically evaluated using colorimetric and gloss measurements, which revealed specific degradation phenomena. Selected spray paints used by the artist were chemically characterized, and their deterioration was further investigated through both molecular-level analysis and accelerated artificial ageing protocols.


May 2023


January 2025


Original spray-paints

These protocols combined photochemical stress with controlled fluctuations in temperature and relative humidity, applied to ETICS mock-ups painted with the same materials used in the mural. A comparative analysis between the naturally aged mural and the artificially aged samples is presented and discussed, offering valuable insights for the development of targeted-conservation strategies.

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2A – Peelable polyvinyl alcohol highly viscoelastic dispersions loaded with nanostructured fluids: a new class of cleaning tools for works of art

E. Carretti, F. Porpora, S. Baldini, L. Dei

Aims

The development, and the structural and mechanical characterization of an new complex system composed by a aqueous 3D Highly Viscous Polymeric Dispersion (HVPD) of poly(vinyl alcohol) (PVA) cross-linked with an innovative green molecule, is the focus of this topic. Similar systems have been studied in the past but the crosslinker used (i.e., the borax) is not considered a safe and green product on the basis of the EU Greendeal.

The high viscosity typical of the system minimizes the capillary penetration of the microemulsion inside the porous matrix constituting the artwork, minimizing the swelling of the binder of the paint layer and the uncontrolled spreading of the liquid phase onto the paint surface. The HVPDs also ensure great control of the cleaning: in fact, the high retention reduces the evaporation of the volatile components confined into the matrix and, once the system carried out its function, it can be easily and completely removed from the painted surface simply by means of a peeling action without leaving any instrumentally detectable residue onto the treated area.

Results

In previous works it has been observed that the PVA-borate systems, thanks to their elasticity and to their high voscosity, do provide selective, surface-controlled cleaning action as well as facile and benign removal from a painting surface by means of a peeling action. By so doing, residues left on the painted surface from the patina and from the cleaning tool are expected to be minimized. Moreover, the rheological properties can be easily modulated by changing the ratio of PVA to borate or their total concentration. Analogous aqueous PVA/borax-based HVPDs loaded with o/w microemulsions are characterized by a similar behavior.

The HVPD have been characterized by Small Angle X Rays Scattering (SAXS) and rheology in order to obtain information about both the structure (i. e. the radius of the nanodroplets and their polydispersity) and the mechanical.

Figure 1 shows the results of a cleaning test carried out on a XIX century Tuscan canvas painting (Figure 1, left) carried out with a the PVA-borate system containing a o/w microemulsion. Contact angle, TOF-SIMS (Figure 1, right), Fourier transform infrared (FTIR), and scanning electron microscopy/energy dispersive spectroscopy (SEM/EDS) data confirmed that microemulsions were effective in removing polymeric organic coatings from painted surfaces of artistical and historical interest, as demonstrated by the results of several cleaning tests performed onto various painted surfaces of artistical and historical interest. These systems require no after-washing to remove residues, their cleaning action is easily controlled, and they can be removed in one piece by peeling.

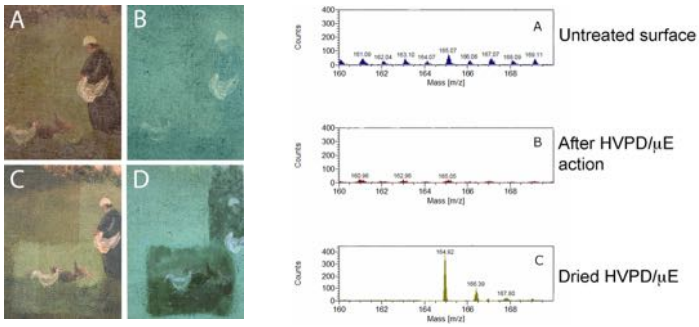
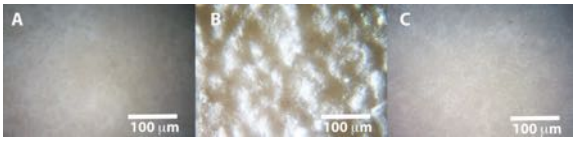


Figure 1: Left: detailed pictures of the XVIII century Tuscan egg-tempera canvas painting before the cleaning test carried out through the HVPD/□E: visible light (A) and UV-induced visible fluorescence (B). The same area of the painting after cleaning procedures: visible light (C) and UV-induced visible fluorescence (D). Right: TOF-SIMS spectra of untreated surface (A), of surface after the interaction time and removal of HVPD/□E (B), and of the HVPD/□E system (C) in the 160-170 m/z mass range.

Moreover, recently, we have found that it is possible to functionalize the HVPDs, apart with organic solvents and o/w microemulsions and other molecules like chelates that increase the range of possible applications and support that can be treated with these systems. In particular the preliminary results indicate the potentialities of these systems for the selective removal of sulphates from the surface of carbonatic stones (Figure 2).



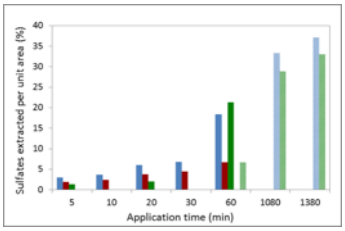


Figure 2: Top: optical micrographs (20x magnification) of the travertine surface before the sulfation treatment (A), the sulfated surface before (B) and after (C) the cleaning test with the HVPD containing 0.5 wt% ammonium carbonate. Bottom: Sulfates extracted per unit area (%) at different contact times based on IC (filled histograms) and ICP (striped histograms) results for the HVPD containing 0.5 wt% ammonium carbonate (light blue), 0.25 wt% EDTA (dark red) and 1 wt% Rochelle salt (green).

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2A – PEMA chemical organogels for the cleaning of artifacts

L. Bellandi, C. Suraci, A. Salvini, R. Giorgi

Aims

Gels are particularly useful for the cleaning of works of art as they allow the controlled delivery of cleaning fluids on solvent-sensitive substrates. Owing to the covalent cross-links between polymer chains, chemical gels exhibit mechanical properties that allow their easy handling and their residue-free removal from artistic surfaces after the cleaning intervention. Here we present several strategies for the synthesis of gels to be loaded with organic solvents, which can be also referred as to organogels.

Results

Poly ethyl methacrylate (PEMA) organogels obtained by solubilizing MMA together with a dimethacrylate cross-linker in organic solvents, e.g. propanol, ethyl acetate (EA), butyl acetate (BA), and metyl ethyl ketone (MEK), were prepared for the removal of aged varnishes from canvas paintings. To achieve successful organogel applications also to the cleaning of solvent-sensitive paper artworks, more retentive systems were developed. As compared to previous formulations, the larger amount of cross-linker and the different solvent-monomer ratio resulted in decreased solvent content and mesoporosity, as proved by Scanning Electron Microscopy and Small Angle X-ray Scattering analysis; this let a more controlled solvent release.

Afterwards to reduce the eco-toxicological impact of both cleaning fluids and gels processing, the cleaning effectiveness of a class of green solvents (i.e., alkyl carbonates, and particularly diethyl carbonate, DEC), loaded into gels was experimented. Because of DEC solubility parameters, efficient interactions between DEC and Pressure Sensitive Tapes (PSTs) components were observed so that PEMA-DEC organogels were tested for the removal of aged PSTs from paper substrates. As proved by Laser Scanning Confocal Microscopy, the embedment of the solvent into the gel network allows a feasible intervention by applying the gel directly on the top surface of PSTs: in this way the solvent gradually penetrates the PST backing and swells the underlying adhesive, so that the detachment of the PST is allowed minimizing both solvent-artwork contact and mechanical effort.

PEMA-DEC systems were then successfully employed in the restoration intervention of a contemporary drawing by Keith Haring (Untitled, Naples Series, 1983): the use of PEMA-DEC gels let the complete removal of aged poly propylene tapes, avoiding drawbacks usually correlated to methods commonly used by restorers. Compatibility of PEMA gels loaded with some essential oils (EOs) are also under investigations to test the efficacy of the gel to control the ability of EOs to solubilize aged varnishes, repaints, and grime.

More recently, novel polyvinyl butyral (PVB)-based chemical gels have been designed, produced and characterized to their use as organogels for cleaning works of art. The gels were synthesized starting from commercially available low environmental impact products and obtaining excellent characteristics without the need for additives to improve the properties of the gel. Rheological tests confirmed strong viscoelastic

properties, and SEM imaging revealed a porous, interconnected structure. Cleaning tests on wood treated with a fluorinated agent and Dammar-varnished canvas demonstrated the effectiveness of these gels, highlighting their potential for cleaning delicate surfaces in the conservation of Cultural Heritage.

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2A – Perfluoroalkyl Substances: Assessment of a Potential Inhibitory Effect and Physico-Chemical Removal Mechanisms

M.C. Collivignarelli, C. Milanese, S. Bellazzi, L.M.R. Calabria, A. Abbà, A. Papetti

Project: Sostanze perfluoroalchiliche: valutazione di un possibile effetto inibente e delle rese prestazionali di tecnologie biologiche. Funding body: AsMia S.r.l.

Aims

This project focuses on the environmental and treatment challenges posed by per- and polyfluoroalkyl substances (PFAS), known for their persistence, toxicity, and resistance to degradation. Widely used in consumer and industrial products, PFAS often enter wastewater treatment plants (WWTPs) via textile industry discharges and landfill leachates. Due to their stability, PFAS are poorly removed by conventional WWTPs, contributing to environmental contamination through treated effluents and sludge. The project has two main goals: (1) assess the potential inhibitory effects of PFAS on aerobic biomasses using respirometric tests with mesophilic and thermophilic sludges, and (2) investigate PFAS removal mechanisms via adsorption on activated carbon to identify the most efficient treatment approaches.

Results

In Block 1, respirometric tests conducted on biomasses A and B analyzed the waste by diluting the high concentrations of PFAS in Waste 1 with the plant input or with tap water, without considering further variables. The results showed that the COD of the substrate is a determining factor in the respirometric tests: the specific OUR (OURs) increased proportionally with the COD concentration of the substrate.

In Block 2, to eliminate the influence of COD variability, respirometric tests were performed by dosing substrates obtained by mixing the waste with the effluent of the reference plant, so that the COD of the substrate was similar to that of the WWTP input (Ing-A for biomasses A and B). This led to very low PFAS concentrations in the substrate: 0.930 mg/L.

In Block 3, respirometric tests were conducted using waste as is, without dilution. In this case, the COD of the waste was compared with that of a substrate with high nutritional value (casein peptone) diluted in water. The results of the single-track tests showed a variable tolerance of the biomasses based on the type of PFAS and the characteristics of the waste.

In general, none of the wastes containing PFAS showed a significant inhibitory effect on the metabolic activity of the biomasses, regardless of the experimental conditions. This result suggests that the presence of perfluoroalkyl compounds in the liquid waste does not seem to directly influence the biological activity of the tested biomasses. Therefore, it appears necessary to adopt more specific and sensitive analytical methods in order to correctly detect and quantify PFAS, regardless of the effect they may have on biomass metabolism.

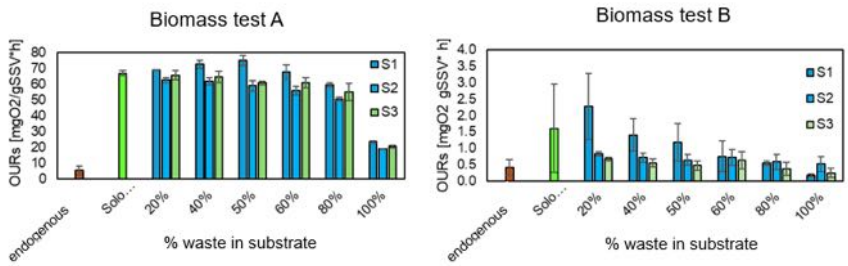

Figure 1. Results of OUR respirometric tests carried out with two different civil biomasses (A and B) placed in contact with wastewater with a high concentration of PFAS.

Among the new generation carbon-based materials, the application of MOFs (Metal-Organic Frameworks) is of particular interest. These materials combine an organic component, characterized by a high carbon content, with a metallic component, giving rise to a porous structure rich in active sites. Thanks to their electrostatic attraction capacity, MOFs are particularly effective in retaining perfluoroalkyl molecules, especially those with longer chains. The presence of the metallic component offers significant advantages, including the possibility of separating the adsorbent material by applying a magnetic field, resulting in easy recovery and regeneration. However, it is important to underline that the active surface of the regenerated material is generally lower than that of the virgin material, resulting in a reduction in the adsorption efficiency. A further critical aspect concerns short-chain perfluoroalkyl molecules, which tend to resist the thermal treatments for carbon regeneration and are frequently detected in exhaust gases, raising environmental concerns. The use of adsorbent materials obtained from recycled sources, such as biochar, represents a sustainable and highly advisable strategy. Biochar derived from agricultural waste have shown excellent adsorbent performances, thanks to their high cellulose content, which provides a large specific surface area. Even residues from wastewater treatment, especially biosolids, can be valorized through pyrolysis, thermal activation or combustion, helping to close the production cycle according to the principles of the circular economy. However, a challenge still open concerns the management of PFAS after their transfer from the liquid to the solid phase: the possibility of reusing or destroying them effectively remains one of the main unsolved issues in current scientific research.

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2A – Retentive cleaning systems for the removal of corrosion products from artistic bronzes and iron-based alloys

T. Guaragnone, A. Casini, D. Chelazzi, E. Fratini, P. Baglioni, R. Giorgi

Aims

Development of plasticized PVA-based polymeric systems and pHEMA/PAA gels loading complexing agents for the safe removal of alteration products from Cu-based and Fe-based alloys.

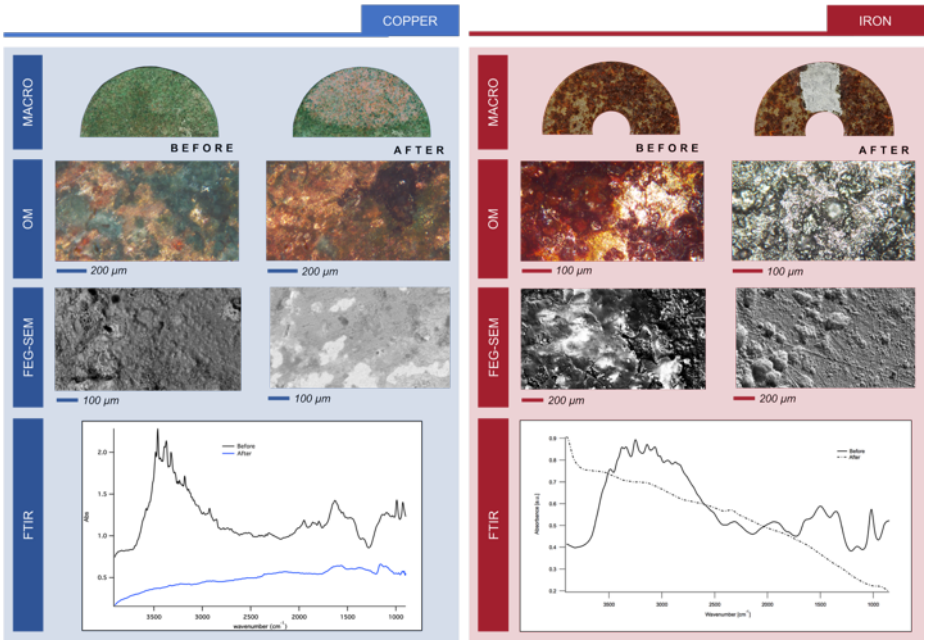
Results

Innovative poly(vinyl)alcohol-based film forming system and poly(2-hydroxyethyl methacrylate) (pHEMA) networks semi-interpenetrated (SIPN) with poly(acrylic acid) (PAA), specifically devised for the controlled and selective cleaning of copper-based and iron-based artifacts were developed.

