Consorzio Interuniversitario per lo Sviluppo dei Sistemi a Grande Interfase

Report 2020

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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

2B: Metals and Ceramics

2C: Biotechnology

CSGI Research Activity

Outline

CSGI (Research Center for Colloids and Nanoscience) was established in Firenze, in December 1993. It has been officially recognized by the Italian Government in 1994, and is under the supervision and control of the Italian Ministry for the University and Scientific Research (MUR). Since its foundation CSGI has been promoting and coordinating scientific initiatives in Italy for the training and technological transfer in the field of chemistry of colloidal systems, and more generally in the field of solid condensed matter. In this context CSGI plans and implements actions that make basic and applied research and technological transfer possible for businesses, facilitating their access to the activity of national, international or "large scale infrastructures" laboratories and to local, national and European projects. CSGI is an internationally recognized network of excellence in Italian chemistry; the positioning in the scientific panorama is validated by the VQR 2011-2014, where CSGI is the consortium with the highest number of members in Chemistry, with over 94% of the products rated as Excellent, I> 0.94.

CSGI is recipient of an annual Government funding that constitutes a multiplier for the attraction of industrial funds and resources obtained on a competitive basis with consortium co-financing. This strategy is particularly effective, given that 80% of CSGI budget is made of funds from collaborations with small-medium and large industries, as well as regional, national and, particularly, European funds.

Scientific Research

CSGI brings together the most important Italian scientific schools in the field of Soft Matter and Functional Surfaces, providing a support infrastructure for the Italian academic network operating in this thematic area.

Over the years CSGI has built an important international network for technological transfer, involving Italian, European and international research bodies and some important industrial multinationals (ENI, Procter & Gamble, Biomeuriex, L’Oreal, pharmaceutical IDI, Dompé, Rottapharm etc.). This third mission activity allowed the creation of strategic synergies between the consortium units and public and private entities. Spin-off are active: LifeCARES srl (Life Cycle Assessment, Renewable Energy and Sustainability) and WeGoNANO (Working Group on carbon-based and Glycan-based NANOstructured materials), aiming to develope multifunctional nanostructured functionalized biocompatible materials, starting from the specific companies needs. Finally, CSGI is coordinator of the European Cluster for cultural heritage ECHOES (Enabling Cultural Heritage-Oriented European Strategies), which contributes to the formation of EU research guidelines in the field of conservation materials.

The CSGI training capacity is also recognized by the European Community through the H2020 Marie Curie projects. CSGI is the only Italian consortium to coordinate an European Industrial Doctorate, in partnership with Procter & Gamble.

In January 2020 the following European projects are active: APACHE - Active & intelligent PAckaging materials and display cases as a tool for preventive conservation of Cultural Heritage, (H2020-NMBP-ST-IND-2018, CSGI coordinator), evFOUNDRY - The Extracellular Vesicle Foundry (H2020-FETOPEN-1-2016-2017, CSGI coordinator), SIMBIT - Single molecule bio-electronic smart system array for clinical testing (H2020-

ICT-2018-2, CSGI coordinator), GEOENVI - Tackling the environmental concerns for deploying geothermal energy in Europe (H2020-LC-SC3-2018), SAMCAPS - Self-Assembled MicroCAPSule: Synthesis, Characterization, and Eco-friendly Application in Home Care Products (Marie Curie European Industrial Doctorate EID, CSGI coordinator), ESPRESSO - Efficient Structures and Processes for Reliable Perovskite Solar Modules (H2020-LCE-2017-RES-RIA-TwoStage), E-RIHS - European Research Infrastructure for Heritage Science (H2020-INFRADEV-2016-2), InnovaConcrete - Innovative materials a nd techniques for the conservation of 20th century concrete-based cultural heritage (H2020-NMBP-2017-two-stage), ICARUS - Innovative Coarsening-resistant Alloys with enhanced Radiation tolerance and Ultra-fine -grained Structure for aerospace application (H2020-FETOPEN -2014-2015-rIA). All these projects gather industrial partners, both small-medium and large; in many cases CSGI is the coordinator of the network, confirming the proactivity and the capacity for involvement and logistical and administrative support of the consortium structure.

Training, Dissemination and Technological Transfer Activities

Most intellectual, scientific and budgetary resources are devoted to these three aspects (e.g. scholarships, Ph.D., research grants, support for dissemination and training initiatives such as workshops, schools, conferences). In fact, the CSGI Consortium aims at the training of specific highly qualified figures in the field of advanced formulations, declined in all areas for which knowledge of Soft Matter and Surface and Interphases Chemistry is primary.

To date, the CSGI is the only Italian center active in three levels of training in the field of chemical-physical formulations, a sector of primary importance both for large industry and for small and medium-sized enterprises.

CSGI is also very active in the training of specialized researchers, has granted several fellowships, PhD supporting programs, post-doc grants, and other educational projects, and has organized several national and international meetings and symposia. In particular, between 2017 and 2020, CSGI members carried out training activities in the supervision of 152 three-year and master's degree theses, in 47 Ph.D. theses (18 financed by CSGI funds). Also noteworthy is the extra-curricular training activity in third level Masters, courses for Ph. D. Schools, organization of schools and workshops.

Among the dissemination/outreach initiatives of 2019, it should be reported:

- CSGI - Procter & Gamble Workshop (May 2019 and December 2019, Florence);
- CHESS School (Conventional And High-Energy Spectroscopies For Inorganic, Organic and Biomolecular Surfaces and Interfaces, An Unconventional School for Ph.D Students and Young Investigators, Florence, December 2-6 2019), organized by CSGI members of Bari and Florence UOs;
- Final workshop of the EU BioClean project ("BIOfilm management and CLEANing by leveraging fundamental understanding of biological, chemical and physical combined approaches", Bari, 1-2 October 2019, open session);
- 1st Clustering Event For Extracellular Vesicles FET-Open Projects, Palermo 6 November 2019, which brought together the 5 EU FET projects on extracellular vesicles, with the participation of 34 research and industrial organizations from 15 European countries;
- EU Symposium, 20 March 2019 (session 3) – RE - designing Access to Cultural Heritage for a wider participation in preservation, (re-) use and management of European culture;

- Meeting May 2019 EU organized by CSGI for "Clustering / Networking / Participation in activities jointly organized with other H2020 projects";
- Material Testing Symposium, 6-8 November 2019, New York City (USA);
- British Museum Conference and Workshops on APACHE Project & Nano-Systems Research and Applications on Cultural Heritage, 4-5 June 2019;
- NanoInnovation 2019, 13 June 2019, Rome (Italy), Innovative nanomaterials for cultural heritage;
- Advanced Materials and Nanotechnologies at the service of Cultural Heritage Conservation, 9 March 2019;
- Apache project presentation, Brazil, April 2, 2019;
- Bright. The European Research Night (various CSGI locations, 27 September 2019).

CSGI has also co-sponsored national and international congresses (Global Women's Breakfast, Fun4Heritage Functional Materials for Cultural Heritage, Chess 2019 - Conventional and High Energy Spectroscopier for Inorganic, Organic and Biomolecular Surface and Interface, Water and Water Systems – The Hydrophobic Effect, Scuola ISPC 2018 – International School of Physical Chemistry).

The CSGI financial plan is solid, with a strong growth of its financial assets, mainly due to EU funding.

The main topics of CSGI research activity are:

- development of processes to produce: nanophasic systems (i) innovative textiles, (ii) nanophasic alloys, (iii) ceramics and nanophasic or nanostructured composites (with low temperature and low energy costs);
- formulation of dispersions in fluids, emulsions and inverted emulsions (paints, adhesives, sealing materials, detergents, etc.);
- development of systems for the confinement of proteins and for the controlled release of pharmaceutics;
- development of food-related industrial processes (for example the treatment of milk and milk derivatives in supercritical phase);
- development of innovative procedures for the conservation and restoration of works of art (paintings, frescoes and stone-based materials).

Fields of Interest

- Nanostructured and ultrafine materials.
- Structure and dynamics of supramolecular assemblies (monolayers, micelles, liposomes, microemulsions, Langmuir-Blodgett films, host-guest systems).
- Nanophasic ternary oxides, Hydrogen storage.
- Structural analysis of biomolecules in solution, interaction processes, recognition of ligands with macromolecular surfaces, theoretical and experimental analysis of cellular metabolism, interactions between metals and ligands, characterization of the interaction sites.
- Formulation of nanophasic systems.
- Innovative methodologies and materials for the conservation and restoration of cultural heritage (stone materials, wood materials, paintings, frescoes, paper, photographic material).

National Agency for the evaluation of Quality of Research: CSGI ranking

CSGI was one of the 9 Consortia that voluntary submitted their candidature, for the second time in a raw, to the Italian evaluation of universities and research centers: Valutazione della Qualità della Ricerca (VQR), an exercise to evaluate the quality of the research efforts. The report was produced by Agenzia Nazionale di Valutazione del sistema Universitario e della Ricerca (ANVUR), the Italian national agency for the Italian research qualification. VQR 2006-2010 and 2011-2014 resulted in the largest-scale evaluations of research in Italy's history (2011-2014 is the last evaluation available, the results for the next evaluation 2015-2020 will be available in 2021).

The VQR examined research outcomes in 14 disciplinary areas of study published between 2011 and 2014 by 96 universities, 18 research centers and 19 other institutions to identify the significance of the Italian research output and how it compares globally. By reviewing a significant number of Italian research outcomes, ANVUR could gain a greater understanding of Italian research strengths, impact and neglected fields of study.

CSGI ranked in the first position among the other Italian Consortia for Chemistry for the period 2011-2014.

In the disciplines related to Chemical Sciences (the core of the CSGI research), CSGI resulted as excellent.

Structure and Organization of CSGI

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

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

President of CSGI
Prof. Giovanni Marletta, Department of Chemical Sciences, University of Catania.

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.csgi.unifi.it/

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 (headquarter)
- 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

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 Perugia
- ○ University of Rome, La Sapienza
- ○ University of Rome, Tor Vergata
- ○ University of Rome - TRE
- ○ University of Venice

Personnel

CSGI gathers about 300 researchers including Full Professors, Associate Professors, University Researchers.

Moreover, CSGI employs 35 researchers and 4 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) Baglioni Piero, Dei Luigi, Ferroni Enzo, Giorgi Rodorico – “Sospensioni stabili di idrossido di calcio”. Italian Patent FI/96/A000255, deposit date 31/10/1996.

2) 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.

3) 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.

4) 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.

5) 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.

6) 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.

7) 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.

8) 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.

9) 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.

10) 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.

11) 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.

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

13) 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.

14) 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.

15) 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.

16) 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.

17) 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.

18) 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.

19) 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.

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”. World Organization Patent WO 2010044118 Priority IT 2008-RM545.

21) 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.

22) 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.

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

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

25) 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.

26) 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.

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

28) 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.

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

30) 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.

31) 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.

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

33) 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.

34) 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.

35) 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.

36) 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.

37) 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.

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

Prospective CSGI Activity in 2021-2022

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 2017-2020

1. {Ru(CO)(x)}-Core complexes with benzimidazole ligands: synthesis, X-ray structure and evaluation of anticancer activity in vivo. Tamasi, Gabriella; Merlino, Antonello; Scaletti, Federica; Heffeter, Petra; Legin, Anton A.; Jakupec, Michael A.; Berger, Walter; Messori, Luigi; Keppler, Bernhard K.; Cini, Renzo DALTON TRANSACTIONS 46, 9, 3025-3040 (2017).
2. A bienzymatic biocatalyst constituted by glucose oxidase and Horseradish peroxidase immobilized on ordered mesoporous silica. Pitzalis, Federica; Monduzzi, Maura; Salis, Andrea MICROPOROUS AND MESOPOROUS MATERIALS 241, 145-154 (2017).
3. A Diabatic Electronic State System to Describe the Internal Conversion of Azulene. Banerjee, Shiladitya; Skouteris, Dimitrios; Barone, Vincenzo COMPUTATIONAL SCIENCE AND ITS APPLICATIONS - ICCSA 2017, PT V 10408, 328-337 (2017).
4. A Hybrid EOF Algorithm to Improve MODIS Cyanobacteria Phycocyanin Data Quality in a Highly Turbid Lake: Bloom and Nonbloom Condition. Tao, Min; Duan, Hongtao; Cao, Zhigang; Loiselle, Steven Arthur; Ma, Ronghua IEEE JOURNAL OF SELECTED TOPICS IN APPLIED EARTH OBSERVATIONS AND REMOTE SENSING 10, 10, 4430-4444 (2017).
5. A hypothesis on different technological solutions for outdoor and indoor Roman wall paintings. Birolo, Leila; Tomeo, Antonella; Trifuoggi, Marco; Auriemma, Finizia; Paduano, Luigi; Amoresano, Angela; Vinciguerra, Roberto; De Rosa, Claudio; Ferrara, Luciano; Giarra, Antonella; Luchini, Alessandra; De Maio, Carla; Greco, Giovanna; Vergara, Alessandro ARCHAEOLOGICAL AND ANTHROPOLOGICAL SCIENCES 9, 4, 591-602 (2017).
6. A MODIS-Based Novel Method to Distinguish Surface Cyanobacterial Scums and Aquatic Macrophytes in Lake Taihu. Liang, Qichun; Zhang, Yuchao; Ma, Ronghua; Loiselle, Steven; Li, Jing; Hu, Minqi REMOTE SENSING 9, 2 (2017).
7. A Modular Implementation for the Simulation of 1D and 2D Solid-State NMR Spectra of Quadrupolar Nuclei in the Virtual Multifrequency Spectrometer-Draw Graphical Interface. Presti, Davide; Pedone, Alfonso; Licari, Daniele; Barone, Vincenzo JOURNAL OF CHEMICAL THEORY AND COMPUTATION 13, 5, 2215-2229 (2017).
8. A single-molecule FRET sensor for monitoring DNA synthesis in real time. Fijen, Carel; Silva, Alejandro Monton; Hochkoeppler, Alejandro; Hohlbein, Johannes PHYSICAL CHEMISTRY CHEMICAL PHYSICS 19, 6, 4222-4230 (2017).
9. A stabilizer-free non-polar dispersion for the deacidification of contemporary art on paper. Poggi, Giovanna; Giorgi, Rodorico; Mirabile, Antonio; Xing, Huiping; Baglioni, Piero JOURNAL OF CULTURAL HERITAGE 26, 44-52 (2017).
10. Accurate Vibrational-Rotational Parameters and Infrared Intensities of 1-Bromo-1-fluoroethene: A Joint Experimental Analysis and Ab Initio Study. Charmet, Andrea Pietropolli; Stoppa, Paolo; Giorgianni, Santi; Bloino, Julien; Tasinato, Nicola; Camimeo, Ivan; Biczysko, Malgorzata; Puzzarini, Cristina JOURNAL OF PHYSICAL CHEMISTRY A 121, 17, 3305-3317 (2017).
11. Adsorption and release of ampicillin antibiotic from ordered mesoporous silica. Nairi, Valentina; Medda, Luca; Monduzzi, Maura; Salis, Andrea JOURNAL OF COLLOID AND INTERFACE SCIENCE 497, 217-225 (2017).
12. Adsorption of Amino Acids and Glutamic Acid-Based Surfactants on Imogolite Clays. Bonini, Massimo; Gabbani, Alessio; Del Buffa, Stefano; Ridi, Francesca; Baglioni, Piero; Bordes, Romain; Holmberg, Krister LANGMUIR 33, 9, 2411-2419 (2017).
13. Alginate-gelatin formulation to modify lovastatin release profile from red yeast rice for hypercholesterolemia therapy. Leone, Gemma; Consumi, Marco; Pepi, Simone; Lamponi, Stefania; Bonechi, Claudia; Tamasi, Gabriella; Donati, Alessandro; Rossi, Claudio; Magnani, Agnese THERAPEUTIC DELIVERY 8, 10, 843-854 (2017).
14. Alteration processes of pigments exposed to acetic and formic acid vapors. Malagodi, Marco; Licchelli, Maurizio; Bottigliero, Silvia; Milanese, Chiara; Cofrancesco, Pacifico; Rovetta, Tommaso 2017 1ST IEEE INTERNATIONAL CONFERENCE ON ENVIRONMENT AND ELECTRICAL ENGINEERING AND 2017 17TH IEEE INDUSTRIAL AND COMMERCIAL POWER SYSTEMS EUROPE (EEEIC / I&CPS EUROPE) (2017).
15. Antimicrobial activity of eumelanin-based hybrids: The role of TiO2 in modulating the structure and biological performance. Vitiello, Giuseppe; Pezzella, Alessandro; Zanfardino, Anna; Silvestri, Brigida; Giudicianni, Paola; Costantini, Aniello; Varcamonti, Mario; Branda, Francesco; Luciani, Giuseppina MATERIALS SCIENCE & ENGINEERING C-MATERIALS FOR BIOLOGICAL APPLICATIONS 75, 454-462 (2017).
16. Antimicrobial Nanoplexes meet Model Bacterial Membranes: the key role of Cardiolipin. Marin-

Menendez, Alejandro; Montis, Costanza; Diaz-Calvo, Teresa; Carta, Davide; Hatzixanthis, Kostas; Morris, Christopher J.; McArthur, Michael; Berti, Debora SCIENTIFIC REPORTS 7 (2017).