Traditional cleaning procedures of metallic artifacts are commonly performed by mechanical and/or chemical methods. Both these methods present some limits related to the poor selectivity and invasiveness of the mechanical procedure, and to the scarce control over the reactions involved in the chemical approach.

In the case of copper-based alloys, the cleaning procedure is particularly delicate, it should aim at the complete removal of the defacing and harmful corrosion products of Cu(II) (copper carbonates, sulphates, chlorides, etc.) but preserving the underlying protective cuprite Cu(I) layer. On the contrary, for the iron-based alloys is important the complete removal of all corrosion patinas that are usually powdery and porous layers and unable to protect the metal beneath. Moreover, the presence of high soluble chlorine salts, such as Fe(III)Cl3, can also bring to new rusting processes.

In the case of PVA-based film forming system, the proposed cleaning procedure consists in the application of a PVA-based polymeric solution able to form an elastic film, which can be gently peeled off from the surface upon drying. Plasticizers (different polyols) were added to the solution to obtain a final film with suitable mechanical properties to facilitate the peeling action, while the composition of the volatile fraction (water and ethanol) was adjusted in order tune both, the viscosity of the system and the time required for the film to form. Finally, a complexing agent was loaded in the polymeric dispersion. The main advantage of these cleaning systems consists in the simultaneous chemical and mechanical action, guaranteed by the presence of the complexing agent and the final removal of the film by peeling off.



In case of brittle and mechanically weak metallic surfaces (i.e. archeological artefacts), where the removal or peeling of surface layers might be risky for the artifact integrity, a gel system allows to have e a very controlled action.
Thanks to its mechanical properties, indeed, a pHEMA/PAA gel can be applied repeatedly with no risks to delicate substrates and simply removed in one piece without leaving detectable residues.
Moreover, the capability of PAA to give strong coordination bonds with metal ions via carboxylate groups in alkaline conditions, can boost the capture and retention of copper and increase the cleaning performances of the chelating agent confined inside the gel.

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2A – Superfluid Alkali-Activated Mortars for Heritage Consolidation

D. Coffetti, S. Rapelli, L. Coppola
(Department of Engineering and Applied Sciences, University of Bergamo, Dalmine (BG), Italy)

Aims

The development of alternative binders to Portland cement is a key challenge in the field of restoration, where material compatibility, sustainability, and long-term durability are essential. Alkali-activated slag (AAS) mortars represent a promising option thanks to their low-carbon footprint and potential for tailored properties. However, their adoption is hindered by poor rheology and uncontrolled setting behaviour, which limit their use in superfluid consolidants and injection grouts (Lu et al. 2021). This study explores a ternary powdered activator system (sodium metasilicate pentahydrate, potassium hydroxide, sodium carbonate at 7:3:1 mass ratio) (Coffetti et al. 2023) combined with polycondensate-type superplasticizers, with the aim of producing highly workable, stable, and durable superfluid mortars suitable for restoration applications.

Results

Workability tests on pastes and mortars confirmed that conventional polycarboxylate ether (PCE) superplasticizers are ineffective in such systems, whereas β-naphthalene sulfonate (BNS) polycondensates provide significant improvements (Tian et al. 2023). Among the tested formulations, sodium-based BNS (Na-BNS) exhibited superior dispersion and adsorption characteristics compared to calcium-based BNS (Ca-BNS). Na-BNS at about 1.0% by weight of slag ensured optimal flowability and retention, enabling superfluid consistency without excessive air entrainment, while Ca-BNS promoted abnormal air incorporation, reducing density and compromising performance (Figure 1).

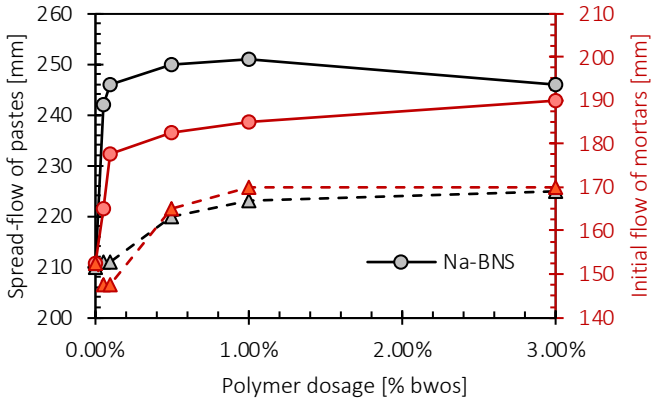

Figure 1: Spread flow of AAS pastes (black line) and initial flow of AAS mortars (red line) containing different amount of BNSs

Setting time measurements showed that Na-BNS induced only moderate retardation, thus maintaining practical working windows essential for on-site restoration works. In terms of mechanical performance, mortars with limited Na-BNS addition achieved higher early and 28-day compressive strength, whereas overdosing or Ca-BNS addition caused significant strength reductions (Figure 2). Microstructural analyses through adsorption isotherms and zeta potential confirmed that Na-BNS achieves stronger anchoring on slag particles, ensuring uniform dispersion and reducing the risk of segregation or flocculation.

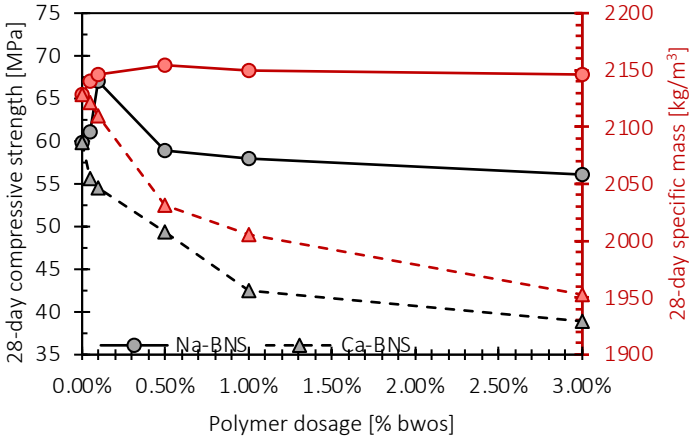

Figure 2. Compressive strength (black line) and specific mass (red line) of mortars containing different amount of BNSs

These results highlight the feasibility of superfluid AAS mortars as consolidants in heritage conservation. Their ability to deeply penetrate cracks and porous matrices, combined with sustainability and improved compatibility compared to Portland-based grouts, makes them suitable for restoration scenarios where durability and reversibility are required.

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2A – Treatment of media of historical and artistic interest

E. Carretti, F. Porpora, L. Dei, S. Baldini, I. Lunghi

Aims

Motion picture films and negative photographs need significant attention due to their historical and artistic value. Structurally, all these documents are characterized by a complex stratigraphy: an emulsion layer made by silver nanoparticles dispersed in a proteinaceous matrix, an anti-halo layer, a subbing layer and a support usually composed by a polymeric material. The first support used as a photographic base since 1890 was celluloid, a mixture of cellulose nitrate and a plasticizer. Nevertheless, due to its strong inflammability and low chemical stability, since the beginning of the motion picture industry (around the first decade of the 20th century) research was carried out to find a safe alternative for cellulose nitrate. Its replacement started around 1904 with the commercialization of cellulose diacetate (CDA) and the production of the first safety films. During the 1930s the first cellulose triacetate (CTA) bases were developed by Eastman Kodak and Geavert. The breakthrough came in 1948 when a formula with optimal optical and mechanical properties was found. Then, in 1951 most inflammable films were replaced by CTA. Unfortunately, also CTA is unstable and subject to deterioration in ordinary room conditions. Principal degradation processes of CTA are due, first to hydrolysis that causes both deacetylation and glycoside bond cleavage, furthermore to loss of plasticizer, oxidation and photodegradation phenomena. To further increase the chemical stability of the support, since the second half of the 1960s polyester gradually replaced CTA as support for photographs and motion picture films. The most important degradation phenomenon affecting CTA-made safety films is the “vinegar syndrome” that is due to the hydrolysis of the ester bond that induces the side chain scission causing the release of acetic acid. This is the most dangerous alteration of CTA filmsand is strictly influenced by temperature, humidity and acidity.

In the early stage (the “induction period”) the reaction rate is determined primarily by heat and humidity. When the acetic acid concentration increases, the acetic acid formed acts as a catalyst for the deacetylation reaction and induces an autocatalytic process. Other factors that contribute to the chemical instability of this support are the residual sulphuric acid, used for the production of CTA, and metal ions, released from enclosures in which CTA-based films are conserved. A secondary effect induced by the acetic acid formed through vinegar syndrome is the hydrolysis of the glycosidic bonds between the saccharide units constituting the CTA backbone. This results in a strong reduction of the molecular weight and a partial impairment of the mechanical properties of the CTA-based film. Then, in addition to the smell, vinegar syndrome’s macroscopic symptoms are the shrinkage of the film with consequent deformation of the emulsion (channeling), the increase of stiffness and the embrittlement of the film that can compromise its usability. Therefore, it is fundamental to define appropriate storage conditions for CTA films in terms of temperature, relative humidity and enclosure’s characteristics and to monitor the artifact’s alteration status. The Image Permanence Institute (IPI) provided a guide to evaluate and plan storage

environments for CTA supports and indicated a method to monitor the acidity based on the use of strips soaked with acid-base indicators that change color when exposed to acid vapors. To limit the diffusion of the vinegar syndrome, it is mandatory to reduce environmental moisture and remove alteration by-products from the storing environment.

Results

On these bases, the goals of this project are multiple:

1. the development of a multi-analytical protocol to understand the conservation status and the degradation mechanism of CTA films by monitoring various parameters such as mass of the film, acetylation degree, free acidity etc; The results of the artificial induction of the “vinegar syndrome” and of its progress (followed by monitoring acetyl content (red), ATR-FTIR ratios (blue), and free acidity (magenta)) on a standard CTA film, data are reported in Figure 1

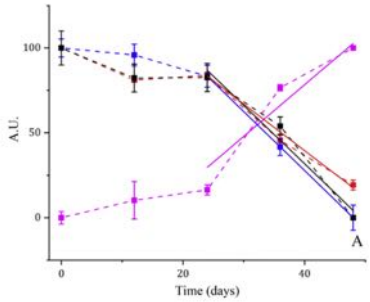

Figure 1: acetyl content (red), ATR-FTIR ratios (blue), and free acidity (magenta) data for (A) LCBF

2. define an effective strategy to prevent and stop the vinegar syndrome, based on the use of nanotechnologies. In detail, some xerogels, effective in the adsorption of acetic acid produced through the “vinegar syndrome” were set up and successfully tested on degraded and not degraded real motion picture films.

A second aim of this topic is the set up of innovative materials (i.e. aerogels and xerogels) for the inhibition of both the chemical and the biological degradation phenomena on ancient photographic documents

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2A – Trypsin-Functionalized Hydrogels for Minimally Invasive Micro-Sampling of Proteinaceous Binders in Cultural Heritage

R. Giorgi, L. Bellandi

Aims

In the field of diagnostics for cultural heritage conservation, non-invasive techniques are nowadays preferable since they do not compromise the integrity of artworks. However, these methods do not provide detailed molecular data on organic materials, such as proteinaceous binders. For this reason, invasive sampling becomes necessary when binder identification is required for conservation or attribution purposes. Traditional procedures require the mechanical removal of small fragments from the artwork [1]. More recently, some studies have shown the potential of hydrogels loaded with free enzyme solutions for micro-sampling, offering a less invasive alternative that preserves the underlying substrate [2]. However, this approach does not address the issue of enzyme residues remaining on the artwork's surface, which may lead to undesired alterations or damage to the heritage material.

Results

To prevent enzyme residues on the artwork surfaces and avoid undesired alterations or damage to the heritage material, an innovative trypsin-functionalized hydrogels as a minimally invasive tool for the in-situ digestion and extraction of protein binders from painted surfaces was investigated. Trypsin was selected for its well-characterized substrate specificity and successful use in prior studies involving historical/artistic substrates [1].

A hydrogel matrix composed of poly(2-hydroxyethyl methacrylate)/poly(acrylic acid) (pHEMA/pAA) was employed, and three strategies for enzyme incorporation were explored: (i) Functionalizing pAA with trypsin and then synthesize a semi-interpenetrated gel based on p(HEMA/pAA-Tryp; (ii) Immobilize trypsin on the surface of the gel; (iii) Synthesize a semi-interpenetrated gel based on p(HEMA)/pAA/free tryp. Fourier-transform infrared spectroscopy confirmed the successful incorporation of trypsin and preservation of its enzymatic structure. The properties of such visco-elastic probe (gel) can be enriched by loading different enzyme solutions able to react with proteins, lipids, or gums, usually found on artworks and already collected in mass spectrometric database. The enzyme solution-loaded gel will operate in a direct ultra micro-sampling of organic material in situ, thanks to the capability to confine the hydrolysis action of enzymes to the very surface layer and to digest and upload few molecules of analytes for further analysis. The strengths of the protocol rely on the ultra micro-invasiveness, the simplicity in gel handling and in its applicability to a large set of object and art materials.

This preliminary phase of the research focuses on evaluating the feasibility and effectiveness of the pHEMA/pAA–trypsin hydrogel system for in-situ digestion and selective recovery of proteinaceous binders. Ongoing tests on model substrates aim to assess digestion efficiency and compatibility with proteomic techniques, such as MALDI-TOF-MS and LC–ESI-MS/MS. The goal is to establish a reliable micro-sampling method that ensures both high analytical performance and minimal impact on the surface of the artworks.

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2A – Twin-Chain Polymer Networks for the cleaning of Modern and Contemporary Art

R. Mastrangelo, D. Chelazzi, G. Poggi, E. Fratini, P. Baglioni

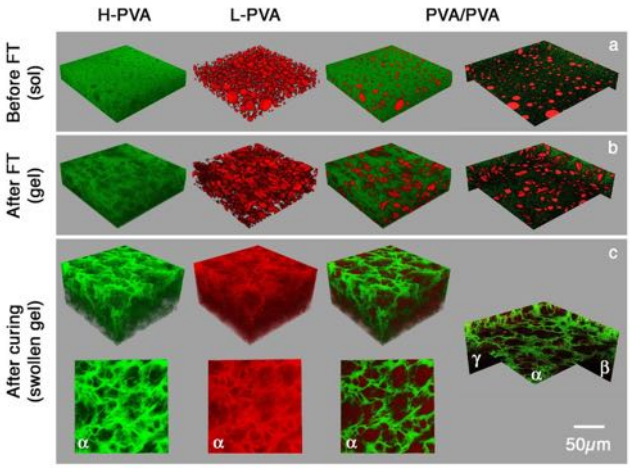
Aims

Artifacts, like easel paintings, are subject to degradation, not only as a result of natural ageing, but also for the exposure to ambient contaminants: grime and soil deposit on surfaces and are often hard to remove. Traditional cleaning techniques in restoration involve the uncontrolled spreading of the cleaning fluid on the surface of the artwork, the use of mechanical methods to remove grime and the possible deposit of residues. The cleaning of Modern and Contemporary paintings is one of the Conservator's most complex tasks: traditional methods are too invasive and risky for their clotted, solvent-sensitive surfaces. The ideal cleaning systems are highly adaptable and retentive gels, with a macroporous structure that allows the diffusion of cleaning fluids throughout the gel matrix and at the gel-substrate interface.

Results

Twin-Chain Polymer Networks (TC-PN) are poly(vinyl) alcohol (PVA)-based cryogels with a sponge-like structure. The micron-sized pores are crucial to ensure high cleaning performances on rough and delicate artistic surfaces. Classically, PVA cryogels are obtained through a freeze-thawing (FT) process. The freezing step induces a water-polymer phase separation: polymer-rich areas are compressed by the growing ice crystals, until PVA crystallites form. PVA crystallites act as junctions, conferring to the hydrogel cohesion and elasticity closer to those of chemical gels. Conversely, ice crystals act as templates in the formation of a ubiquitous porosity. Free water content and water retentiveness are far higher than those characterizing traditional gels used in restoration. In TC-PN, the spontaneous phase separation occurring between a highly hydrolyzed (H-PVA) and a partially hydrolyzed PVA (L-PVA) was exploited to obtain sponge-like hydrogels: L-PVA concentrates in blobs in the pre-gel solutions, acting as a porogen during cryostructuration. H-PVA behaves, instead, as the main structural component. The characterization of the systems morphology at the micron-scale was performed though confocal microscopy and SEM, while the nanoscale features were investigated through SAXS measurements. The porogen causes an increase of the average pores size and a decrease of the correlation length, describing polymer chains crowding in the gels walls. The number of FT cycles drastically affect the rheological response, as gels crystallinity increases, making the gels stiffer.

The cleaning performances of H-PVA gels and TC-PN were compared on rough and flat surfaces: TC-PN performed better in the removal of artificial soil from glass and mock-ups specifically prepared to mimic Jackson Pollock's dripping technique.



Gels of this type were successfully used in the restoration of Pollock's masterpieces *Two* and *Eyes in the Heat*, on display at the *Peggy Guggenheim Collection*, in Venice. More recently, in the framwork of the EU project GREENART, we have focused on the replacement of PVA can be partially replaced in the gels to explore other synthetic or bio-derived "green" polymers, modulating the properties of the gels (in the present report, a specific section is dedicated to that). Another topic that has been recently addressed is the role of tortuosity in the cleaning capability of these gels; controlling tortuosity means control of interfacial processes in countless applications, with vast potential impact. Further details are reported in the contribution indicated above.

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2A – Valorization and Recovery of Residuals from Wastewater Treatment Plant

M.C. Collivignarelli, C. Milanese, S. Bellazzi, L.M.R. Calabria, A. Abbà

Project: DORIAN (Modellazione Digitale a supporto del progetto ambienti sicuri, sostenibili e resilienti) Funding body: Ministero dell'università e della ricerca (MIUR) 2023-2027

Aims

This project promotes a circular economy in wastewater treatment by transforming waste residues into valuable resources. Solid residues from pre-treatment are washed and reused as aggregates in green concrete, reducing landfill use and raw material extraction. Treated effluent, meeting regulatory standards, is reused in agriculture (for irrigation) and industry (for non-potable uses), conserving freshwater. Treated sewage sludge, rich in nutrients, can serve as fertilizer if safety standards are met. Pyrolysis of sludge produces biochar, which is useful in both water treatment and agriculture. The project also explores alternative organic substrates to optimize denitrification, enhancing nitrogen removal and overall process sustainability.

Results

The results are reported focusing mainly on the sludge residue. The sludge was collected from a municipal WWTP, dried at 105°C (A), pyrolyzed at 650°C and 950°C (B) and subsequently activated at 650°C (C). The sample was then neutralized, filtered and finally dried in an oven (D).

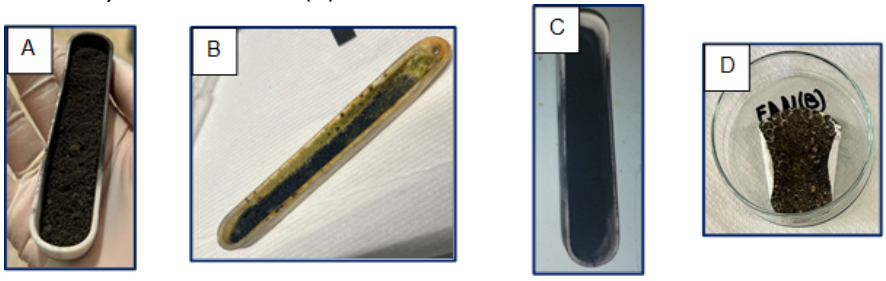

Figure 1: Production of Biochar through pyrolysis and chemical activation of biological sewage sludge.

Subsequently, from the characterization by X-ray diffraction and IR spectroscopy of the biochar produced, it was not possible to achieve a precise and complete analysis since the sewage sludge is a highly heterogeneous matrix and contains numerous compounds and components (carbon, oxygen, nitrogen and phosphorus, calcium and iron). From the treatment point of view, the biochar produced was used as an "adjuvant" (1) of aerobic biomass to remove both conventional and emerging parameters (AOX) and as a final chemical-physical treatment (2). From this experimentation, it emerged that the introduction of biochar as an adjuvant within the activated sludge process effectively improved the removal of the AOX that is difficult to biodegrade (dichlorophenol), especially for moderate concentrations. The reuse of biochar as a final treatment of the activated carbon pyrolyzed at 650°C

demonstrated a higher adsorption capacity than that treated at 950°C, especially for moderate concentrations of AOX. However, as shown in Figure 2, adsorption decreases dramatically for pollutant concentrations above 50 mg/L, confirming that the effectiveness of biochar strongly depends on the dosed amount and concentration of the tested pollutants.

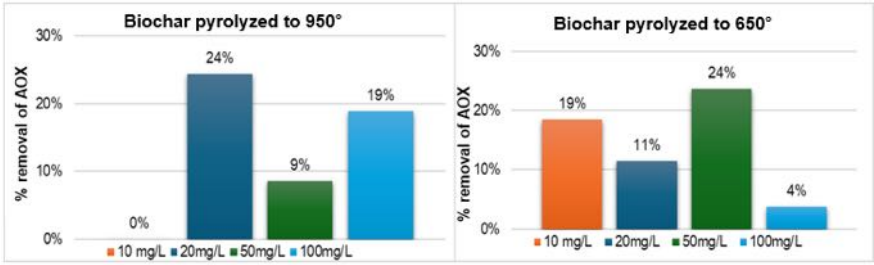

Figure 2. Results of adsorption tests using biochar pyrolyzed at 950°C and 650°C.

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2B – Cathodes and anodes materials for lithium and sodium ion batteries

M. Bini, M. Ambrosetti, C. Milanese, A. Girella et al.

Aims

The large-scale diffusion of electric vehicles and electronic portable devices requires a huge energy amount. The renewable resources (wind or solar) could be a good choice for providing energy, but they are intermittent, so requiring energy storage systems for the stationary applications. To this aim, the most diffuse and performing systems are the batteries, particularly lithium ion batteries (LIBs), already marketed by many years, that should however be replaced for well-known issues by more sustainable alternatives, such as sodium ion batteries (SIBs). We synthesized anodes materials to improve the electrochemical performances of SIBs and to unravel the mechanisms at the base of electrochemical performances for LIBs.

Results

Different kind of synthesis routes (wet or solid-state methods) were typically used, with the aim to compare the performances of the synthesized materials and to find the better experimental conditions to obtain peculiar features. The use of doping or substitutions with transition elements could help to improve the structural stability and the electrochemical performances, as well as the nano-dimensions, thanks to the shortening of Li+ or Na+ diffusion paths. All the materials were usually characterized from the physical-chemical (X-ray diffraction measurements with Rietveld structural refinements, SEM/EDS, Raman, FT-IR, EPR and Mössbauer spectroscopies) and electrochemical (cyclic voltammetry, galvanostatic measurements and impedance spectroscopy) point of view and they were tested in semi-cells. The determination of the involved reaction mechanisms could be based on Large Facilities measurements, such as operando diffraction.

This kind of characterization was applied to different materials, allowing to obtain important results (see references). We studied $ZnFe_2O_4$, a spinel phase applied as anode in LIBs. It was prepared by co-precipitation and template syntheses, obtaining samples with different morphologies and crystallite sizes. The electrochemical features were interpreted on the basis of the physical-chemical features. The higher electrode area of the template ZFO, with smaller particles, is responsible for better reactivity in the first cycles, but, in the long term, a lower crystallinity of active material, leading to nano-crystalline reaction products, could determine a better reversibility. More recently, the focus was on pure and doped (Mn, Mg or Sn) $GeFe_2O_4$ applied as anode in SIBs, that was obtained with hydrothermal and mechano-chemical syntheses. The spinel cubic structure of pure $GeFe_2O_4$ is maintained in doped samples. The expected redox processes, involving Fe and Ge ions, are present in the electrochemical tests. The Sn doping demonstrated a beneficial effect on the long-term cycling (providing 150 mAh/g at 0.2 C after 120 cycles) and on the capacity values (346 mAh/g at 0.2 C with respect to 300 mAh/g of the pure one), while the Mg substitution was less effective. The Mn substitution was also effective with respect to the pure sample, but less than the Sn one.

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2B – Electrode materials for enhanced electrochemical performances in SIBs

D. Capsoni, D.M. Conti

Aims

Rechargeable batteries play a basic role in the transition to renewable energy systems. Lithium-ion batteries dominate the market, thanks to their valuable performances in terms of energy and power density, cycling stability and rate performances. However, they exhibit some drawbacks: (i) current performance is not sufficient to satisfy the power demand for energy grids and electric vehicles, due to the limited capacity of commercial electrodes; (ii) availability of Lithium source. Sodium-ion batteries represent a promising choice, as Na is abundant on Earth crust, but they have two distinctive drawbacks: low cycling stability and poor rate performance at high C-rate. In the present research project, we synthesized active materials/CNFs self-standing electrodes. The foreseen advantages of the free-standing electrodes, compared to conventional tape-casted ones are: (i) the metal current collector and support is avoided; ii) the CNFs porous matrix allows the intimate contact of the electrolyte with the active material; iii) the synergic effect of the conducive and porous matrix and the homogeneous dispersion of the active material enhance the specific capacity and cycling performance, especially at high C-rate. First, we synthesized and characterized LiFePO4/CNFs composites to test the synthetic procedure and active material amount on well-known cathode for LIBs. Then, ZnS, and NASICON-type Na3MnTi(PO4)3 and Na3MnZr(PO4)3 electrode materials for SIBs were investigated.

Results

The self-standing LiFePO4/CNFs cathodes were prepared by electrospinning the dispersion of commercial LiFePO4 into a polyacrylonitrile in a N,N-dimethylacetamide solution. The obtained sheets underwent stabilization and carbonization processes, and the free-standing cathodes were obtained. The tested active material amount (12.3 and 34.5 wt%) is lower than the conventional tape-casted cathodes (70–85 wt%). The LiFePO4 maintains the olivine-type structure and results homogeneously dispersed into and within the carbon nanofibers. The self-standing electrode (34.5 wt% of active material) displays high Li+ diffusion coefficient (1.36 × 10−11 cm2/s), improved reversibility, lower capacity fading, good reversibility and stability, enhanced capacity values at C-rates higher than 5C, and good lifespan when cycled 1000 cycles at 1C and further cycled up to 20C, compared to the LiFePO4 tape-casted cathode (80 wt% of active material), appositely prepared for comparison.

To prepare the self-standing Na3MnTi(PO4)3/CNFs electrodes, we pre-synthesized the active material, and followed the electrospinning procedure assessed for LiFePO4. The active material effective loading is only 10 wt%, as some sedimentation of Na3MnTi(PO4)3 occurred along the tube connecting the pump and the needle of the horizontal spinneret, possibly due to the poor dispersibility of the pre-synthesized active material aggregates in the PAN-based polymer solution. The Na3MnTi(PO4)3 particles are homogeneously spread into and within CNFs and preserve the NASICON structure. Despite the low amount of active material loaded into CNFs, the

electrochemical performances are appealing compared to a tape-casted electrode appositely prepared, especially at high C-rates: the capacity value at 20C is 77.60 mAh/g, the electrode exhibits good cycling performance and a capacity retention of 59.6% after 1000 cycles at 1C.

In the case of the Na3MnZr(PO4)3/CNFs composites, the self-standing cathodes were prepared by electrospinning using both the dip–drop method (precursors of the active material were dip-drop coated on pre-electrospun CNFs), and the dispersion of pre-synthesized Na3MnZr(PO4)3 in the PAN solution to be electrospun. Different electrospinning settings (horizontal and vertical) were also employed. The different approaches aim at obtaining higher active material loading into CNFs, by overcoming the sedimentation problems encountered for free-standing Na3MnTi(PO4)3/CNFs electrodes. Among the applied strategies, the electrospinning (vertical setting) of the polymeric solution containing pre-synthesized Na3MnZr(PO4)3 powders resulted effective to quantitatively load the active material (30 wt%). The Na3MnZr(PO4)3 aggregates connected to the CNFs, covered their surface, and were also embedded, as demonstrated by TEM and EDS. Compared to the self-standing cathodes prepared with the horizontal setting or dip–drop coating methods, the vertical setting electrode exhibited the highest capacity values, and good cycling life, compared to the tape-casted counterpart.

Finally, we synthesized and characterized ZnS–graphene composites/CNFs self standing anodes for SIBs. The characterization techniques confirm that nanocrystalline ZnS (sphalerite) covered by the graphene sheets are obtained. The active material is homogeneously dispersed in the CNFs' matrix. Two self-standing anodes (active material amount: 11.3 and 24.9 wt%) display enhanced electrochemical performance compared to a tape-casted electrode counterpart (active material amount: 70 wt%).

The obtained results demonstrate that improved electrochemical performances at high C-rates are obtained by applying a feasible and simple synthetic strategy (ex situ synthesis of the active material and addition to the carbon precursor for electrospinning), by using low amount of active materials. The results evidence the relevant role of the CNF matrix, which hosts the active material, promotes electrolyte permeation and contact with the active material, and increases the electronic conductivity.

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2B – Influence of welding parameters and heat treatments on aluminium joints produced by Additive Manufacturing

D. Asperti, M. Locatelli, S. Ferrari, S. Lorenzi, M. Cabrini, T. Pastore
(Department of Engineering and Applied Sciences, University of Bergamo, Dalmine (BG), Italy)

Aims

Additive Manufacturing (AM) allows the production of lightweight aluminium components with complex geometries and high mechanical performance. However, when hybrid structures combining additively manufactured and conventionally wrought alloys are required, reliable welding processes become crucial. Aluminium alloys present significant challenges in fusion welding, mainly due to their high thermal conductivity, residual stresses, and susceptibility to hydrogen-induced porosity. This work investigates the mechanical and corrosion behaviour of hybrid joints between LPBF-processed AlSi10Mg and wrought AW6061 alloy. The effect of welding parameters, joining technique and pre/post heat treatments was analysed with the aim of identifying correlations between microstructure, hardness distribution and corrosion susceptibility.

Results

Hybrid welds were produced using Gas Tungsten Arc Welding (GTAW) with Al 5356 filler, joining AlSi10Mg parts in both as-built and heat-treated conditions to AW6061 plates. Welding was performed by continuous TIG and pulsed TIG at 80–100 Hz, followed in some cases by post-weld T6 ageing. Microstructural analyses revealed that pre-weld solution treatment significantly reduced hydrogen-related porosity in the weld bead, in agreement with observations reported for AM aluminium alloys in literature (Dixit et al., 2022). As illustrated in Figure 1, the as-built specimen shows numerous pores while the heat-treated sample exhibits a much denser structure.

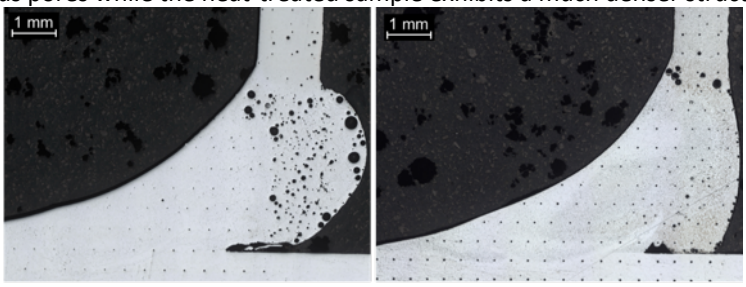

Figure 1: Cross-sections of specimens welded with pulsed TIG at 100 Hz in as built (a) and heat-treated condition (b).