17. Antimicrobial peptides at work: interaction of myxinidin and its mutant WMR with lipid bilayers mimicking the P. aeruginosa and E-coli membranes. Lombardi, Lucia; Stellato, Marco Ignazio; Oliva, Rosario; Falanga, Annarita; Galdiero, Massimiliano; Petraccone, Luigi; D'Errico, Geradino; De Santis, Augusta; Galdiero, Stefania; Del Vecchio, Pompea SCIENTIFIC REPORTS 7 (2017).
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5. Baglioni, P. CHINA TIME NEWS, Taiwan, 2017. Article
6. Baglioni, P. Curso Materiales y métodos para la conservación del patrimonio cultural, Universidad de Costa Rica, San Josè (Costa Rica) 15-27 February 2017. “Materiales y métodos para la conservación del Patrimonio”. Invited lecture.
7. Baglioni, P. Frontiere della Chimica, Scuola Normale Superiore, Pisa 02 May 2017. Invited lecture.
8. Baglioni, P. Gels for Cleaning, Washington (USA), 18-24/08/2017. Invited lecture.
9. Baglioni, P. Japan Colloid Conference, Tokyo (Japan), National Research Institute for Cultural Properties 04-19/09/2017. 4 Invited lectures.
10. Baglioni, P. Modena 07/04/2017. “Francesco Selmi: profilo ed eredità di un intellettuale e patriota nell’Italia pre e post unitaria”. Invited lecture.
11. Baglioni, P. Nano-systems: research and applications on Cultural Heritage, Centro Conservazione e Restauro La Venaria Reale, Turin 13-15 June 2017. Conference Introduction to nanoscience and nanomaterials in the conservation of Cultural Heritage; Conference “Nanoscience and its contribution to the conservation of Cultural Heritage”. Invited lecture.
12. Baglioni, P. NSRRC - OPEN HOUSE, Taipei (Taiwan) 26-30 July 2017. Invited lecture.
13. Baglioni, P. Physical Chemistry Chemical Physics, Cambridge Royal Society 9-11/11/2017. Overwiew on Nanorestart Project. Invited lecture.
14. Baglioni, P. RBNI Monthly Seminar Series 2017, Russel Berrie Nanotechnology Institute, Israel 1 November 2017. Invited lecture.
15. Baglioni, P. RBNI Monthly Seminar Series, Tel Aviv (Israel), Russell Berrie Nanotechnology Institute 01/11/2017. “Colloid and Surface Chemistry for the conservation of Cultural Heritage”. Invited lecture.
16. Baglioni, P. Science for Art, Pistoia, 06 November 2017. “Ricerche di frontiera per lo sviluppo di nuovi materiali nano-technologici per il restauro e la consevazione delle opere d'arte”. Invited lecture.
17. Baglioni, P. XLVI Winter Meeting on Statistical Physics, Taxco (Mexico) 07-14/01/2017. Invited lecture.
18. Baglioni, P. Wood in Chemistry, Grenoble (France), 22-24/03/2017. Invited lecture.
19. Baglioni, P.; Giorgi, R. TechnoHeritage, Cadiz (Spain) 21-24 May 2017. “Materials and methods for the conservation of cultural heritage”. Invited lecture.
20. Baglioni, P.; Giorgi, R. Workshop “Nanotechnologies for conservation of cultural heritage”, Pratt Institute, NY (USA) 25-28 January 2017. Invited lecture and Practical Session.
21. Baglioni, P.; Giorgi, R.; Chelazzi, D.; Poggi, G.; Bonelli, N.; Mirabile, A.; Pensabene, L.; Petruzzellis, M.L.; Di Carlo, G.; Lavorgna, M.; Salzano De Luna, M.; Ingo, G.M.; Iacopino, D.; Bordes, R.; Shashoua, Y.; Semenzin, E. Nano-systems: research and applications on Cultural Heritage, Centro Conservazione e Restauro La Venaria Reale, Turin 11-12 May 2017. “Nanoscience and its contribution to the conservation of Cultural Heritage”; “Gels and emulsions: theoretical aspects”. Training.
22. Baglioni, P.; Giorgi, R.; Pensabene, L. Workshop: Nanotechnology and Conservation, The Solomon Guggenheim Collection, 23-26 January 2017. “Nanotechnologies for conservation of cultural heritage”. Talk and practical session.
23. Baglioni, P.; Mirabile, A. Primer Simposio Ibericoamericano de Innovacion, Ciencia y Nueva Tecnologias para el estudio, divulgacion y conservacion del patrimonio cultural, Universidad Militare Nueva Granada, Bogota (Colombia) 14-16 Noviembre 2017. “Nanoscience and its contribution to the conservation heritage”. Lectio Magistralis and training.
24. Baglioni, P.; Mirabile, A. Workshop Nanorestart “New materials for Modern and Contemporary Art

Conservation", Centre Pompidou, France 19 -20/04/2017. "Nanoscience and its contribution to the conservation of Cultural Heritage"; "Gels and emulsions: theoretical aspects". Training.

25. Baglioni, P.; Mirabile, A.; Di Carlo, G.; Schrekker, H. Nanorestart – Nanotecnologia para a Conservação e Restauração do Patrimônio Cultural, UFRGS, Porto Alegre (Brazil), 2017. "Materiais e métodos para a conservação do patrimônio cultural". Invited lecture and training.
26. Baglioni, P.; Pensabene, L. Article on Sette - Magazine del Corriere della Sera, 2017. "Il Picasso che non ti aspetti, ritrovato sotto una mano di bianco". Article.
27. Balbi, A.; Skouteris, D.; Tasinato, N.; Puzzarini, C.; Barone, V. ERC AdG – Barone DREAMS: final meeting, Pisa 29/11 – 2/12 2017. "The formation pathway of aminoacetonitrile in the interstellar medium". Poster.
28. Balbi, A.; Tasinato, N.; Mendolicchio, M.; Puzzarini, C.; Barone, V. The 25th Colloquium on High Resolution Molecular Spectroscopy, Helsinki (Finland) 20-25/08/2017. "Accurate quantum-chemical spectroscopic characterization of interstellar methanimidic acid". Poster.
29. Baratto, M.C.; Harir, M.; Al Khatib, M.; Basosi, R.; Pogni, R. XXVI Congresso Nazionale della Società Chimica Italiana, Paestum 10-14/09/2017. "Spectroscopic and biochemical characterization of a new Tyrosinase from Streptomyces cyaneofuscatus". Poster.
30. Barone, V. 40th edition of the Colloquium Spectroscopicum Internationale (CSI XL), Pisa 11-16/06/2017. Oral presentation.
31. Barone, V. ERC-Chem Day, Accademia dei Lincei, Roma 16/03/2017. "Chimica creatività". Lectio Magistralis.
32. Barone, V. International Workshop CAT-ICBCS 2017, Università degli Studi della Calabria, Rende (CS) 3-4/2017. Oral presentation.
33. Barone, V. SEMINARI di BIOGEM, Approfondimenti Culturali e Scientifici Unità di Ricerca Scienza e Società, Ariano Irpino (AV) 26/04/2017. "Linguaggi comuni per sistemi complessi: nuovi ponti attraverso antiche frontiere". Oral Presentation.
34. Barone, V. Seminari INFN Sezione di Perugia, Perugia 07/04/2017. "Virtual and real in molecular sciences: the devil and holy water?". Oral Presentation.
35. Barone, V. Seminario internazionale Ricerca ed innovazione in chimica dei beni culturali, Accademia delle Scienze dell'Istituto di Bologna, Bologna 02/11/2017. "Reale e Virtuale, Arte e Scienza: nuovi ponti, attraverso antiche frontiere". Oral presentation.
36. Barone, V. XLIII Congrès des Chimistes Théoriciens d'Expressio", Paris (France) 3-7/07/2017. "The Virtual Multifrequency Spectrometer: status and perspectives of an undergoing project". Oral presentation.
37. Basosi, R. Congresso Naz. ATI, Lecce 8/09/2017. "Gli indirizzi per l'Energia dell'Unione Europea, l'impegno italiano in Horizon 2020 e SET Plan e le opportunità di fondi EU nel WP 18-19". Plenary lecture.
38. Basosi, R. Congresso Naz. Rete LCA, Siena 23/06/2017 "EU Energy Policies toward Sustainability after COP 21". Oral presentation.
39. Basosi, R. Ecomondo, Rimini 7-10/11/2017. "I percorsi di innovazione tecnologici per l'Energia: il contributo italiano in Horizon 2020 e SET Plan". Plenary lecture.
40. Basosi, R. ENEA 6/12/2017. "I nuovi scenari EU per l'ENERGIA: Horizon 2020, SET Plan e Mission Innovation". Invited lecture.
41. Basosi, R. EXPO 2017 Future Energy, Astana (Kazakistan) 26/06/2017. "ENERGY: Introductory remarks on European and Italian Energy Policies toward Sustainable Development". Plenary lecture.
42. Basosi, R. Firenze, INSTM 18/05/2017. "Energy Technologies in EU H2020 and SET Plan". Oral presentation.
43. Basosi, R. GIURI, Bruxelles (Belgium) 12/06/2017. "EU Energy Policies in Research". Oral presentation.
44. Basosi, R. INSEAN, CNR Roma 10/07/2017. "Il SET Plan europeo e lo sviluppo del Wind OFFSHORE". Oral presentation.
45. Basosi, R. Montebelluna 6/04/2017. "Gli indirizzi per l'Energia dell'Unione Europea e le opportunità dei progetti Horizon 2020". Oral presentation.
46. Basosi, R. Roma, CNR 19/06/2017. "Il SET Plan europeo e lo sviluppo del PV". Oral presentation.
47. Basosi, R. Science Park, Trieste 17/02/2017. "ENERGIA: la partecipazione italiana a HORIZON 2020 e le opportunità dei fondi EU". Oral presentation.
48. Basosi, R. Università di Bologna 2017. "Le politiche europee dell'Energia dopo COP 21". Oral presentation
49. Basosi, R. Università di Napoli "Federico II" 10/10/2017. "Le opportunità di fondi EU nel WP 18-19 di H2020". Oral presentation.
50. Basosi, R. Università di Venezia "Ca' Foscari" 25/01/2017. "Il nuovo Bando Energia WP 2017-18 di H2020". Oral presentation.