Hardness mapping highlighted strong heterogeneities across the weld bead. Regions closer in composition to AW6061 were characterised by lower hardness values, while Si-rich areas displayed higher hardness due to eutectic networks and coarse Mg_2Si precipitates. Similar behaviour has been described in previous studies on dissimilar AlSi10Mg welds (Scherillo et al., 2018). Corrosion tests performed according to EN ISO 11846 confirmed the influence of these microstructural differences on the local corrosion behaviour. The cross-sections of the corroded specimens, reported in Figure 2, show that the weld bead is composed of distinct zones with variable susceptibility to selective attack.

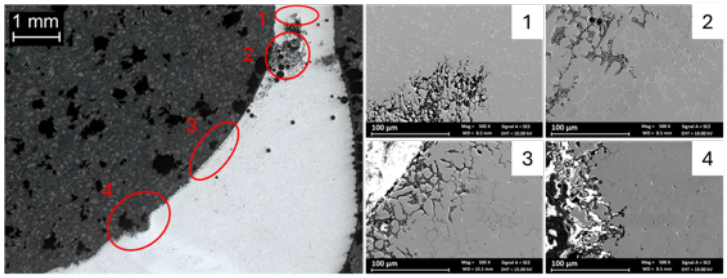

Figure 2: (a) Cross-section of the weld bead in the Cont HT specimen, highlighting four distinct zone exhibiting different susceptibility. (b) Low-magnification FESEM micrograph of the corresponding zones.

In particular, areas enriched in Mg were the most prone to localised dissolution, while Si-rich regions exhibited a more resistant behaviour. These findings are consistent with the strong correlation between local composition and corrosion performance highlighted in other studies on welded AM alloys (Cui et al., 2023). The correlation between microsegregation and corrosion depth, summarised in Table 1 (see Figure 2), underlines the difficulties of ensuring homogeneous behaviour in hybrid joints. The study demonstrated that pre-weld heat treatment of AM alloys effectively reduces porosity and improves weld bead quality, while microstructural inhomogeneities resulting from dissimilar alloy mixing generate local variations in hardness and corrosion behaviour. Hybrid welding of AM and wrought alloys therefore remains challenging, and further optimisation of welding parameters and post-processing strategies is required to ensure both mechanical integrity and corrosion resistance.

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2B – Investigation of elastic-plastic mechanical behavior in Hydrogen-promoting environment

L. Gritti, M. Pelucchi, S. Lorenzi, M. Cabrini, T. Pastore
(Department of Engineering and Applied Sciences, University of Bergamo, Dalmine (Bg), Italy)

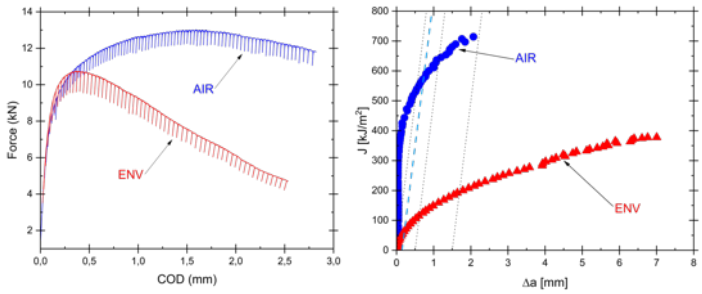
Aims

The conversion of existing natural gas pipelines into hydrogen transport systems is crucial for the sustainable energy transition. To assess the impact of hydrogen-promoting environments on mechanical behavior, it is essential to conduct in-situ testing where hydrogen charging, and mechanical testing are performed concurrently. Hydrogen can form on the surface of pipeline metals through dissociation from the gas phase or electrochemical reduction of hydrogen ions via cathodic protection or over protection. Once atomic hydrogen enters the material, it can diffuse rapidly through the metal lattice, accumulating at critical concentrations and leading to hydrogen embrittlement (HE). The steels used in gas pipelines are immune to HE, however this phenomenon can occur under conditions of slow plastic deformation, often due to soil movement. Therefore, this research project investigates the mechanical behavior of pipeline steel under hydrogen charging, in conjunction with mechanical testing to simulate these complex conditions.

Results

Elastic-plastic fracture mechanics extends classical fracture mechanics by accounting for both elastic and plastic deformation near the crack tip. A key parameter in this framework is the J-integral, which quantifies the energy absorbed per unit crack growth and serves as a measure of the material's resistance to fracture(Rice, 1968). Unlike linear elastic fracture mechanics, the J-integral remains valid in the presence of significant plasticity. To estimate crack extension, the compliance method is used, allowing for an indirect measurement based on load–displacement data. This approach enables a more accurate assessment of crack growth under realistic loading conditions, where both plastic and elastic contributions are significant. The mechanical tests were conducted within situ hydrogen charging. The sample was submerged in solution and connected at the potentiostat. It was applied the cathodic protection during all mechanical tests.

The experimental results of loading curves, as reported in the *Figure* (a), indicated a quite difference between the test conducted in air (AIR) and in environment under cathodic polarization (ENV), after reaching the maximum load. This difference it was imputed at cathodic hydrogen supply. Thus, the presence of hydrogen leads to embrittlement phenomena when reaching the predominant plastic behavior of the sample, as confirmed by (Fukunaga, 2024).



(a) (b)

Figure 1: (a) Experimental curves of elastic-plastic tests in air and cathodic polarization; (b)J-integral elaboration of tests

The J-integral curves, elaborated by experimental data, confirm the effect of hydrogen embrittlement on the environment test (Figure (b)). The J-curve performed in air shows much more energy to propagate the defect than the one performed in the environment. Therefore, the material acts more fragile, and the crack propagates at lower energy level provided. These results are confirmed by analysis of fracture surface in Figure . The air test denoted a typical ductile fracture characterized by dimples in different sizes and high surface deformation. Therefore, more energy (work) had to be done to deform the material and propagate the crack. The presence of hydrogen charging from the environment involves a surface associated with a brittle aspect with semi-cleavage facets, and the secondary cracks along perpendicular plane to principal propagation direction. The fracture is affected by poor plastic deformation and crack propagate plane cleavage facets. The propagation crack required less energy to take place as confirmed by J-curve. Tests are in progress to evaluate the effect of gaseous charging and on different materials used in the industry of transport of energy.

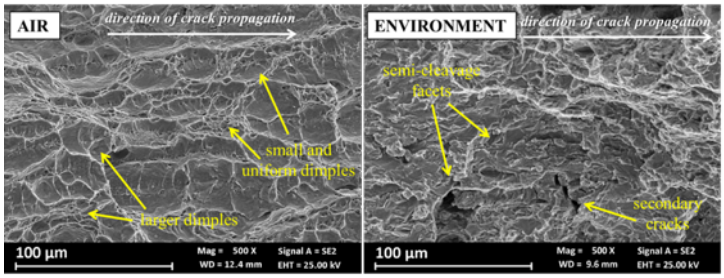


Figure 2: Fractographic analysis of sample surface

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2C – Advances in Fluorescence Spectroscopy for Tracing Organic Carbon Transport and Transformation

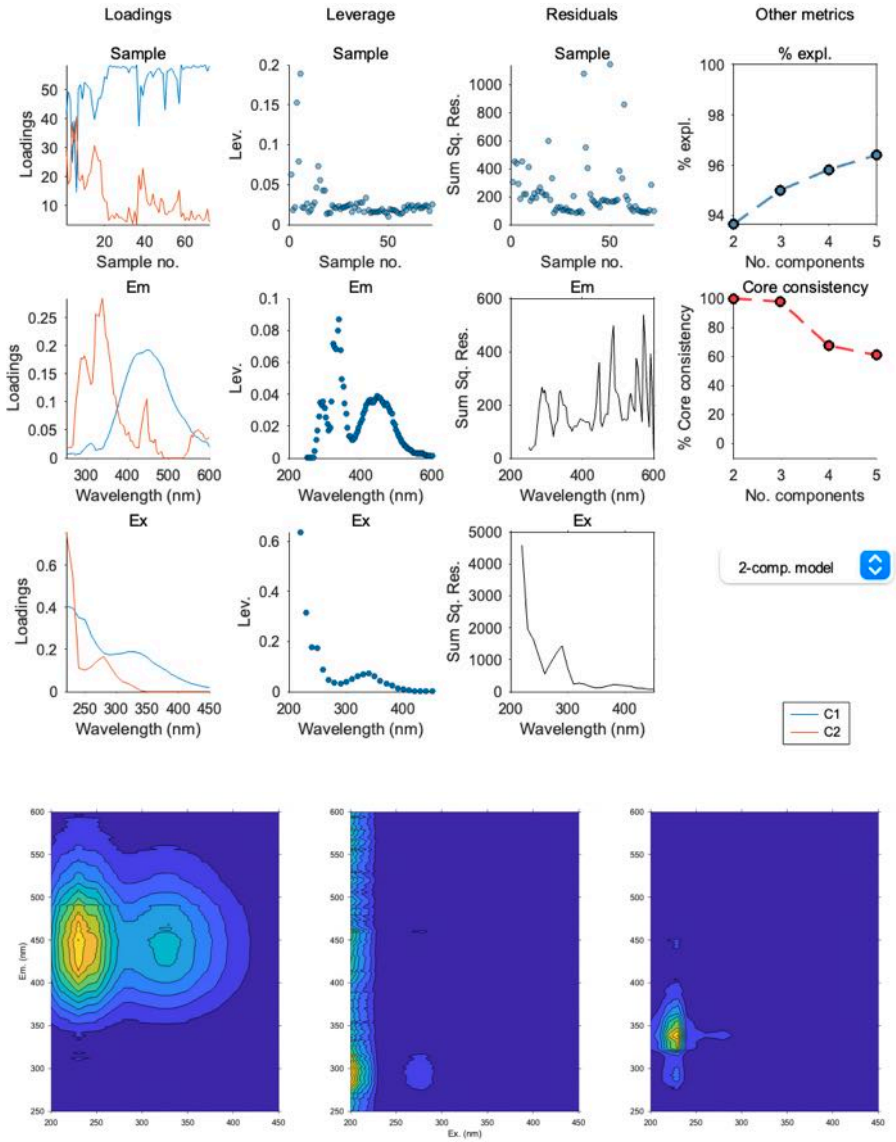
S. Loiselle, A. Boldrini, A. Polvani, L. Galgani, X. Liu, R.G. Cirrone, B. Gumiero, F. Di Grazie

Aims

Fluorescence spectroscopy is emerging as a powerful and versatile tool in environmental analytical chemistry, offering new opportunities to better understand the dynamics of dissolved organic matter (DOM) and pollution sources—particularly in river catchments impacted by both diffuse and point-source pollution, such as agricultural runoff and sewage treatment works (1).

Results

We highlight opportunities and recent developments in the use of continuous fluorescence sondes to capture high-frequency changes in DOM alongside conventional water quality parameters. We also present the development of a low-cost spectrofluorometer designed for rapid in-situ measurements, with a particular focus on enabling use by citizen scientists (2). Furthermore, we demonstrate how integrating multivariate analysis techniques, including parallel factor analysis (PARAFAC), with fluorescence measurements can help identify pollution signatures with high temporal and spectral granularity. In particular, we show how the ratio of tryptophan-like to humic-like fluorescence can serve as a useful indicator to distinguish between labile and refractory DOM sources (3). These combined approaches illustrate how fluorescence-based sensing and chemometric analysis can deliver detailed, responsive, and scalable insights into aquatic carbon dynamics. In the context of a changing climate—where changes to DOM sources and sinks are evident—such innovations provide a timely and impactful approach to support adaptive management and environmental resilience.



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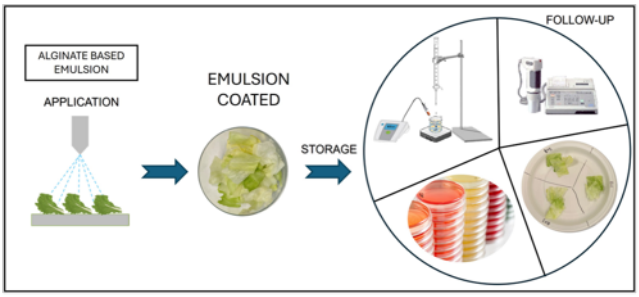
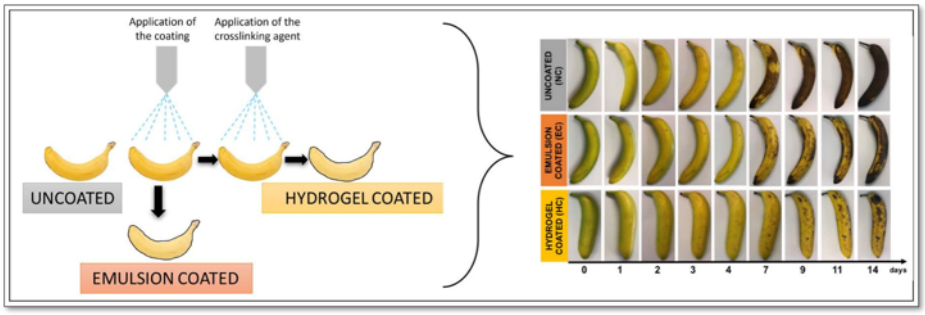
2C – Alginate-Based Emulsions for Extending the Shelf-Life of Fruit and Vegetables

M. Cofelice, F. Cuomo, S. Iacovino , A. De Leonardis, A. Ceglie, F. Lopez

Aims

The food industry is looking for solutions to reduce and replace traditional petroleum-based plastic packaging to reduce the perishability of fresh products. In this investigation, the effectiveness of an edible emulsion coating based on lemongrass essential and alginate was tested to extend the shelf life of *Lactuca sativa* salad leaves and banana fruit (*Musa* from the *Musaceae* family). The edible coatings formulated aims to offer good mechanical and gas barrier properties to slow down spoilage of fresh-cut or whole fruit and vegetables.





Results

First, the edible coating formulations were characterized using rheology, and then they were applied to commodities. The emulsion was sprayed onto fresh-cut salad or whole bananas, and the effect of the treatment was assessed by comparing it with uncoated samples. The quality characteristics of the fresh-cut Lactuca sativa salad were analysed in terms of weight, pH, titratable acidity, phenol content, visual appearance, and microbiological contamination. Regarding bananas, the effect of coating application on the peel during ripening was evaluated in terms of peel colour, pulp titratable acidity, total soluble solids, firmness and sensory acceptability.

The obtained data confirmed that the coating retained a higher total phenol content in Lactuca sativa salad. Furthermore, an enhanced product quality was observed in

terms of microbiological contamination during the first eight days of storage, with evidence of reduced psychrotrophic and mesophilic bacteria. Compared to the uncoated fruit, coated bananas remained uniform in appearance (peel colour) for longer, show reduced weight loss, had a delay in the formation of total soluble solids, and in the consumption of organic acids. The shelf life of the coated fruit was extended by up to 11 days, at least 5 days more than uncoated fruits.

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2C – Annurca apple extract and RYR synergistic effect on hypercholesterolemia

S. Pepi, L. Talarico, G. Leone, C. Bonechi, G. Tamasi, M. Consumi, F. Bisozzi, A. Magnani
(Department of Biotechnology, Chemistry and Pharmacy, University of Siena)

Aims

Recently, European Authorities imposed that any product for daily consumption shall provide less than 3 mg of monacolins from red yeast rice (RYR). This obliges to find new formulations able to guarantee an effect on cholesterol levels close to that performed by 10 mg of monacolin K. Two different formulations based on chitosan and xanthan gum containing 10 mg of lovastatin from RYR and a combination of lovastatin (3 mg) from RYR and annurca apple extract (AC), respectively, were compared to verify their antihyper cholesterol action in terms of inhibition of HMG-CoA reductase enzyme, protection of high-density lipoprotein (HDL) and low-density lipoprotein (LDL) from oxidation and total free cholesterol depletion.

Results

Two series of formulations were obtained combining chitosan and xanthan gum in different percentages. The obtained formulations were loaded with RYR or AC or a combination of them to evaluate their efficacy in lowering cholesterol.