51. Basosi, R. Workshop CRITIS, IMT Lucca 13/10/2017. “European Energy Policies toward Sustainable Development”. Invited lecture.
52. Basosi, R.; Capra, M. 13/12/2017. “Le politiche europee dell’Energia per la ricerca e l’innovazione: SET Plan e Mission Innovation”. Oral presentation.
53. Basosi, R.; Capra, M. 4/09/2017 “Le politiche europee dell’Energia dopo COP 21, H2020, SET Plan e Mission Innovation”. Oral presentation.
54. Bergese, P. Ai confini della biologia: dalla genomica agli esosomi attraverso il gene editing. Università Cattolica del Sacro Cuore, facoltà di scienze agrarie, alimentari e ambientali, Piacenza 18-12-2017. “The colloidal side of cell communication”. Invited talk.
55. Bergese, P. Workshop on isolation and characterization of extracellular vesicles obtained from different biological fluids. IGTP Campus, Badalona, Barcelona (Spain) 27th February to 2nd March 2017. “The colloidal side of extracellular vesicles”. Invited talk.
56. Bergese, P. International School of Physical Chemistry. Materials for Biomedical Applications, Island of San Servolo, Venice July 02-07 2017. “Fundamentals of Surfaces and Surface Modifications”. Invited talk.
57. Bhattacharjee, N.; Zazza, C.; Brancato, G. Theoretical Physics Tools and Complex Network Physics applied to Biology and Social Systems - Incontro Nazionale delle Iniziative INFN di Gruppo IV: BIOPHYS e PLEXNET - Scuola Normale Superiore, Pisa September 25-26, 2017. “Carbon nanotube as artificial channel: Ion translocation behavior with respect to concentration and nanotube size”. Oral presentation.
58. Bini, M.; Tondo, C.; Capsoni, D.; Mozzati, M.C.; Albini, B.; Galinetto P. 21th International Conference on Solid State Ionics, Padua 18-23/06/2017. “Tuning the superparamagnetic behavior of ZnFe2O4 nanoparticles: the role of Ca and Gd doping”. Poster.
59. Bonini, M. North University of China, Taiyuan (China) 26/09/2017. “Colloids, nanostructures and composites: towards functional materials”. Invited oral presentation.
60. Bonini, M. RIDCI - China Research Institute of Daily Chemical Industry, Taiyuan (China) 28/09/2017, “Colloids, nanostructures and composites: towards functional materials”. Invited oral presentation.
61. Bonini, M. Shanxi University, Taiyuan (China) 25/09/2017. “Colloids, nanostructures and composites: towards functional materials”. Invited oral presentation.
62. Bonini, M. Taiyuan University of Science and Technology, Taiyuan (China) 27/09/2017. “Colloids, nanostructures and composites: towards functional materials”. Invited oral presentation.
63. Bonini, M.; Discovering Advanced AFM – International Workshop on Atomic Force Microscopy, Bologna 12/10/2017. “The AFM contribution towards the mechanistic understanding of surface cleaning”. Invited oral presentation.
64. Boussessi, R.; Tasinato, N.; Pietropolli Charmet, A.; Stoppa, P.; Barone, V. ERC AdG – Barone DREAMS: final meeting, Pisa 29/11–2/12 2017. “Benchmark Analysis on the Performances of Segmented Polarization Consistent Basis Sets for Spectroscopic Applications”. Poster.
65. Bozdag, M.: 3rd Satellite Meeting on Carbonic Anhydrase, Montecatini Terme 24-27/05/2017. “Novel tumor associated Carbonic Anhydrase Inhibitors: derivatives of SLC-0111”. Oral presentation.
66. Brancato, G. First Workshop on "Hybrid Methods in Molecular Simulation", Cagliari April 3-4 2017. “A QM/MM Approach for Simulating Non-Periodic Molecular Systems in the Liquid Phase”. Oral presentation.
67. Brancato, G. University of Groningen, Groningen, The Netherlands March 6, 2017. “Molecular Modeling of Engineered Protein Channels: MscL, Hemolysin and Ferritin as Test Cases”. Oral presentation.
68. Bruni, G.; Pardi, F.; Capsoni, D.; Bini M.; Valle G.; Berbenni V.; Milanese C.; Girella A.; Marini A. 1st Journal of Thermal Analysis and Calorimetry Conference and 6th V4 Thermoanalytical Conference, Budapest (Ungheria) 6-9/06/2017. “Discovery and physico-chemical characterization of a new polymorph of febantel”. Poster. Chairman of the Pharmaceutical Section.
69. Bua, S.: 3rd Satellite Meeting on Carbonic Anhydrase, Montecatini Terme 24-27/05/2017. “Design and Synthesis of Novel Nonsteroidal Anti-Inflammatory Drugs and Carbonic Anhydrase Inhibitors Hybrids (NSAIDs−CAIs) for the Treatment of Rheumatoid Arthritis”. Poster contribution.
70. Bua, S.: 50 anni in MS-tandem, dove siamo arrivati e dove andiamo?”, Firenze 12/12/2017. “Development of LC-MS/MS methods and application of LEDA post-processing tool to resolve coeluting isomers of Novel Nonsteroidal Anti-Inflammatory Drugs-Carbonic Anhydrase Inhibitors Hybrids in plasma”. Poster contribution.
71. Bua, S.: Convegno Monotematico 2017 “Pharmacological basis of novel pain therapeutics”, Firenze 4-5/05/2017. “Design and Synthesis of Novel Nonsteroidal Anti-Inflammatory Drugs and Carbonic Anhydrase Inhibitors Hybrids (NSAIDs−CAIs) for the Treatment of Rheumatoid Arthritis”. Poster contribution.

72. Bufalo, G.; Cinelli, G.; Cuomo, F.; Ambrosone, L. Workshop “Chimica per la protezione dell’Ambiente”, SCI Sezione Campania e del Dipartimento di Scienze e Tecnologie Ambientali, Biologiche e Farmaceutiche, Caserta 28/09/2017. “Uso alternativo degli ultrasuoni per ridurre l’impatto ambientale delle concerie”. Oral presentation.
73. Cabrini, M.; Lorenzi, S.; Pastore, T.; D’Urso, G.; Giardini, C. Joint EUROCORR 2017 & 20th ICC & Process Safe Congress, Prague 8Czech Republic) 3-7/09/2017. “Evaluation of corrosion behavior of AA2424 T4 welded by means of FSW”. Oral presentation.
74. Cabrini, M.; Lorenzi, S.; Pastore, T.; Pesenti Bucella, D.; Paggi, A.; Parravicini Bagliani, E.; Darcis, P. Bar, wire and tube drawing (IWD), Bergamo 30/11-01/12/2017. “Development of new tests to assess sulfide stress corrosion cracking of linepipes”. Oral presentation.
75. Cabrini, M.; Lorenzi, S.; Pastore, T.; Testa, C.; Manfredi, D.; Calignano, F.; Lorusso, M.; Fino, P. XII Giornate Nazionali sulla Corrosione e Protezione dei Materiali, Milano 28-30/06/2017. “Corrosion behavior of aluminum alloys obtained by Direct Metal Laser Sintering”. Oral presentation.
76. Cabrini, M.; Lorenzi, S.; Pastore, T.; Testa, C.; Manfredi, D.; Lorusso, M.; Calignano, F.; Fino, P. Joint EUROCORR 2017 & 20th ICC & Process Safe Congress, Prague (Czech Republic) 3-7/09/2017. “Corrosion behavior of aluminum-silicon alloys obtained by Direct Metal Laser Sintering”. Oral presentation.
77. Capsoni, D.; Boni, P.; Bini, M.; Quinzeni, I.; Bruni, G.; Mustarelli, P. 21th International Conference on Solid State Ionics, Padova 18-23/06/2017. “Silicon doped LiNi0.5Mn1.5O4 as high-voltage cathode for Li-ion batteries”. Poster.
78. Catte, A.; Bhattacharjee, N.; Akhunzada, M.J.; Verbeek, D.S.; Kocer, A.; Brancato, G. Theoretical Physics Tools and Complex Network Physics applied to Biology and Social Systems - Incontro Nazionale delle Iniziative INFN di Gruppo IV: BIOPHYS e PLEXNET - Scuola Normale Superiore, Pisa September 25-26, 2017. “Modeling of artificial and natural ion channels”. Oral presentation.
79. Ceselin, G.; Tasinato, N.; Puzzarini, C.; Pietropolli Charmet, A.; Stoppa, P.; Giorgianni, S. The 25th Colloquium on High Resolution Molecular Spectroscopy, Helsinki (Finland) 20-25/08/2017. “N2-, O2- and air-pressure broadening coefficients of SO2 for {1 band and ground state transitions for atmospheric applications”. Poster.
80. Ceselin, G.; Tasinato, N.; Puzzarini, C.; Pietropolli Charmet, A.; Stoppa, P.; Giorgianni, S. The 25th Colloquium on High Resolution Molecular Spectroscopy, Helsinki (Finland) 20-25/08/2017. “Determination of SO2-H2, -He and -CO2 pressure broadening coefficients in the infrared and millimeter/sub-millimeter spectral regions”. Poster.
81. Cinelli, G.; Cuomo, F.; Venditti, F.; Ambrosone, L.; Ceglie, A.; Lopez, F. XXVI Congresso Nazionale della Società Chimica Italiana, Paestum (SA) 10-14/09/2017. “Ultrasound-assisted emulsification microextraction for analytical determination”. Poster.
82. Cioffi, N. NALS 2017 Nanomaterials Applied to Life Sciences, Gijon (Spain) December 12-15 2017. “Nanoantimicrobials. Progress and prospects”. Plenary lecture.
83. Cofelice, M.; Cuomo, F.; Ceglie, A.; Lopez, F. XXVI Congresso Nazionale della Società Chimica Italiana, Paestum (SA) 10-14/09/2017. “On the sodium alginate aqueous solutions and nanodispersions flow behavior”. Poster.
84. Cofelice, M.; Cuomo, F.; Lopez, F. XVI European Student Colloid Conference ESC 2017, Florence 19-22/06/2017. “Supramolecular systems for producing edible coatings and films”. Poster.
85. Colleoni, C.; Esposito, F.; Guido, E.; Migani, V.; Trovato, V.; Rosace, G. 17th World Textile Conference AUTEX 2017. Corfu (Greece) 29-31/05/2017. “Ceramic coatings for water-repellent textiles”. Oral presentation.
86. Coppola, L. 2nd International Congress on Materials and Structural Stability, Rabat (Morocco) 22-25/11/2017. “Alkali activated materials and geopolymers in the future of sustainable construction”. Oral presentation.
87. Coppola, L.; Antonietti, S.; Coffetti, D.; Felici, A.; Maccoppi, A. IX Giornate di Studio sui Geopolimeri, Napoli 26-27/01/2017. “L’utilizzo dei geopolimeri nel restauro dei beni culturali e monumentali”. Oral presentation.
88. Coppola, L.; Antonietti, S.; Coffetti, D.; Felici, A.; Montereali, L. IX Giornate di Studio sui Geopolimeri, Napoli 26-27/01/2017. “L’utilizzo dei geopolimeri nel ripristino delle strutture esistenti in calcestruzzo armato”. Oral presentation.
89. Coppola, L.; Coffetti, D.; Lorenzi, S. 10th ACI/RILEM International Conference on Cementitious Materials and Alternative Binders for Sustainable Concrete, Montreal (Canada) 2-4/10/2017. “Innovative carboxylic acid waterproofing admixture for self-sealing watertight concretes”. Oral presentation.
90. Coppola, L.; Coffetti, D.; Lorenzi, S. 10th ACI/RILEM International Conference on Cementitious Materials and Alternative Binders for Sustainable Concrete, Montreal (Canada) 2-4/10/2017. “CSA-