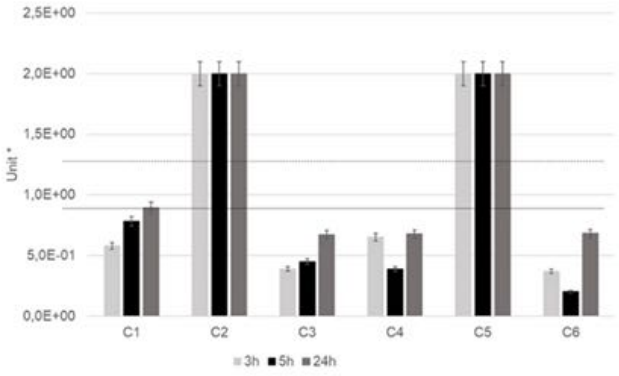
Table 1: Composition of analyzed formulations

Sample	*Chitosan-Xanthan gum (%)*	*Monacolin K (mg)*	*AC (mg)*
C1	20–80	10.01	0.00
C2	20–80	0.00	200
C3	20–80	2.992	200
C4	80–20	10.01	0.00
C5	80–20	0.00	200
C6	80–20	2.992	200
Rosuvastatin 5 mg	/	/	/

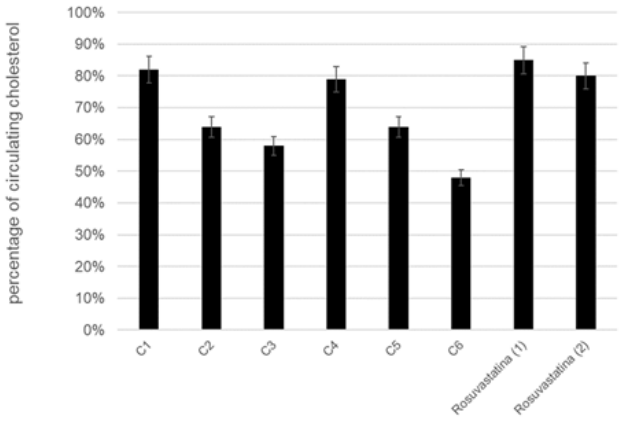
[1]Corresponding to 200 mg of RYR; [2] corresponding to 59.8 mg of RYR

The combination of Annurca apple extract and RYR showed a synergistic effect in terms of inhibition of HMG-CoA reductase, antioxidant activity towards both HDL and LDL and depleting free cholesterol. In figure is reported (a) the Inhibitory activity versus HMG-CoA reductase of all formulations as a function of kinetics release (One unit will convert 1.0 mmole of NADPH to NADPþ per 1 minute at 37°C; *The unit specific activity is defined as mmol/min/mg-protein; The lower the value the higher the inhibiting action. Continuous line: aliquots obtained after digestion of two tablets

of Rosuvastatin 5 mg dotted line: aliquots obtained after digestion of one tablet of Rosuvastatin 5 mg) and (b) Percentage of free cholesterol after incubation with different formulations. Rosuvastatin (1): 1 tablet of rosuvastatin 5 mg; Rosuvastatin (2): 2 tablets of rosuvastatin 5 mg [2].



(a)



(b)

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2C – Biodiversity valorization: development of new active food ingredients

G. Moretto, R. Colombo, A. Papetti

Aims

Italy has one of the most significant biodiversity heritages in Europe, and therefore it is important to preserve and enhance it as a source of goods and resources to ensure the maintenance of healthy ecosystems and coexistence between humans and nature. The beneficial properties of plants on human health have always been known, even before the chemical composition of the drugs used was clear. Scientific advances over time have enabled the identification of biologically active compounds, commonly referred to as secondary metabolites, to which various biological properties are attributed. In particular, several studies showed how plants and their metabolites play a role in the prevention and treatment of chronic degenerative diseases, such as diabetes, and neurodegenerative diseases, such as Alzheimer's. Uncontrolled hyperglycaemia is considered the main cause of diabetic complications, such as microvascular and macrovascular disorders, because of the formation of advanced glycation products. In addition, glycation can modulate the self-assembly and fibrillogenesis of Amyloid β (Aβ)-peptides, leading to the formation of AGE- Aβ-peptides, which appear to be more toxic and appear to accelerate the advancement of Alzheimer's disease, characterized by deposition of amyloid beta plaques at the extracellular level. This is further important in light of the identification of diabetes as a major risk factor for Alzheimer's. The aim of the present research project is to enhance the plant biodiversity by obtaining food ingredients for food supplement market. A selection of the most promising plant extracts able to interfere with the glycation reaction and with Aβ-aggregation will be performed. All the tested extracts are included in the Belfrit list (reference belfrit list). Considering that a food ingredient should be stable and its components bioaccessible, bioaccessibility studies and physico-chemical and stability tests will be performed and, if necessary, suitable food waste carriers used to stabilize and prolong the shelf-life of the ingredient.

Results

Althaea officinalis, Salvia pratensis, Succisa pratensis, Diospyros kaki, Sanguisorba officinalis, Verbaschum thapsus, Aloysia citriodora, Arthemisia abrotanum and Beta vulgaris were tested for their ability to interfere with the formation of the Advanced Glycation End products (AGEs) at different stages of the glycation reaction. Different in vitro assays have been carried out. In a screening phase of the research, NBT and BSA-MGO assays, and MGO/GO TRAPPING capacity have been performed to evaluate the anti-glycative properties at the initial and middle steps, respectively, in order to identify the most promising extracts. The results indicated that all extracts have high GO and MGO trapping capacity at 1 mg/ml (Diospyros > Sanguisorba > Succisa > Verbaschum > Salvia > Althaea). Specifically, an increase in both trapping MGO and GO capacity with increasing the incubation time for Succisa, Salvia, and Sanguisorba was observed only in GO trapping capacity for Verbaschum. Similarly, Diospyros showed high trapping MGO and GO capacity as early as after 24 hours which remained

almost constant after 96 h of incubation (96,33%) for MGO and increased to 99% for GO. Conversely, Althaea is the least active species, which showed good MGO trapping capacity but poor GO trapping capacity. In addition, all extracts counteract the AGEs formation in the middle stage of glycation (Diospyros > Succisa > Verbaschum > Sanguisorba > Althaea), with the exception of Salvia officinalis. In fact, data showed an increase in anti-glycative activity with increasing doses for each incubation time and for all extracts. Also in this case, Diospyros kaki was the most active specie, since it was able to efficiently inhibit both the formation of Argpyrimidine-like and Versperlysine-like AGEs after 1 day of incubation, followed by Succisa pratensis (with an inhibition rate of 65% and 53% after 1 day). Conversely, data showed that only Succisa, Diospyros, Salvia, and Althaea were able to inhibit the fructosamine formation at the early stage, while Sanguisorba and Verbaschum have no activity. Based on these results, Diospyros kaki and Succisa pratensis can be considered the most active and promising species and the investigation has been extended. Therefore, BSA-GLU, BSA-FRU, and OPA tests have been performed to explore the anti-glycative activity even at the final step of the reaction. Succisa and Diospyros inhibited the AGEs formation in the presence of fructose almost after 14 days of incubation. On the other hand, it has been observed a total reduction in AGEs formation after 7 days of incubation in the system glycated (BSA-GLU) in presence of Diospyros kaki and about 70% after 21 days. In parallel, the Diospyros capacity to protect the primary amino groups involved in the glycation reaction (i.e. lysine) has been evaluated by the OPA test. In accordance with the data obtained from BSA-GLU assay, the OPA test revealed 70% free lysine after 21 days of incubation. Finally, the anti-glycative activity of the second group of selected extracts (Aloysia citrodora, Arthemisia abrotanum, Beta vulgaris) has so far been studied only at the middle step. However, the results obtained indicated high trapping MGO and GO capacity, especially for Aloysia citrodora, for which a 97% and 99% reduction in MGO and GO concentration, respectively, was observed after 96 h of incubation (Aloysia>Arthemisia>Beta).

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2C – Characterization of extracts of coffee leaves (Coffea arabica L.) by spectroscopic and chromatographic/spectrometric techniques

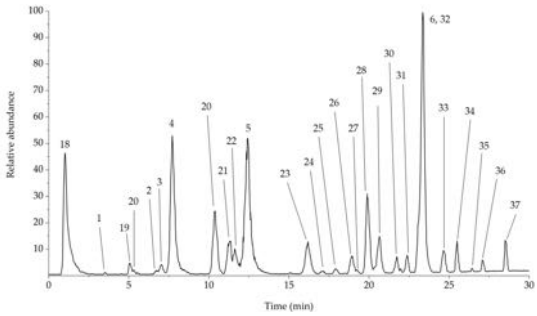
C. Bonechi, G. Leone, M. Consumi, M. Andreassi, A. Magnani, C. Rossi, G. Tamasi
(Department of Biotechnology Chemistry and Pharmacy, University of Siena)

Aims

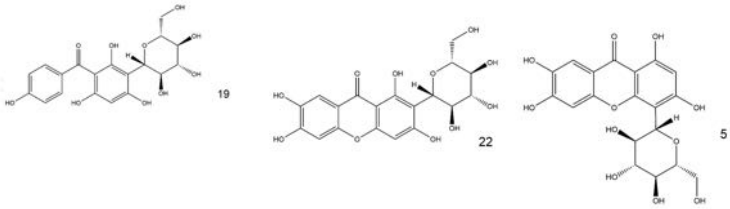
Coffea arabica L. leaves represent a viable alternative to the canonical matrices used for preparation of beverages, such as tea leaves and grounded coffee beans. Coffee leaves infusions are rich in antioxidant phenolic compounds and have a lower concentration of caffeine. Due to increasing interest in this field, a complete study of the bioactive compounds as chlorogenic acids, xanthones and alkaloids is noteworthy. C. arabica leaves were subjected to ultrasound-assisted extraction, and the extracts were studied via nuclear magnetic resonance spectroscopy (NMR) and chromatographic techniques coupled with mass spectrometry (HPLC-MS^n) to identify and quantify the secondary metabolites profile through an untargeted data dependent approach.

Results

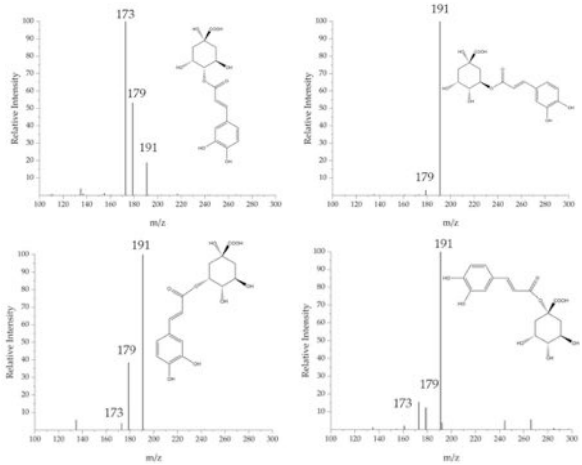
A combined NMR and HPLC-MS approach was developed with the aim to identify and quantify bioactive components in plant matrices belonging to the Coffea arabica L. family, Castillo variety. These molecules are important components of the pool of natural compounds responsible for the main beneficial effects of coffee leaves, as regards antioxidant activity. The results emphasize how coffee leaves represent an important source of bioactive compounds as functional foods. The combined use of two powerful techniques, chromatography coupled with tandem mass spectrometry and NMR spectroscopy, allowed a sound characterization of the secondary metabolites.
As example, a chromatogram is here after reported, showing peaks referred to compounds that are members of different categories of compounds: xanthones, flavonoids, chlorogenic acids, and lignans (Figure 1).



A quantitative analysis was performed for the major components (chlorogenic acids, mangiferin, caffeine and trigonelline) via HPLC-MS in Single Ion Monitoring (SIM) mode. In total, 39 compounds were identified.
In particular, the first compound related to the xanthone structure was compound 19. The deprotonated molecule shows a $[M–H]^-$ ion at m/z 407, producing ions at m/z 287 and 317 in MS^2 and 193, 243, 167 in MS^3 fragmentations. The compound was identified as iriflophenone-3-C-glucoside. Other xanthone molecules were eluted at Rt of 11.63 and 12.42 min, respectively; the molecules show the same MS^n fragmentation with a $[M–H]^-$ ion at m/z 421, and were identified as isomangiferin (22) and mangiferin (5).



The class of chlorogenic acids molecules is represented by 5-caffeoyl-quinic acids and is composed by esters of hydroxycinnamic acids (ferulic, caffeic, p-coumaric acids) with quinic acid. Mono caffeoyl-quinic acids have $[M–H]^-$ ions at m/z 353, in this study, four different species were isolated and identified as 3-CGA (1), 1-CGA (2), 4-CGA (3) and 5-CGA (4). The MS^2 fragmentation of mono caffeoyl-quinic acids are here after reported, as (a) 4-CGA, (b) 5-CGA, (c) 3-CGA, (d) 1-CGA.
The presence of these bioactive compounds provided the strong potential of C. arabica leaves as functional food and as an alternative to classic infused beverages.



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2C – Extracellular Polymeric Substances (EPS) extracted from anammox bacteria: structural, mechanical and applicative properties

E. Carretti, D. Berti, T. Lotti, C. Lubello, B. Pagliaccia

Aims

Recovering and converting Extracellular Polymeric Substances (EPS) from sewage sludge into bio-based products could enhance both the economic and environmental sustainability of biological wastewater treatment processes. In fact, utilizing waste sludge from these treatments in other industrial sectors could significantly improve the overall sustainability of the process and support the transition to a circular economy. One promising avenue for EPS valorization is their use as biosorbents for the removal of heavy metals—such as lead, copper, nickel, and zinc—commonly found in municipal and industrial wastewater.

To explore this potential, batch equilibrium biosorption tests were conducted using EPS extracted from waste anammox granular sludge, applied to both single- and multi-metal aqueous solutions. The sorption properties of the recovered EPS were compared to those of pristine anammox granules in order to better understand the adsorption mechanisms of extracted versus non-extracted EPS in the biomass. These mechanisms were further investigated using a combination of spectroscopic techniques.

The primary objective of this work is to demonstrate the feasibility of converting EPS recovered from waste anammox sludge into value-added biomaterials suitable for treating heavy metal-contaminated wastewater. Moreover, based on an in-depth analysis of the adsorption characteristics of anammox EPS, the study proposes guidelines for their potential application at an industrial scale.

Figure 1 illustrates the full pathway from waste granular sludge through EPS extraction and recovery to their use in heavy metal adsorption from urban and industrial wastewaters.

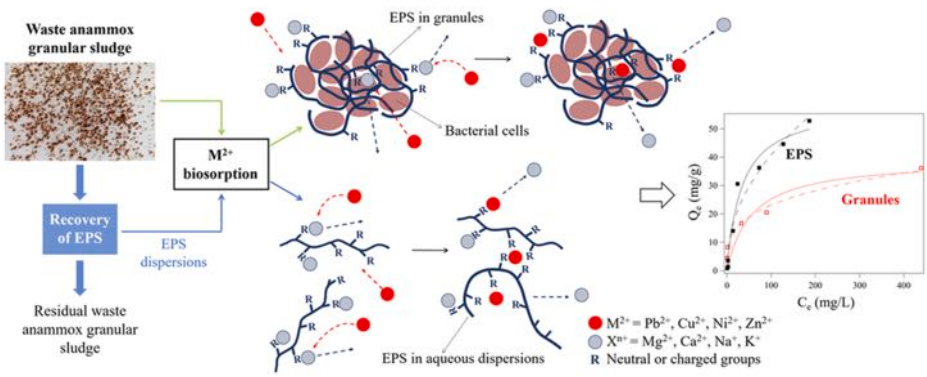

Figure 1: Extraction and application of EPS for the absorption of heavy metals

Results

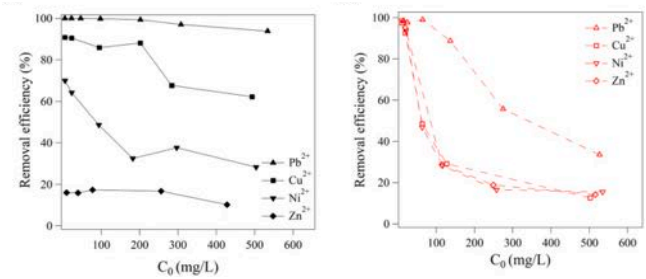

Figure 2: Removal efficiencies (%) observed for anammox EPS (right) and pristine granules (left) towards the selected heavy metal ions (Pb2+, Cu2+, Ni2+ and Zn2+) at increasing initial heavy metal concentrations (C0=5–500 mg/L).

To better understand the adsorption mechanisms of both extracted EPS and the native granular biomass, a comparison was made between extracted EPS and pristine anammox granules. The results revealed differing adsorption capacities: extracted EPS showed values of 84.9, 52.8, 21.7, and 7.4 mg/g (TSEPS), while pristine anammox granules exhibited 103.7, 36.1, 48.2, and 49.8 mg/g (TSgranules) for Pb^{2+}, Cu^{2+}, Ni^{2+}, and Zn^{2+}, respectively. In addition to the possible metal uptake by other components within pristine granules (e.g., adsorption on cell surfaces, intracellular accumulation, etc.), the metal-binding ability of EPS may be influenced by chemical alterations introduced during the extraction process, as well as by the increased mobility of EPS in aqueous dispersion, which allows for spatial rearrangement not possible in native granules.

Given their strong metal-binding properties in both single-metal and multi-metal contaminated aqueous systems, anammox EPS show promising potential for the treatment of heavy metal-contaminated wastewater.

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2C – Geographical identification of Sangiovese grapes and leaves trough elemental contents via ICP-MS analysis

R. Nardin[a], G. Tamasi[a], M. Baglioni[a], F. Bisozzi[a], M. Consumi[a], J. Costa[a], G. Fattori[a], F. Borghini[a,b], R. Esposito[a], A. Boldrini[a], C. Tozzi[b], A. Riccaboni[b,c], C. Rossi[a]

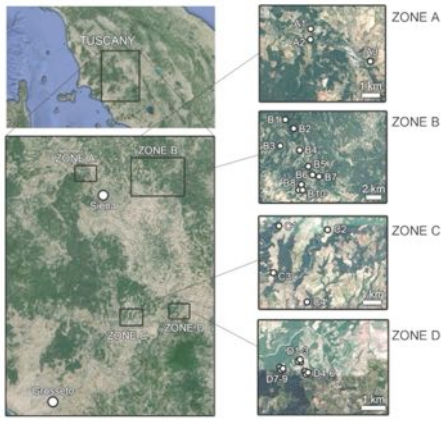
[a]*Department of Biotechnology Chemistry and Pharmacy*
[b]*Santa Chiara Lab*
[c]*Department of Business and Law, University of Siena*

Aims

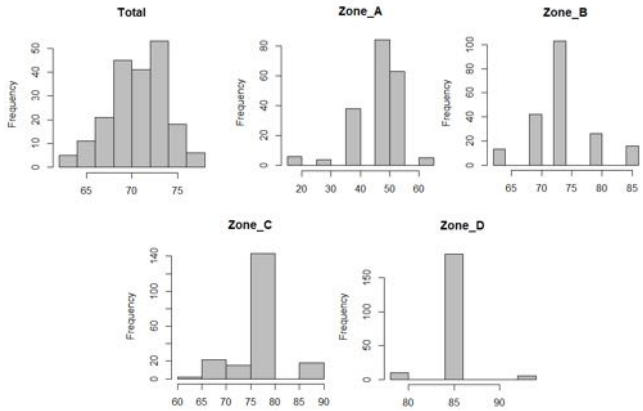
Sangiovese is a red grape variety originating from Italy and extensively cultivated in Tuscany, where it is one of the most common. It is the major component of the Chianti Classico and Chianti Wine (in which it must be present at a concentration of at least 80%), both of which are denomination protected by geographical indicators (GI). Both are protected by the PDO (Protected Designation of Origin) GI which specifies that every part of the production, processing and preparation process must take place in the specific region (Tuscany) and, for wine, that the grapes must come exclusively from the geographical area (Tuscany) indicated. This is, in fact, an aspect often overlooked in zoning studies, which usually mainly focus on finished products rather than on raw materials. Due to the importance for the region on an economic scale, to fight counterfeits and to protect the consumer, an interest in certifying the origin of agricultural goods has been growing in the last years. In this context, part of the Italian PNRR-founded Agritech center (Centro Nazionale per le Tecnologie dell'Agricoltura) that focuses on the quality and traceability of agricultural goods strives to increase the accuracy and reduce the zoning range. With Inductively coupled plasma mass spectrometry (ICP-MS) analysis, trace and ultratrace elements can be measured, and these parameters can be used to investigate the geographical origin of samples.

Results

Samples were collected in four Tuscany areas (Figure 1) to perform ICP-MS analyses of metals, metalloids and rare earth elements (REESs) on soils, leaves and grapes. Finally, the experimental data were explored applying multivariate models (principal component analysis, linear discriminant analysis, LDA, ..). Analysis of soils, showed that the concentration of toxic metals is generally low in the investigated areas, with some minor exception due to the proximity to urban centres or roads. A PCA approach was used to discriminate between soils coming from different areas, showing that Zone A is easily distinguishable from the other zones; Zones B and C are similar, yet present a statistically significant difference in their mineral composition, while Zones C and D are practically indistinguishable. A certain degree of linear correlation was found between the mineral content in soils and in leaves (especially for REEs), which is partially lost when comparing soils and grape berries. Barium was the element showing the highest soil/plant correlation both for leaves and for grapes.



A PCA-LDA approach was used to create predictive models for leaves and grapes (Figure 2), using CV to test their accuracy, and encouraging results were obtained in both cases, with an almost perfect accuracy in the case of leaves. The elements that mainly contribute to the discrimination in the LDA model computed for leaves were found to be Cs and Rb, followed by Y, Li, Ba, Pb, and ∑REEs. On the other hand, the LDA model computed for grapes mainly bases on the contribution of Pb, Zn, Sr, Ba, Li, and Cs. This was achieved, at a certain level of confidence, despite the extreme closeness of some of the sampled vineyards (10-20 km) by computing a multivariate model using selected elements.



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2C – Geographical Origin Authentication of Leaves and Drupes from Olea europaea via ^{1}H NMR and Excitation–Emission Fluorescence Spectroscopy: A Data Fusion Approach

D. Tatini[1], F. Bisozzi[1], S. Costantini[1], G. Fattori[1], A. Boldrini[1], M. Baglioni[1], C. Bonechi[1], A. Donati[1], C. Tozzi[2], A. Riccaboni[2], G. Tamasi[1], C. Rossi[1]

[1]Department of Biotechnology, Chemistry and Pharmacy, University of Siena, Via Aldo Moro 2, 53100 Siena, Italy

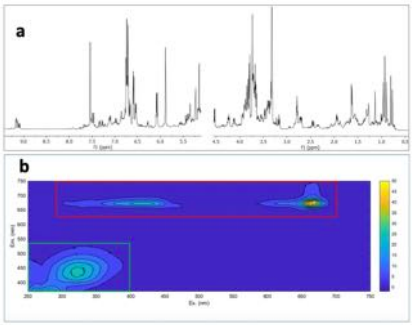
[2] Santa Chiara Lab, University of Siena, Via Valdimontone 1, 53100 Siena, Italy

Aims

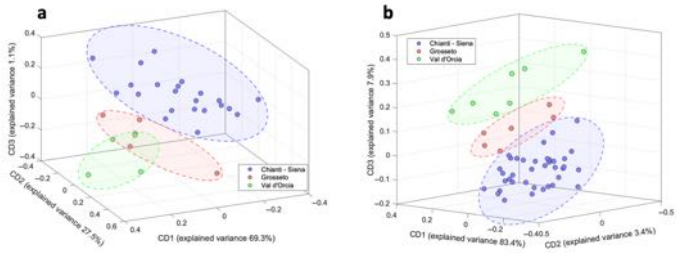
Ensuring the geographical authenticity of agricultural products is a key aspect of food quality, traceability, and consumer protection. This study explores the potential of combining ^{1}H NMR spectroscopy and excitation–emission matrix (EEM) fluorescence spectroscopy for the authentication of the geographical origin of Olea europaea leaves and drupes. While both techniques have been independently applied to olive-derived matrices, this research explores their integration using mid-level data fusion through the Common Dimensions (ComDim) algorithm. The primary goal is to determine whether this multiblock approach can enhance the classification performance over single-technique models, particularly for samples from closely related subregions of Tuscany (Chianti–Siena, Grosseto, Val d'Orcia). In addition, the study introduces a SIMCA-based class-modeling framework built on ComDim outputs, aiming to improve the reliability of one-class classification on merged datasets and explore its feasibility in practical food authentication.

Results

A total of 82 samples (51 drupes and 31 leaves) were collected across three Tuscan subregions (Chianti–Siena, Grosseto, Val d'Orcia). Samples were extracted using a methanol/water solution and analyzed using both ^{1}H NMR (a) and EEM fluorescence spectroscopy (b). Exploratory PCA revealed a partial clustering according to the geographical origin in leaf samples, particularly in ^{1}H NMR data, while drupe samples showed more complex and overlapping patterns. Parallel Factor Analysis (PARAFAC) applied to EEM data allowed the identification of fluorophores such as chlorogenic acid, tocopherols, and polyphenols.



SIMCA models based on ^{1}H NMR achieved excellent classification for olive leaves (100% sensitivity and specificity in calibration, 83% accuracy in test). EEM-based SIMCA models showed weaker performance, especially for drupes. Consequently, a ComDim-based mid-level data fusion approach was implemented, achieving a significantly improved geographical differentiation compared to the results obtained from the single-block PCA approach, as evidenced in the figure below for leaves (a) and drupes (b). Moreover, the resulting ComDim scores and residuals were used to build a multiblock SIMCA-like classification model. For leaves, the ComDim-SIMCA model performed comparably to the single ^{1}H NMR model. However, for drupes, data fusion significantly improved sensitivity and test set accuracy up to 90%.



These findings suggest that combining spectroscopic data via data fusion improves the classification performances, particularly for complex matrices such as drupes. Importantly, the study introduces the use of ComDim-SIMCA as a multiblock extension of traditional one-class classification and demonstrates its potential in agrifood traceability. The proposed classification strategy demonstrated its effectiveness at subregional level, underscoring the value of integrating complementary spectroscopic techniques to detect the chemical markers associated with geographical origin.

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2C – Human D-lactate dehydrogenase: functional and structural characterization

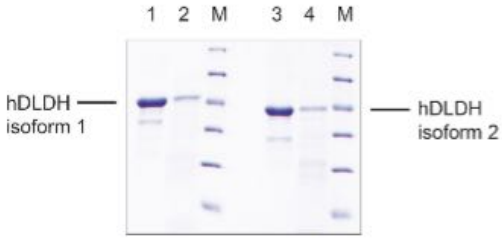
A. Stefan, A. Mucchi, A. Hochkoeppler

Aims

In humans, in addition to the well-known NADH-dependent LLDH isoforms, a gene coding for two isoforms of a D-lactate dehydrogenase has been identified. However, no information on these enzymes is available at the protein level. We describe here a procedure to overexpress in *E. coli* and to purify DLDH-1 and DLDH-2 isoforms (differing by 2.7 kDa) in order to deeply analyse some of their functional and structural features.

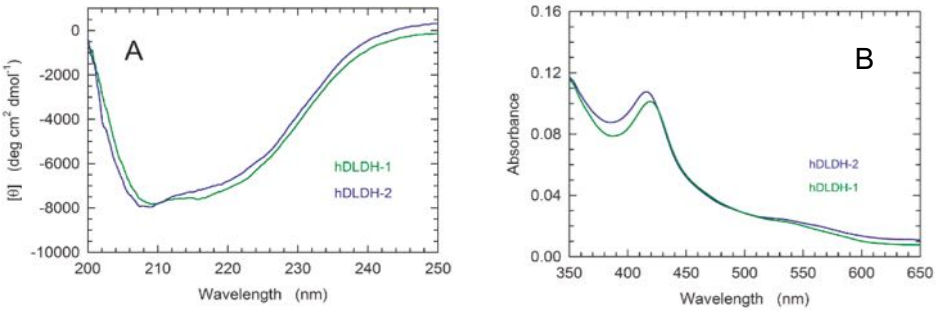
Results

To overexpress the isoforms of hDLDH, two genes, optimized for *E. coli* codon usage, were synthesized, cloned into the pET9a vector and the constructs accordingly obtained were used to transform *E. coli* BL21(DE3). Bacterial cultures were induced with 1 mM IPTG for 15h at 30 °C, then cell pellets were harvested and used for the following extraction. The procedure involves these steps: i) the insoluble fraction was resuspended with 1% (w/v) N-lauroylsarcosine for 15 h at 4°C; ii) the supernatant obtained after centrifugation was treated with Amberlite XAD-4; iii) the final soluble solution was concentrated and loaded on a Superdex-200 column. The best fractions of purified oligomeric and monomeric isoforms were pooled, quantified (ca 250 mg/L) and analysed by SDS-PAGE (Fig. 1).



To further inspect the oligomeric states of hDLDH, we performed Dynamic Light Scattering (DLS) experiments. Remarkably, when hDLDH-1 was analysed, an excellent agreement was observed between the molecular mass values estimated by gel filtration chromatography and DLS (ca 296±166 kDa, corresponding to a hexameric quaternary structure). On the contrary, the DLS experiments indicate a tetrameric structure of hDLDH-2, with a molecular mass of 213±7 kDa.

The secondary structure of both hDLDH isoforms was then analysed by means of CD spectroscopy (Fig. 2A). The two spectra are very similar with a minimum at 208 nm more pronounced in the case of hDLDH-2. Accordingly, both purified enzymes were appropriately refolded after their solubilisation by sarkosyl from inclusion bodies.



To identify the cofactor associated to purified hDHLDH-1 and hDHLDH-2 we recorded the UV–Vis absorption spectra over the 350–650 nm wavelength interval (Fig. 2B). We did not detect an absorption spectrum diagnostic of FAD, featuring a maximum at 450 nm. On the contrary the two spectra showed a single sharp band with maximal absorption shifted to shorter wavelengths (ca. 420-416 nm).

When the catalytic activity was studied, we found that both isoforms are strictly stereoselective, being unable to oxidize L-lactate. Independent assays using different concentration of D-lactate in the presence of DCPIP as electron acceptor indicate that hDLDH-1 is more efficient than hDLDH-2. Table 1 shows the kinetic parameters for both enzymes.

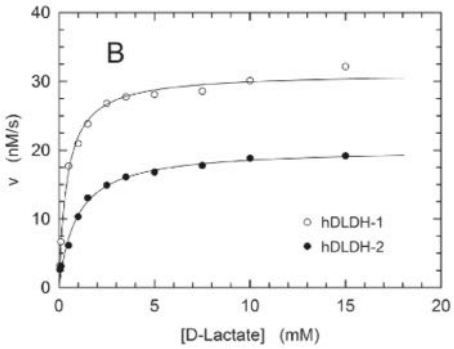


Table 1
Kinetic parameters of hDLDH-1 and hDLDH-2 determined under steady-state conditions.