based ternary binders for a sustainable concrete”. Oral presentation.

91. Coppola, L.; Coffetti, D. SIMP-SGI-SOGEI-AIV Congress on Geosciences: a tool in a changing world, Pisa 3-6/09/2017. “One-part alkali activated slags for environmentally friendly cement-free repair mortars for conservation, restoration and retrofitting of existing concrete structures”. Oral presentation.
92. Cordaro, G.; Donazzi, A.; Pelosato, R.; Cristiani, C.; Dotelli, G.; Natali Sora, I. 15th International Symposium on Solid Oxide Fuel Cells (SOFC-XV) Hollywood, FL (USA) 23-28/07/2017. “Electrochemical and chemical characterization of NdBa1-xCo2-yFeyO5+δ cathodes for IT-SOFCs”. Oral presentation.
93. Cuomo, F.; Ceglie, A.; Ambrosone, L.; Lopez, F. XXVI Congresso Nazionale della Società Chimica Italiana, Paestum (SA) 10-14/09/2017. “Encapsulation and release of hydrophilic and lipophilic molecules from layer by-layer assembled capsules”. Poster.
94. Cuomo, F.; Lopez, A.; Ceglie, A. 7th Symposium on Polyelectrolytes, Coimbra (Portugal) 16-19/06/2008. “Liposomal formulation for polynucleotides delivery”. Poster.
95. De Leonardis, A.; Macciola, V.; Niro, S.; Cuomo, F.; Panfili, G.; Lopez, F. EuroFed Lipid Congress, Uppsala (Sweden) 27-30/08/2017. “Ethnic Food Market in Europe: A Study on Chemical Composition, Nutritional Feature and Oxidative Stability of the West-African Virgin Red Palm Oil”. Poster.
96. D’Errico, G.; De Santis, A.; Russo Krauss, I.; Paduano, L. GEM XIX: International Congress of French Group of membrane studies, Roscoff (France) 5-8/11/2017. “Structural characterization of model membranes containing DHA: the role of a unique molecule”. Oral communication.
97. De La Fuente García, E.; Carrara, V.; Fontana, F.; Natali Sora, I. ICheaP13 - 13th International Conference on Chemical & Process Engineering, Milano 28-31/05/2017. “Simulated weathering tests of photocatalytic paint containing LaFeO3”. Oral presentation.
98. De Santis, A.; Russo Krauss, I.; Paduano, L.; D’Errico, G. 30th Conference of the European Colloid and Interface Society (ECIS), Madrid (Spain) 3-8/09/2017. “Structural characterization of model membranes containing DHA: the role of a unique molecule. Oral communication.
99. De Santis, A.; Russo Krauss, I.; Paduano, L.; D’Errico, G. XXVI Congresso Nazionale della Società Chimica Italiana (SCI), Paestum (SA) 10-14/09/2017. “Micro-structural characterization of model membranes containing DHA” Oral communication.
100. Ditaranto, N.; Longano, D.; Bonerba, E.; Tantillo, G.; Sabbatini, L.; Torsi, L.; Cioffi, N. XII ECHEMS Meeting 2017 - Electrochemistry in… ingenious molecules, surfaces and devices. “Electrosynthesized benzalkonium chloride-copper nanoparticles for developing smart antimicrobial surfaces”. Poster.
101. Ditaranto, N.; Orlando, I.; Curci, A.; Cioffi, N.; Margiotta, N.; Natile, G. SCI 2017, XXVI Congresso Nazionale della Società Chimica Italiana. “Synthesis And Analytical Characterization Of A Dual-Acting Pt(IV) Prodrug With potential Antitumor And Anti-Inflammatory Activities”. Poster.
102. Ditaranto, N.; Sportelli, M.C.; Picca, R.A.; Sabbatini, L.; Cioffi, N. CSI–XL 2017, Colloquium Spectroscopicum Internationale XL. “Spectroscopic characterization of second-generation nanostructured antimicrobials”. Oral presentation.
103. Ferrara, C.; Ferrari, S.; Capsoni, D.; Bini, M.; Pell, A.; Pintacuda, G.; Mustarelli, P. 21th International Conference on Solid State Ionics, Padua 18-23/06/2017. “Structural investigation of Li2(Fe/Mn)SiO4: a combined NMR –XRD study”. Poster.
104. Ferri, M.; Trueba, M.; Trasatti, S.P.; Cabrini, M.; Lo Conte, A. Joint EUROCORR 2017 & 20th ICC & Process Safe Congress, Prague (Czech Republic) 3-7/09/2017. “Investigation of the repassivation behavior of al 7075-T6 under constant bending load and dynamic slow strain conditions”. Oral presentation.
105. Ferri, M.; Trueba, M.; Trasatti, S.P.; Cabrini, M.; Lo Conte, A. XII Giornate Nazionali sulla Corrosione e Protezione dei Materiali, Milano 28-30/06/2017. “Effetto Della Sollecitazione Meccanica a Flessione sul Comportamento A Corrosione Di Leghe Di Al Strutturali”. Oral presentation.
106. Gelli, R.; Del Buffa, S.; Tempesti, P.; Ridi, F.; Bonini, M.; Baglioni, P. XXVI Congresso Nazionale della Società Chimica Italiana, Paestum (SA) September 10-14, 2017. “Investigation of gelatin-based composites as scaffolds for bone tissue engineering”. Poster.
107. Gelli, R.; Mati, L.; Ridi, F.; Baglioni, P. XXVI Congresso Nazionale della Società Chimica Italiana, Paestum (SA) September 10-14, 2017. “Effect of cellulose ethers on the formation and properties of magnesium phosphate-based cements for biomedical applications”. Oral presentation.
108. Giaccherini, A.; Baroni, T.; Cioffi, N.; De Luca, A.; Picca, R.A.; Di Benedetto, F.; Innocenti, M. XII ECHEMS Meeting 2017 - Electrochemistry in… ingenious molecules, surfaces and devices. “Sulphides heterojunction grown by means of E-ALD: an SXRD operando structural characterization”. Poster.
109. Holzer, B.; Manoli, K.; Ditaranto, N.; Macchia, E.; Torsi, L. 7th IEEE International Workshop on Advances in Sensors and Interfaces, 2017. “Characterization of modified working electrodes for sensing applications”. Oral communication.

110. Innocenti, M.; Di Benedetto, F.; Salvietti, E.; Giaccherini, A.; Giurlani, W.; Carlà, F.; Cioffi, N.; Picca, R.A.; Berretti, E.; Felici, R. SCI 2017, XXVI Congresso Nazionale della Società Chimica Italiana. "Microscopic and Spectroscopic Analysis with Synchrotron Light of Modified Surfaces of Technological Interest". Oral communication.
111. Izzi, M.; Clemente, M.; Sportelli, M.C.; Volpe, A.; Picca, R.A.; Conte, A.; Del Nobile, M.A.; Ancona, A.; Cioffi, N. CHESS 2017, Conventional and high-energy spectroscopies for inorganic, organic and biomolecular surfaces and interfaces. "Characterization of new composites for food-packaging applications". Poster presentation.
112. Loiselle, S. EFC/FAO Mountain Watersheds, Prague (Czech Republic) 8/2017. "Combining in situ and remote methods for river and catchment management". Oral presentation.
113. Lo Nostro, P.; Tatini, D.; Sarri, F.; Ambrosi, M.; Carretti, E. 31st ECIS (European Colloid and Interface Science) Conference, Madrid (Spagna) 03-08/09/2017. "Innovative eco-compatible approaches for shale gas extraction". Poster.
114. Lopetuso, R.; Picca, R.A.; Giaccherini, A.; Salvietti, E.; Cioffi, N.; Innocenti, M. CHESS 2017, Conventional and high-energy spectroscopies for inorganic, organic and biomolecular surfaces and interfaces. "XPS characterization of thin layered semiconductors grown by electrochemical atomic layer deposition (E-ALD)". Poster presentation.
115. Lopez-Lorente, A.I.; Picca, R.A.; Di Franco, C.; Sportelli, M.C.; Mizaikoff, B.; Kranz, C.; Valentini, A.; Palazzo, G.; Cioffi, N. NALS 2017, Nanomaterials Applied to Life Sciences. "Gold nanoparticles obtained by stainless steel assisted synthesis: characterization and applications". Oral presentation.
116. López-Lorente, A.I.; Picca, R.A.; Minervini, G.; Di Franco, C.; Sportelli, M.C.; Mizaikoff, B.; Kranz, C.; Valentini, A.; Palazzo, G.; Cioffi, N. N&N 2017, Nanoscience & Nanotechnology INFN Meeting 2017. "What's new and good in the aqueous synthesis of colloidal gold nanoparticles (AuNPs)? A critical overview of AuNPs 'green' synthetic methods". Invited oral communication.
117. López-Lorente, Á.I.; Tricase, A.; Picca, R.A.; Di Franco, C.; Sportelli, M.C.; Mizaikoff, B.; Kranz, C.; Valentini, A.; Palazzo, G.; Cioffi, N. SCI 2017, XXVI Congresso Nazionale della Società Chimica Italiana. "What's new and good in the aqueous synthesis of colloidal gold nanoparticles (AuNPs)? A critical overview of AuNPs synthetic methods and their Analytical applications". Oral presentation.
118. Lopez, F.; Cuomo, F.; Venditti, F.; Ambrosone, L.; Ceglie, A. XXVI Congresso Nazionale della Società Chimica Italiana, Paestum (SA) 10-14/09/2017. "Olive mill wastewaters phenol photocatalytic degradation by visible light activated carbon doped titanium". Oral presentation.
119. Lorenzi, S.; Cabrini, M.; Pastore, T.; Testa, C.; Calignano, F.; Manfredi, D.; Biamino, S.; Lombardi, M.; Fino, P. 68th annual meeting of the International Society of Electrochemistry, Providence, RI (USA) 27/08-01/09/2017. "Electrochemical Study of the Corrosion Resistance of the AlSi10Mg Alloy Obtained by means of LPBF". Oral presentation.
120. Luchini, A.; Vitiello, G.; Gerelli, Y.; Fragneto, G.; Paduano, L. Workshop Neutrons in Structural Biology (NISB2017), Grenoble (France) 7-9/06/2017. "Novel insights into cardiolipin-contaning lipid bilayers". Poster.
121. Macchia, E.; Alberga, D.; Manoli, K.; Mangiatordi, G.F.; Palazzo, G.; Torsi, L. Solid State Ionics 2017, Padua 18-23 June 2017. "Organic bioelectronics probing conformational changes in surface confined proteins". Oral presentation.
122. Macchia, E.; Alberga, D.; Manoli, K.; Mangiatordi, G.F.; Palazzo, G.; Lattanzi, G.; Torsi, L. XXVI Congresso Nazionale SCI 2017, Peastum (SA) September 10-14 2017. "Organic bioelectronics probing conformational changes in surface confined proteins". Oral presentation.
123. Macchia, E.; Ghittorelli, M.; Torricelli, F.; Torsi, L. IWASI 2017, Vieste 15-16 June 2017. "Electrochemical organic transistor immuno-sensor operating at the femto-molar limit of detection", Poster.
124. Macchia, E.; Ghittorelli, M.; Torricelli, F.; Torsi, L. Orbitaly-Organic Bioelectronics Italy, Cagliari 25-27 October 2017. "Organic electrochemical transistor immuno-sensor operating at the femto-molar limit of detection". Poster.
125. Macchia, E.; Torsi, L.; Alberga, D.; Manoli, K.; Mangiatordi, G.F.; Palazzo, G.; Lattanzi, G. E-MRS Spring Meeting 2017, Strasbourg (France) 22-26 May 2017. "Organic Bioelectronics: a powerful tool to investigate biological interfaces", Oral presentation.
126. Maranghi, S.; Borghetti, F.; Basosi, R.; Busi, E. XI Convegno della Rete Italiana LCA, Siena, June 22-23, 2017. "Self-cleaning nano-technology application on a new antibacterial insect screen: an attributional LCA study for quantifying energy and water savings." Poster.
127. Maranghi, S.; Parisi, M.L.; Sinicropi, A.; Basosi, R. XI Convegno della Rete Italiana LCA, Siena, June 22-23, 2017. "Sviluppo di un approccio integrato per la valutazione ambientale di sistemi fotovoltaici di nuova generazione: le perovskiti." Poster.
128. Margiotta, N.; Orlando, I.; Trapani, A.; Dellaquila, D.; Tripodo, G.; Mandracchia, D.; Ángeles Esteban,

M.; Cioffi, N.; Ditaranto, N. N&N 2017, Nanoscience & Nanotechnology INFN Meeting 2017. “Designing nanostructured prodrugs and drug carriers: the importance of a thorough analytical characterization”. Invited oral communication.