Donor	Acceptor	Isoform	V_{max} (nM/s)	k_{cat} (s^{-1})	K_m (mM)
0.05–15 mM D-Lactate	50 μM DCPIP	hDLDH-1	31.2 ± 0.5	0.031	0.43 ± 0.04
0.05–15 mM D-Lactate	50 μM DCPIP	hDLDH-1	29.3 ± 0.8	0.029	0.49 ± 0.07
0.05–15 mM D-Lactate	50 μM DCPIP	hDLDH-2	20.2 ± 0.6	0.020	0.92 ± 0.11
0.05–15 mM D-Lactate	50 μM DCPIP	hDLDH-2	16.6 ± 0.3	0.017	0.80 ± 0.07

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2C – Influence of Soil Microelement Availability and potential of novel antifungal substances against Esca Disease Incidence in Grapevines

M.T. Gelaw, J. Costa, M.C. Baratto, A.M. Atrei, F. Bigazzi, L. Mugnai, R. Pogni (Department of Biotechnology, Chemistry and Pharmacy, University of Siena, Italy; Department of Agricultural, Food, Environmental and Forestry Science and Technology (DAGRI), Plant pathology and Entomology section, University of Florence,Italy)

Aims

To determine the differences in microelements in soils between asymptomatic and symptomatic soils and how to combat the disease using different antifungal substances.

Results

V. vinifera production and productivity are severely challenged by esca complex of diseases and *F. Mediterranea* is among the primary wood degradation agents causing significant yield losses globally. This study was designed to evaluate the potential effects of several antifungal substances (lignin-coated magnetic nanoparticles (LMNPs), Tagatose, and Choline Pelargonate ionic liquids) against *F. Mediterranea* under in vitro conditions using different rates of concentrations. The study was conducted under laboratory conditions using appropriate growth medium in a completely randomized design (CRD) with three replications. All antifungal substances significantly reduced the radial mycelium growth of *F. Mediterranea.* The lower rates of lignin-coated iron-based magnetic nanoparticles concentrations (25 ppm and 50 ppm) were more effective in reducing radial mycelium growth of *F. Mediterranea* than other treatments. The lowest and highest concentrations of Choline Pelargonate ionic liquid and Tagatose completely (100%) inhibited the radial mycelium growth of *F. Mediterranea.* Further in vivo efficacy and mechanistic analysis of the different antifungal substances may ascertain the future applicability. Furthermore soil samples underwent both EPR spectroscopy and ICP-MS analysis to determine the presence and concentration of 20 microelements. Preliminary ANOVA results indicate statistically significant differences in several elements between high- and low-incidence areas. These findings support the need for further investigation into soil chemistry as a contributing factor in Esca development.

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2C – Lignans from flaxseed: biological properties and recovery technologies

P. Sangiorgio[a], S. Errico[a], A. Verardi[a], S. Moliterni[a], G. Tamasi[b], C. Rossi[b], R. Balducchi[a]

[a]ENEA, Italian National Agency for New Technologies, Energy and Sustainable Economic Development, Trisaia Research Centre

[b]Department of Biotechnology Chemistry and Pharmacy, University of Siena)

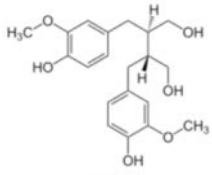
Aims

Flaxseed lignans frequently feature in the literature, however, much remains to be discovered about the mechanisms underlying their functional and therapeutic properties. Furthermore, it is necessary to identify systems for lignan production and detoxification that are sustainable, cost-effective, easy to use, and scale up. These systems can address the needs of the nutraceutical, cosmetic, and pharmaceutical sectors and lead to competitive commercial products. This study analyzes the biological effects of lignans as anticancer, antioxidants, and modulators of estrogen activity. It also focuses on lignan extraction and recovery sustainable methods that are suitable as products for human consumption.

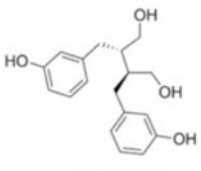
Results

Flaxseeds are one of the plant matrices richest in lignans, and have attracted interest in the last decade, due to their health-beneficial compounds, especially in the functional and vegan food sector. The flaxseed lignan industry is booming due to the therapeutic potential of flaxseed in the treatment of high-incidence chronic diseases in industrialized countries. Furthermore, flaxseed lignans can be successfully used as nutraceutical ingredients or incorporated into functional products to combat diseases associated with an unhealthy lifestyle by adopting as natural a strategy as possible. In the last 20 years, research has led to the development of numerous technologies for the extraction and detoxification of lignans from flaxseed, and to multiple patented inventions.

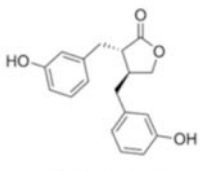
Lignans are phenolic compounds, having a strong antioxidant capacity, which inextricably links them to beneficial effects on human health. Moreover, secoisolariciresinol (SECO), like the other lignans found in flaxseed (matairesinol, lariciresinol, and pinoresinol), are mammalian estrogen precursors that are converted to enterolignans, enterodiol, and enterolactone, by the anaerobic intestinal microflora.



SECO



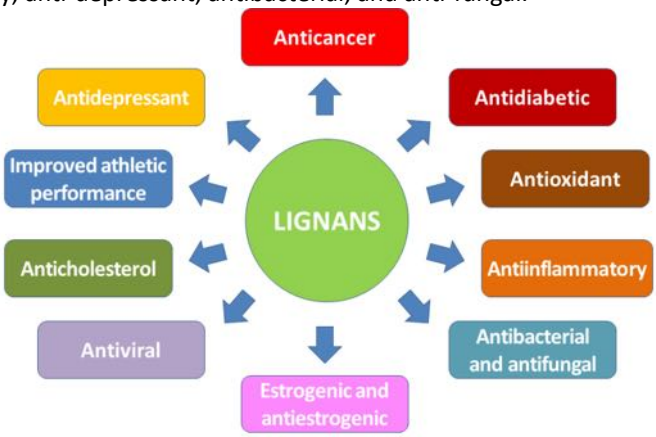
Enterodiol



Enterolactone

The most relevant beneficial effects of lignans are summarized in the next figure and span from anticholesterol, antiviral, anticancer, antioxidant, supplemental for

improved athletic performance, antidiabetic, estrogenic and anti-estrogenic, anti-inflammatory, anti-depressant, antibacterial, and anti-fungal.



Another important point of interest is the selection of methodology based on the solvent extraction of flaxseed lignans that increases efficiency if supported by unconventional technologies, such as ultrasound and microwave. In this case, it is possible to use green or low toxic solvents, such as water and ethanol. However, further studies are needed to develop more sustainable, efficient, and effective recovery methods for obtaining purified and detoxified lignans at a large scale.
In this way, it will be possible to further explore the biological activities of lignans and respond to the growing market demand.

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2C – Metabolomics as a Tool to Explore Adaptive and Pathological Processes

F. Cesare Marincola[1], V. Fanos[2], A. Dessì[2]
[1]*Department of Chemical and geological sciences, University of Cagliari-CSGI*
[2]*Dipartimento di Scienze Chirurgiche, University of Cagliari*

Aims

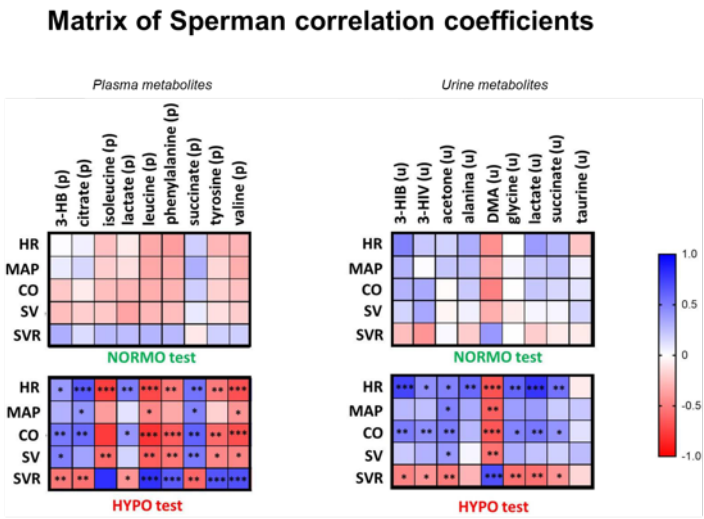
Metabolomics provides a systems-level view of biochemical dynamics by detecting low-molecular-weight metabolites that reflect physiological and pathological states. In the present research, ^{1}H NMR spectroscopy, integrated with multivariate and univariate statistical approaches, was applied to two different biomedical questions. The first study investigated the metabolic response to an acute bout of mild dynamic exercise performed under normobaric moderate hypoxia, with the aim of identifying metabolic pathways influenced by oxygen availability and linking them to hemodynamic changes. The second focused on the urinary metabolome of newborns from diabetic mothers, exploring the impact of maternal therapy (diet versus insulin) on early postnatal metabolic profiles and the potential for biomarker discovery. Both projects aimed to demonstrate the utility of metabolomics in characterizing adaptive and pathological processes in early and adult life.

Results

In the study on newborns of diabetic mothers, urine samples were collected from 26 newborns: 21 children of diabetic mothers, comprising 13 in diet therapy and 8 in insulin therapy and 5 control children of non-diabetic mothers (CTR). Urine samples were collected at five time points: at birth, on the third day of life, one week, one month and six months postpartum. At birth, infants of insulin-treated diabetic mothers showed altered levels of seven urinary metabolites, including acetate, lactate, glycylproline/proline, isocitrate, *N,N*-dimethylglycine, *N*-acetylglucosamine, and *N*-carbamoyl-aspartate, compared with diet-treated infants and controls. These differences involved key pathways such as the citrate cycle, amino acid metabolism (glycine, serine, threonine, arginine, proline), amino sugar metabolism, and pyruvate metabolism. However, the alterations were no longer detectable at later time points, suggesting that early nutrition, from maternal or formula milk, may have influenced the normalization of the metabolomic profile.

In the hypoxia–exercise study, plasma and urine samples from 13 healthy volunteers were collected before and after exercise performed under normoxia (Normo test) and hypoxia (Hypo test). Multivariate statistical analysis revealed distinct metabolic signatures depending on oxygen availability. Hypoxia was associated with enhanced glycolytic flux, evidenced by increased lactate, and alanine, while changes in tricarboxylic acid (TCA) intermediates such as citrate and succinate suggested a shift in mitochondrial energy metabolism. Correlation analysis with hemodynamic parameters demonstrated links between metabolic responses and cardiovascular adaptations, highlighting metabolomics as a sensitive tool to monitor hypoxia-induced stress.

Overall, these findings support the translational potential of metabolomics in understanding adaptive physiology and identifying early biomarkers of risk.



HR, Heart rate; CO, cardiac output; MAP, mean arterial pressure; SV, stroke volume; SVR, systemic vascular resistance. 3-HB, 3-hydroxybutyrate; 3-HIB, 3-hydroxyisobutyrate; 3-HIV, 3-hydroxyisovalerate.

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2C – Minimization of Biological Sludge through the TAMR (Thermophilic Aerobic Membrane Reactor) Process

M.C. Collivignarelli, C. Milanese, S. Bellazzi, L.M.R. Calabria, A. Abbà

Project: Progetto STABIRA - Funding body: Unione Europea (NextGenerationEU)

Aims

This project develops an innovative thermophilic fluidized bed biological reactor, integrated with membrane filtration, for treating sludge from mixed municipal and industrial wastewater. It aims to drastically reduce sludge at the source, recover energy and nutrients, and promote agricultural reuse. The technology allows near-complete sludge reduction and maximized recovery of organic matter and thermal energy, supporting the transition to circular economy models. Its integration into the sludge line for in-situ treatment is a novel application. Additionally, the project emphasizes digitalization in wastewater management and includes strategies for full-scale validation and market implementation, highlighting its international innovation potential.

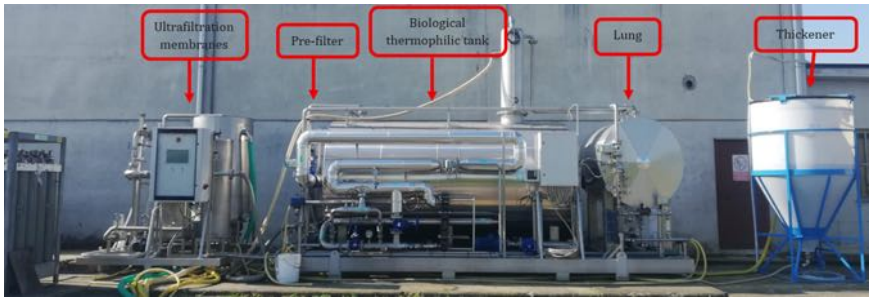

Figure 1: TAMR pilot Plant.

Results

The TAMR pilot plant showed good performance even under complex and unfavorable operating conditions.
In particular, three fundamental strengths emerged:
• PROCESS “RESILIENS”: the thermophilic biomass operated stably right from the start despite the high variability in the qualitative characteristics (COD) of the incoming thickened sludge, demonstrating great adaptability and process continuity.
• HIGH PERFORMANCE: already in the first week of operation, very good values were obtained both in terms of total solids reduction and COD removal, confirming that the TAMR process is immediately effective and does not require long acclimatization periods.
• QUICK RESTART CAPABILITY AFTER EXTENDED SHUTDOWNS: the TAMR process

demonstrated good resilience, being able to quickly reactivate biological activity even after weeks without organic substrate feeding; with temperatures below optimal thermophilic levels and no oxygen supply.
Regarding respirometric tests, it emerged that the thermophilic biomass showed good "acclimatization" during the plant startup phase, as evidenced by the trend in endogenous respiration:
The healthy state of the thermophilic biomass was confirmed by the rather high values of endogenous OUR.
The comparison between exogenous OUR values on the permeate by the two biomasses (thermophilic and mesophilic) highlighted, on the one hand, a significant complementarity of action between the thermophilic and mesophilic biomass, and on the other, confirmation that the HRT in the thermophilic tank is sufficient for the degradation of the organic matter (Figure 2).

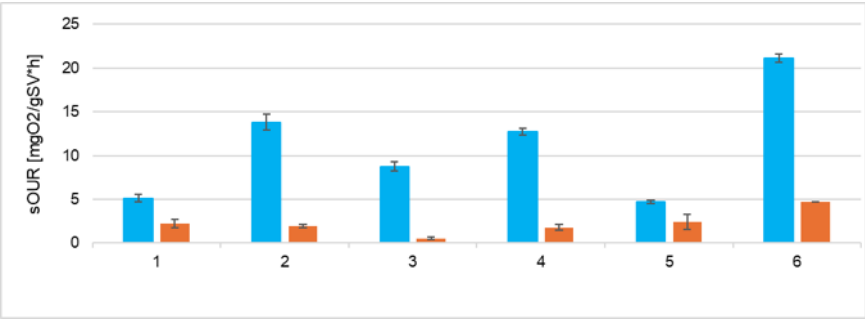

Figure 2: Results of the OUR respirometric tests conducted on thermophilic and mesophilic biomass to evaluate exogenous respiration in contact with the permeate from the TAMR plant.

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2C – Peptides inhibiting the assembly of monomeric human L-lactate dehydrogenase into catalytically active homotetramer

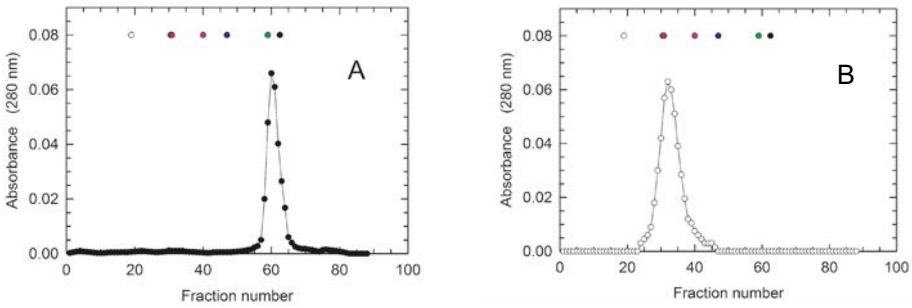
A. Stefan, L. Gentilucci, F. Ruffolo, V. Rossi, S. Sordi, T. He, G. di Stefano, F. Santino, M. Brigotti, C. Scotti, L. Iamele, H. de Jonge, F. Dal Piaz, D.R. Santarcangelo, A. Hochkoeppler

Aims

Human lactate dehydrogenase A (hLDH-A), responsible for the reduction of pyruvate to lactate, is overexpressed in different types of cancers and therefore represents an appealing therapeutic target. Since the activity is exerted by the tetrameric form, the dissociation of the homotetramer can lead to a loss of activity. Here we report on the unprecedented isolation of recombinant monomeric hLDH-A at neutral pH, and on its use to identify peptides inhibiting the assembly of the tetrameric enzyme.