129. Margiotta, N.; Orlando, I.; Trapani, A.; Dellaquila, D.; Tripodo, G.; Mandracchia, D.; Ángeles Esteban, M.; Cioffi, N.; Ditaranto, N. NALS 2017 Nanomaterials Applied to Life Sciences, Gijon (Spain) December 12-15 2017. “Nanostructured pharmaceutical drug carriers and prodrugs: design and analytical characterization”. Oral communication.
130. Mendolicchio, M.; Tasinato, N.; Barone, V. DREAMS@Anacapri, Anacapri (NA) 20-22/04/2017. “MSR: a new software for the calculation of accurate molecular structures”. Oral presentation.
131. Mendolicchio, M.; Tasinato, N.; Barone, V. ERC AdG – Barone DREAMS: final meeting, Pisa 29/11–2/12 2017. “Development and implementation of new computational methods for the calculation of accurate equilibrium molecular structures”. Oral presentation.
132. Mendolicchio, M.; Tasinato, N.; Barone, V. XXVI Congresso Nazionale della Società Chimica Italiana, Paestum (SA) 10-14/09/2017. “New Models and Computational Strategies for Molecular Structure Prediction”. Oral presentation.
133. Mendolicchio, M.; Tasinato, N.; Boussessi, R.; Barone, V. The 25th Colloquium on High Resolution Molecular Spectroscopy, Helsinki (Finland) 20-25/08/2017. “New computational tools for the determination of molecular structures: the MSR software”. Poster.
134. Messia, M.C.; Cuomo, F.; Oriente, M.; Falasca, L.; Marconi, E. XI Convegno dell’Associazione Italiana di Scienza e Tecnologia dei Cereali (AISTEC), Roma 22-24/11/2017. “Valutazione del comportamento reologico della mucillagine di chia (Salvia hispanica L.) all’interno di impasti a base di cereali”. Poster.
135. Messina, G.M.L.; De Zotti, M.; Formaggio, F.; Marletta, G. MRS FALL MEETING 2017, Boston (USA) 26/11-01/12-2017. “Molecular muscle based on pH-driven stretching-shrinking of peptides”. Oral presentation.
136. Messina, G.M.L.; Dettin, M.; Marletta, G. E-MRS SPRING MEETING 2017, Strasbourg (France) 22-26/05/2016. “Smart peptides for bioresponsive surfaces”. Invited keynote
137. Messina, G.M.L.; Dettin, M.; Marletta, G. EURO BIOMAT 2017, Weimar (Germany) 09-10/05/2017. “Self-assembling peptide hydrogel for 3D architecture for mesenchymal stem cells culture”. Oral presentation.
138. Milanese, C. Gordon Research Conference “Hydrogen-Metal Systems”, Stonehill College, Easton (MA, USA) 16-21/07/2017. “Exploring H and Li dynamics and hydrogen absorption mechanism in lithium fullerides”. Invited lecture.
139. Milanese, C. Indiscienza: le scienze dell’energia, Collegio Ghislieri (Pavia) 15/05/2017. “Idrogeno: l’elemento più leggero alleggerirà i problemi energetici e ambientali?” Invited lecture.
140. Milanese, C. was in the scientific committee of the Symposium “Multifunctionality of Metal Hydrides for Energy Storage – Developments and Perspectives” and in the committee for the evaluation of the EMRS symposium PhD prize.
141. Milanese, C.; Rueda, M.; Girella, A.; Gioventù, M.; Cofrancesco, P.; Sanz-Moral, L.M.; Martín, A.; Marini, A.; Pontiroli, D.; Gaboardi, M.; Magnani, G.; Riccò, M. Gordon Research Conference “Hydrogen-Metal Systems”, Stonehill College, Easton (MA, USA), 16-21/07/2017. “Magnesium borohydride confined in silica aerogel: innovative preparation methods and characterization”. Poster.
142. Milanese, C.; Rueda, M.; Girella, A.; Gioventù, M.; Sanz-Moral, L.M.; Martín, A.; Marini, A. E-MRS 2017 Fall Meeting, Warsaw (Poland) 18-21/09/2017. “Magnesium borohydride confined in silica aerogel: innovative preparation methods and characterization”. Oral presentation.
143. Mohammadpourasl, S.; Dessì, A.; Zani, L.; Reginato, G.; Basosi, R.; Sinicropi, A. Italian Photochemistry Meeting, Perugia 14-16/12/2017. “In silico design of near-IR D-A-π-A sensitizers for dye sensitized solar cells”. Poster.
144. Mosca, M.; Ambrosone, L.; Ceglie, A. XXXVII Congresso Nazionale di Chimica Fisica, Camogli (GE) 24-29/02/2008. “Antioxidant dispersion in biocompatibile oils”. Oral presentation.
145. Murgia, S; Caltagirone, C; Lippolis, V; Monduzzi, M; Prodi, L. XIII Congresso Nazionale di Chimica Supramolecolare, Pula (CA), 18-21/06/2017. “Drug loaded, fluorescent cubic liquid crystalline dispersions designed for applications in cancer therapy”. Oral presentation.
146. Murgia, S. BioNanoMed 2017 (8th International Congress), Krems (Austria) 20-22/03/2017. “Cubic liquid crystalline nanoparticles as potential therapeutic and diagnostic tools”. Oral presentation.
147. Natali Sora, I.; Carrara, V. 5th European Conference on Environmental Applications of Advanced Oxidation Processes (EAAOP5) Prague (Czech Republic) 25-29/06/2017. “Enhanced photocatalytic degradation of ibuprofen in aqueous solution under visible-light irradiation: effects of LaFeO3 and Cu-doped LaFeO3”. Poster.
148. Niccolucci, V.; Mozzillo, M.; Parisi, M.L.; Basosi, R.; Bastianoni, S. VI Convegno della Associazione Rete

Italiana LCA, Siena 22-23/06/2017. “Aumentare la consapevolezza nel consumatore può indurre un cambiamento nelle abitudini alimentari? Un progetto dell’Università di Siena sui fontanelli per la distribuzione di acqua potabile”. Poster.

149. Panzella, L.; d'Ischia, M.; D’Errico, G. 7th International Colloids Conference, Sitges (Spain) 18-21/06/2017. “Rational design of bioinspired polyphenolic materials: Electronic structure, mesoscopic organization and antioxidant activity”. Oral communication.
150. Parisi, M.L.; Bravi, M.; Baratto, M.C.; Basosi, R. VI Convegno della Associazione Rete Italiana LCA, Siena 22-23/06/2017. “Valutazione LCA per la minimizzazione dell'impatto ambientale nello sfruttamento della risorsa geotermica”. Oral presentation.
151. Parisi, M.L.; Bravi, M.; Baratto, M.C.; Basosi, R. XI Convegno della Rete Italiana LCA Resource Efficiency e Sustainable Development Goals: il ruolo del Life Cycle Thinking, Siena 22-23/06/2017. “Valutazione LCA per la minimizzazione dell’impatto ambientale nello sfruttamento della risorsa geotermica”. Oral presentation.
152. Parisi, M.L.; Maranghi, S.; Vesce, L.; Sinicropi, A.; Di Carlo, A.; Basosi, R. DSSC strikes back − 1st Dyenamo DSSC Conference, Uppsala (Sweden) 16-17/10/2017. “Life Cycle Assessment of industrial-scale dye sensitized solar module manufacturing process: a consequential approach for mass production potential evaluation”. Oral presentation.
153. Parisi, M.L.; Pogni, R.; Basosi, R. VI Convegno della Associazione Rete Italiana LCA, Siena (SI) 22-23/06/2017. “Technological breakthrough for energy efficiency in dyes production: bio-synthetic pathway versus chemical process”. Poster.
154. Pelosato, R.; Cordaro, G.; Donazzi, A.; Cristiani, C.; Dotelli, G.; Natali Sora, I.; Fontana, F. VII Workshop Nazionale AICIng - Smart Materials for Technology: Preparation, Self-Assembly, Characterization, Modeling, Milano 12-13/06/2017. “Iron doping and Ba deficiency in NdBaCo2O5+δ cathodes for IT-SOFCs”. Oral presentation.
155. Pelosato, R.; Donazzi, A.; Cordaro, G.; Natali-Sora, I.; Cristiani, C.; Dotelli, G. International Conference on Solid State Ionics (SSI-21), Padova 18-23/06/2017. "Iron doping in NdBa1-xCo2O5+d layered perovskite cathodes: a structural and electrochemical investigation”. Oral presentation.
156. Perugini, L.; Cinelli, G.; Ceglie, A.; Lopez, F.; Cuomo, F. XXVI Congresso Nazionale della Società Chimica Italiana, Paestum (SA) 10-14/09/2017. “Food-grade nanocarriers for protection and delivery of bioactive compounds”. Poster.
157. Perugini, L.; Cuomo, F.; Lopez, F. XVI European Student Colloid Conference ESC 2017, Florence 19-22/06/2017. “Food-grade nanoemulsion for encapsulation and delivery of curcumin”. Poster.
158. Perugini, L.; Cuomo, F.; Venditti, F.; Lopez, F.; Cinelli G. 5th MS Food Day, Bologna 11-13/10/2017. “Ultrasound Assisted Dispersive Liquid-Liquid Micro-extraction Coupled with GC Ion Trap Mass-Spectrometry for Rapid Determination of Bisphenol A in Hydro-alcoholic Solution and Wine”. Poster.
159. Picca, R.A.; Giaccherini, A.; Salvietti, E.; Cioffi, N.; Innocenti, M.. SCI 2017, XXVI Congresso Nazionale della Società Chimica Italiana. “XPS characterization of (Mo/Se) films grown by electrochemical atomic layer deposition”. Poster.
160. Picca, R.A.; Sportelli, M.C.; Manoli, K.; Palazzo, G.; Torsi, L.; Cioffi, N. XII ECHEMS Meeting 2017 - Electrochemistry in… ingenious molecules, surfaces and devices. “Designing ultrastable OTFT-based biosensors by incorporation of electrosynthesized ZnO nanoparticles”. Oral presentation.
161. Picca, R.A.; Sportelli, M.C.; Manoli, K.; Palazzo, G.; Torsi, L.; Cioffi, N. SSI 2017, 21st International Conference on Solid State Ionics. “Understanding the stability of FBI-OFET devices modified with electrosynthesized ZnO nanoparticles”. Oral presentation.
162. Pogni, R.; Spinelli, D.; Fatarella, E.; Baratto, M.C.; Basosi, R.; Atrei, A. XXVI Congresso Nazionale della Società Chimica Italiana, Paestum 10-14/09/2017. “Nanomaterials for enzymatic immobilization”. Poster.
163. Puzzarini, C.; Barone, V. Spin-2017: The 8th Conference On Nitroxides, Padova 10-14/09/2017. “Prebiotic molecules in interstellar space: rotational spectroscopy and quantum chemistry”. Oral presentation.
164. Puzzarini, C.; Barone, V. XVII International Conference on Science, Arts and Culture - Sailing through the Wonders of Astrobiology, Veli Losinj (Croatia) 25-29/07/2017. "Formation mechanisms of prebiotic molecules in the interstellar medium". Oral presentation.
165. Puzzarini, C.; Melli, A.; Tasinato, N.; Bloino, J.; Barone, V. XXVI Congresso Nazionale della Società Chimica Italiana, Paestum (SA) 10-14/09/2017. “Astrochemistry: A Computational Spectroscopy’s View”. Oral presentation.
166. Rampino, S. Invited seminar at Scuola Normale Superiore within the seminar cycle “Frontiere della Chimica”, Pisa 20 ottobre 2017. “Chemical bonding and spectroscopic observables in coordination complexes: insights and analysis through immersive virtual reality”. Invited oral.
167. Rampino, S. Joint Technology Transfer Office JoTTO Fair 2017, Pisa 15 settembre 2017. “Chemical

bonding and spectroscopic observables in coordination complexes". Oral communication.