Results

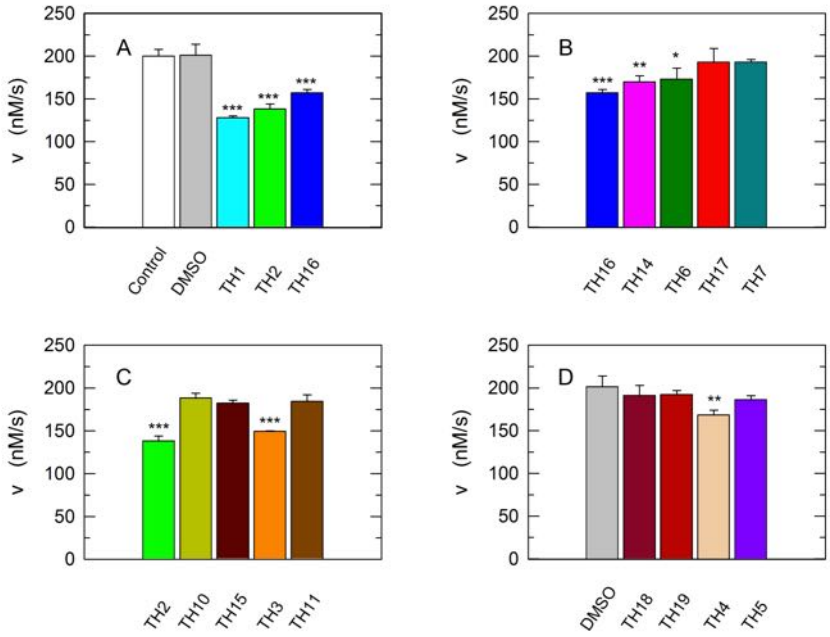
To overexpress hLDH-A in *Escherichia coli* we used a synthetic gene optimized for the codon usage of the bacterial host. The target protein was overexpressed in a soluble form and then purified with standard chromatographic methods. In particular, the first purification step was carried out with a Cibacron Blue column, a further separation from contaminants was obtained by means of hydrophobic interaction chromatography and the final step involved a gel filtration chromatography. Intriguingly, the monomeric LDH-A was eluted from the column in the presence of 10 mM Tris-HCl or 10 mM HEPES (pH 7.5) (Fig. 1A), while we obtained the tetrameric enzyme under condition of high ionic strength (150 mM NaCl, Fig. 1B). Dynamic Light Scattering experiments (DLS) confirmed this observation and revealed that the addition of β-NADH and oxamate triggers the assembly of LDH-A monomers into the



tetrameric form (LDH-5).

Activity assays performed in 10 mM Tris-HCl in the presence of 100 μM β-NADH and 500 μM of pyruvate showed a reaction rate lower for the monomeric enzyme when compared to the tetrameric form suggesting a partial assembly of the LDH-A monomers into the tetrameric enzyme.

Structurally speaking, the four subunits of LDH-5 are arranged as a binary association of dimers, with their N- and C-terminal regions reciprocally engaged in dimer-dimer interactions. Therefore, we selected the N-terminal region of LDH-A as a target of peptides hopefully able to interfere with the assembly of LDH-5. Accordingly, we designed several peptides (Fig. 2), featuring a linear or cyclic structure, unprotected or protected, to be tested in vitro in the presence of the monomeric enzyme. We performed activity assays under steady-state conditions, in Tris-BisTris (10 mM each) buffer (pH 7.5) in the presence of 6 nM monomeric enzyme, 125 µM β-NADH, 0.5 mM pyruvate and 80 µM peptide. The LDH activity was also detected in the absence of any peptide. We found that the octameric linear peptide TH1 (sequence GQNGISDL) was able to decrease the observed LDH activity by 36 %.



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2C – Phenolic profiles of olive leaves from Tuscany cultivars and their use as a marker for varietal and geographical origin

F. Borghini[a,b], G. Tamasi[a], S.A. Loiselle[a],M. Baglioni[a], F. Bisozzi[a], S. Costantini[a], D. Tatini[a], R. Esposito[a], A. Boldrini[a], C. Tozzi[b], A. Riccaboni[b,c], S. Ferrari[d], C. Rossi[a]

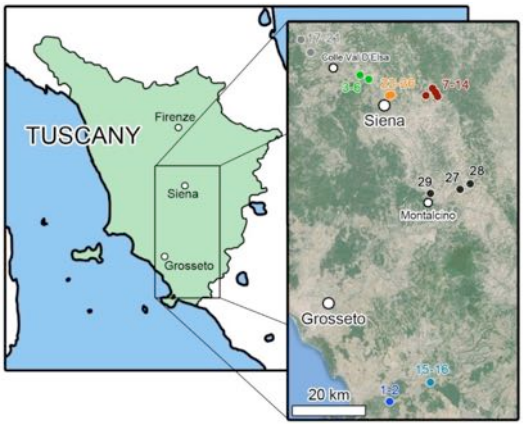
[a]*Department of Biotechnology Chemistry and Pharmacy*
[b]*Santa Chiara Lab*
[c]*Department of Business and Law, University of Siena*
[d]*ISVEA laboratories, Poggibonsi, Siena*

Aims

Olive leaves are a rich source of polyphenols with healthful properties and represent one of the most abundant waste products of olive oil production. The aims of this research were to explore the phenolic composition of olive leaves from the three main Tuscan cultivars (Leccino, Moraiolo and Frantoio) collected in Siena and Grosseto provinces and to investigate the possible use of these compounds as varietal and geographic origin markers. Discriminant factorial analysis (DFA) was used for distinguishing between different cultivars and locations. Apigenin and caffeoylsecologanoside showed significant differences between cultivars. DFA showed that ligstroside, apigenin and luteolin have the most influence in determining the differences between sites, whereas total polyphenols, olacein and hydroxytyrosol acetate allowed for separation between leaves from the same province.

Results

Samples of olive leaves belonging to the Leccino, Moraiolo and Frantoio varieties were collected in different Tuscany areas (Figure 1), and targeted high resolution mass spectrometry analysis, through an Orbitrap 120 instrument (Thermo Scientific) was performed.

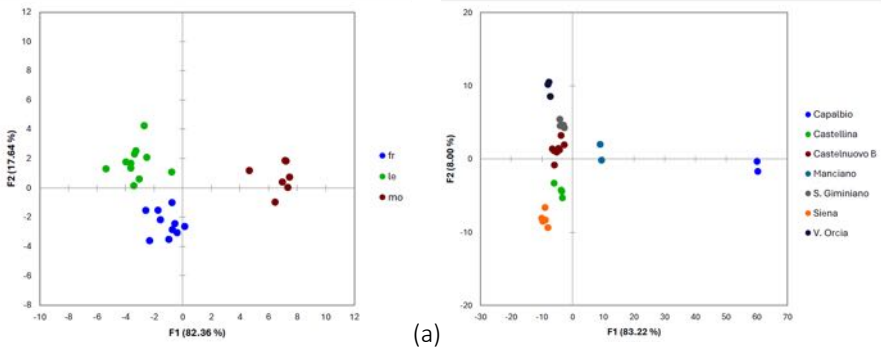


	Site	Cultivar	Altitude
1	Capalbio	Leccino	250
2	Capalbio	Moraiolo	250
3	Castellina in Chianti	Frantoio	292
4	Castellina in Chianti	Leccino	292
5	Castellina in Chianti	Leccino	268
6	Castellina in Chianti	Moraiolo	292
7	Castelnuovo Berardenga	Frantoio	304
8	Castelnuovo Berardenga	Frantoio	300
9	Castelnuovo Berardenga	Frantoio	304
10	Castelnuovo Berardenga	Leccino	300
11	Castelnuovo Berardenga	Leccino	304
12	Castelnuovo Berardenga	Leccino	313
13	Castelnuovo Berardenga	Moraiolo	304
14	Castelnuovo Berardenga	Moraiolo	300
15	Manciano	Frantoio	300
16	Manciano	Leccino	300
17	San Gimignano	Frantoio	282
18	San Gimignano	Frantoio	299
19	San Gimignano	Leccino	282
20	San Gimignano	Leccino	299
21	San Gimignano	Moraiolo	299
22	Siena	Frantoio	305
23	Siena	Frantoio	296
24	Siena	Leccino	305
25	Siena	Leccino	296
26	Siena	Moraiolo	305
27	Val d'Orcia	Frantoio	339
28	Val d'Orcia	Leccino	359
29	Val d'Orcia	Moraiolo	495

Discriminant factorial analysis (DFA) was firstly performed using all variables (n = 29) and then was repeated by eliminating the multicollinearity highlighted by the analysis of the VIF and the correlation matrix (n = 16). The DFA of phenolic profiles showed a clear separation between cultivars along the two factors, with Moraiolo separated well on F1, while Frantoio and Leccino separated along F2 (Figure 2a). In fact, F1, accounting for most of variation (82%), was dominated by flavonoids, luteolin-7-glucoside (correlation 0.407), apigenin (0.368), hydroxytyrosol glucoside (0.350), secoiridoid ligstroside (0.386) and the triterpene maslinic acid. The second factor (F2) was dominated by caffeoyl-secologanoside (0.483) and maslinic acid (−0.404), showing the ability of these compounds to separate more similar cultivars.

DFA was also used to explore dominant phenols characterizing sampling sites (Figure 2b). The first factor (F1) accounted for the majority of the variation between sites (83%), while the second one accounted for 8%. The leaves sampled in Manciano and Capalbio (Grosseto province) show positive values of F1, whereas all those taken in Siena province have negative values. Sites within the same provinces also showed some separation: along F1 for the two Grosseto sites and along F2 for the Siena sites. F1 was dominated by ligstroside (0.753, λ = 0.27), apigenin (0.470, λ = 0.61) and luteolin (0.389, λ = 0.56), while F2 was defined by TPC (0.717, λ = 0.42), olacein (0.566, λ = 0.42) and hydroxytyrosol acetate (0.563, λ = 0.47).

The results of the present study indicate that concentrations of phenolic compounds, measured through high-resolution mass spectrometry, can be used as a marker for both the cultivar and of geographical origin of olive leaves, and possibly of olive-related products, as well as across small geographic scales (less than 50 km distance between sites).



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2C – Tyrosine inhibits the Mycobacterium tuberculosis protein tyrosine phosphatase MptpA

A. Stefan, C. Palazzetti, A. Hochkoeppler

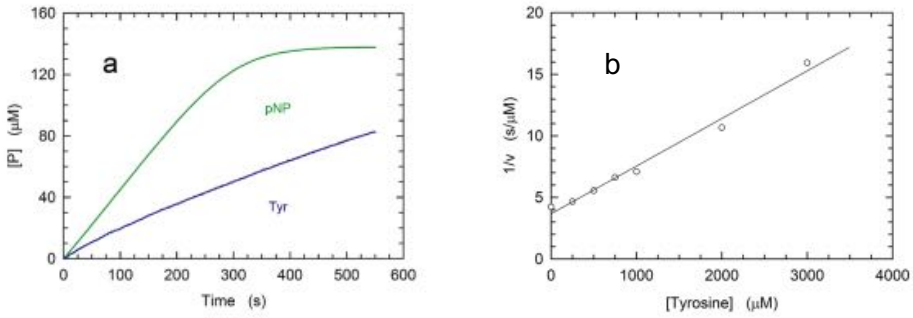
Aims

The catalytic action of the low-molecular weight protein tyrosine phosphatase (MptpA) expressed by *Mycobacterium tuberculosis* is essential for the pathogenicity of the bacterium capable to escape the host immune system. In particular, this LMW-PTPase (17,9 kDa) is able to inactivate the host VPS33B protein thus inhibiting the phagosome-lysosome fusion. Consequently, MptpA is an appealing target for the search of anti-tuberculosis drugs. In this study we show that the enzyme activity at the expense of phosphotyrosine (pTyr) is promptly inhibited by tyrosine, whereas the p-nitrophenol antagonizes the enzyme to a limited extent. This suggests a significant inhibitory role of the α-aminocarboxylic acid moiety of the aromatic amino acid. This may, in turn, recommend the design of MptpA competitive inhibitors targeting the portion of the enzyme active site which is distal from the phosphate-binding region.

Results

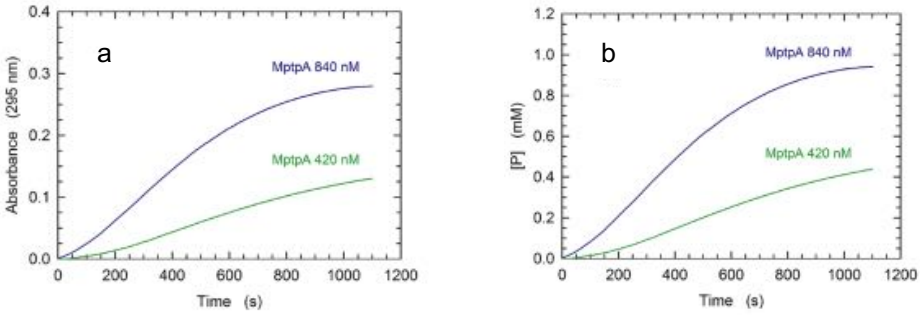
We report the outcome of experiments performed in TBE buffer (25 mM Tris-HCl, 25 mM Bis-Tris, 2 mM EDTA, pH 7.5) in the presence of 420 nM MptpA, using 10 mM pTyr or 10 mM pNPP as substrate. Absorbance changes at 282 nm were observed using a Cary 300 Bio UV–VIS spectrophotometer. A Δε of 0.96 mM−1 cm−1 between tyrosine and phosphotyrosine at 282 nm and a ε of 18.3 mM−1 cm−1 for p-nitrophenol at 405 nm were used.

In the presence of pTyr the reaction kinetics was early subjected to a significant slowdown in sharp contrast to the output detected when the substrate was pNPP (Fig. 1a). We then tested whether or not tyrosine significantly inhibited the catalytic action of MptpA by monitoring changes in Absorbance at 286 nm triggered by the addition of 5 mM pTyr to MptpA, in the absence or in the presence of increasing concentrations of tyrosine (up to 3 mM, Fig. 1 b).



We obtained a value of Ki of MptpA for tyrosine equal to 512±26 µM, one order of magnitude lower than the corresponding previously determined Ki for orthophosphate (Stefan et al. 2020).

We further tested the efficacy of tyrosine as inhibitor of MptpA by using an enzyme-coupled assay in the presence of tyrosinase (50 U/mL), 10 mM pTyr and 420 or 840 nM MptpA (in TBE buffer at pH 7). The generation of L-DOPA from L-tyrosine was measured at 295 nm (at this wavelength the interference by tyrosine is minimal). This assay showed an initial lag phase lasting for 250-300s followed by a linear phase (Fig. 2a). Conversion of the Absorbance values (using a Δε of 0.297 mM−1 cm−1 between L-DOPA and tyrosine at 295 nm) indicates a linear phase up to 200 and 400 µM of reaction product (Fig. 2b). This observation confirms that tyrosine is quite an effective inhibitor of MptpA.



Overall, our observations suggest that the α-aminocarboxylic acid moiety of tyrosine is responsible for the inhibitory competence of this amino acid. These observations could help in the design of inhibitors targeting MptpA, which is an essential determinant of *M. tuberculosis* pathogenicity.

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Author Index

A

B

C

D

E

F

G

H

I

J

K

L

M

N

O

P

Q

R

S

T

U

V

Z