168. Rampino, S. Problems in discrete dynamics: from biochemical systems to rare events, networks, clustering and related topics, Arcidosso 17-18 febbraio 2017. "Dynamics of gas-phase elementary processes in the classical and quantum regime". Invited oral.
169. Rampino, S. SOSC17 School on open Science Cloud, Perugia 5-9 giugno 2017. "Quantum Dynamics". Invited lecture.
170. Rampino, S.; Calderini, D.; Bloino, J.; Skouteris, D.; Barone, V. DREAMS@Anacapri - Workshop ERC "Development of a Research Environment for Advanced Modeling of Soft Matter, Anacapri 20-22 aprile 2017. "Thermodynamic and kinetic properties from fully-coupled anharmonic densities of states: a survey on different anharmonic perturbative treatments". Oral communication.
171. Rampino, S.; Fusè, M.; Salvadori, A.; Mancini, G.; Barone, V. XXVI Congresso Nazionale della Società Chimica Italiana, Paestum 10-14 settembre 2017. "Chemical bonding and spectroscopic observables in coordination complexes: analysis techniques and applications". Oral communication.
172. Riccardi, C.; Musumeci, D.; Russo Krauss, I.; Paduano, L.; Montesarchio D. 9th International Symposium on Nano and Supramolecular Chemistry, Napoli (Italy) 4-7/09/2017. "Conformational behaviour and molecularity studies of natural and modified AS1411 aptamers". Oral communication.
173. Ridi, F.; Gelli, R.; Gigli, L.; Scudero, M.; Bonini, M.; Baglioni, P. XXVI Congresso Nazionale della Società Chimica Italiana, Paestum (SA) September 10-14, 2017. "Synthesis and characterization of immunologically relevant calcium and magnesium phosphate amorphous nanostructures and strategies for their stabilisation". Oral presentation.
174. Rosace, G.; Colleoni, C.; Trovato, V.; Iacono, G.; Malucelli, G. 17th World Textile Conference AUTEX 2017. Corfu (Greece) 29-31/05/2017. "Intumescent flame-retardant properties of graft copolymerized vinyl monomers onto cotton fabric". Oral presentation.
175. Russo Krauss, I.; Picariello, A.; Luchini, A.; Paduano, L. 30th Conference of the European Colloid and Interface Society (ECIS), Madrid (Spain) 3-8/09/2017. "Understanding protein-nanoparticle interaction: one step forward the development of biomedical nanosystems". Poster.
176. Salis, A. 7th World Congress on Chemistry, Athens (Greece), November 13-15 2017. "Recent Experimental and Theoretical Developments of Ion Specific 'Hofmeister' Phenomena". Oral presentation.
177. Sarcina, L.; Garcia Manrique, P.; Matos, M.; Ditaranto, N.; Cioffi, N.; Blanco Lopez, M.C. NALS 2017 Nanomaterials Applied to Life Sciences, Gijon (Spain) December 12-15 2017. "Inclusion of electro-synthetized Cu nanoparticles in vescicular systems for antibacterial treatment". Poster.
178. Spada, L.; Tasinato, N.; Bosi, G.; Vazart, F.; Barone, V.; Puzzarini, C. The 25th Colloquium on High Resolution Molecular Spectroscopy, Helsinki (Finland) 20-25/08/2017. "Weak O–H···F vs. C–H···F hydrogen bonds in cooperation with C–H···O interactions: the case of difluoromethane - tert-butyl alcohol complex". Poster.
179. Spada, L.; Tasinato, N.; Vazart, F.; Barone, V.; Caminati, W.; Puzzarini, C. The 25th Colloquium on High Resolution Molecular Spectroscopy, Helsinki (Finland) 20-25/08/2017. "The Pyridine–Ammonia Hydrogen Bonded Cluster: A High Level Quantum Chemical and Rotational Spectroscopy Study". Poster.
180. Spada, L.; Tasinato, N.; Vazart, F.; Barone, V.; Caminati, W.; Puzzarini, C. ERC AdG – Barone DREAMS: final meeting, Pisa 29/11–2/12 2017. "Non-Covalent Interactions and Internal Dynamics in Pyridine-Ammonia: A Combined Quantum-Chemical and Microwave Spectroscopy Study". Oral presentation.
181. Sportelli, M.C.; Volpe, A.; Izzi, M.; Clemente, M.; Picca, R.A.; Conte, A.; Del Nobile, M.A.; Ancona, A.; Cioffi, N. SCI 2017, XXVI Congresso Nazionale della Società Chimica Italiana. "Analytical characterization of new composites for food packaging applications". Oral presentation.
182. Tadini-Buoninsegni, F. Annual Conference of the Australian Physiological Society and the Australian Society for Biophysics, Adelaide (Australia) 04-07/12/2016. "Functional characterisation of P-type ATPases using solid-supported membrane based electrophysiology". Invited oral presentation.
183. Tadini-Buoninsegni, F. The Novo Nordisk Prize Symposium 2017, Aarhus (Denmark) 18-19/05/2017. "Recording of ion pump activity on solid supported membranes". Invited oral presentation.
184. Tadini-Buoninsegni, F. XXVI Congresso Nazionale della Società Chimica Italiana, Paestum (SA) 10-14/09/2017. "Electrophysiological measurements on a solid supported membrane to investigate the transport activity of sarcoplasmic reticulum Ca2+-ATPase". Oral presentation.
185. Tamasi, G.; Bonechi, C.; Magnani, A.; Leone, G.; Donati A.; Pepi, S.; Rossi C. HYPOTHESIS XII, Siracusa 28-30/06/2017. "Alcohols reforming for hydrogen production: a thermodynamic approach". Oral presentation.
186. Tasinato, N.; Ceselin, G.; Stoppa, P.; Pietropolli Charmet, A.; Giorgianni, S. XXVI Congresso Nazionale della Società Chimica Italiana, Paestum (SA) 10-14/09/2017. "Unveiling the Adsorption Interaction of Glycolaldehyde on TiO2 - Anatase (1 0 1) by Quantum Chemical Calculations". Poster.

187. Tasinato, N.; Licari, D.; Spada, L.; Puzzarini, C.; Barone, V. The 25th Colloquium on High Resolution Molecular Spectroscopy, Helsinki (Finland) 20-25/08/2017. “Crossing the line between computational and laboratory spectroscopy: The Virtual Multifrequency Spectrometer”. Poster.
188. Tasinato, N.; Spada, L.; Puzzarini, C.; Barone, V. XXVI Congresso Nazionale della Società Chimica Italiana, Paestum (SA), 10-14/09/2017. “Computational Tools for the Interpretation of Rotational Spectra within the Virtual Multifrequency Spectrometer”. Oral presentation.
189. Tonelli, M.; Moscatelli, R.; Sebastiani, M.; Martini, F.; Calucci, L.; Geppi, M.; Borsacchi, S.; Ridi, F. 16th European Student Colloid Conference, Firenze June 19-22, 2017. “Interaction of phosphate-based additives with MgO/SiO2 cements”. Poster.
190. Tonelli, M.; Moscatelli, R.; Sebastiani, M.; Martini, F.; Calucci, L.; Geppi, M.; Borsacchi, S.; Ridi, F. XXVI Congresso Nazionale della Società Chimica Italiana, Paestum (SA) September 10-14, 2017. “Interaction of phosphate-based additives with MgO/SiO2 cements”. Oral presentation.
191. Torsi, L. 13th International Conference on Organic Electronics – ICOE 2017, Russia 04-06/06/2017. “Label-free protein electronic detection with an electrolyte-gated organic field-effect transistor-based immunosensor”. Invited presentation.
192. Torsi, L. 14th European Conference on Molecular Electronics (ECME 2017), Germany 29/08-02/09/2017. “Label-free protein electronic detection with an electrolyte-gated organic field-effect transistor-based immunosensor”. Oral presentation.
193. Torsi, L. AMRS 2017, Africa 11-15/12/2017. “Organic Bioelectronics for ultra-sensitive bio-markers detection”. Invited presentation.
194. Torsi, L. CeNS-Colloquium 07/07/2017, Germany. “Highly performing organic bioelectronic sensors”. Oral presentation.
195. Torsi, L. ITC 2017, USA 23-24/02/2017. “Ultra-sensitive bio-markers detection with an electrolyte gated organic transistor”. Invited presentation.
196. Torsi, L. Joint Chemical Physics and Materials and Interfaces Seminar 30/07/2017, Israel. “Label-free protein electronic detection with an electrolyte-gated organic field-effect transistor-based immunosensor”. Seminar.
197. Torsi, L. LOPEC 2017, Germany 28-30/03/2017. “Ultra-low detection limits and selectivity with organic bio-electronic sensors”. Short course.
198. Torsi, L. Organic Bioelectronic Italy OrBItaly 2017, Italy 25-27/10/2017. “Organic Bioelectronics for ultra-sensitive bio-markers detection”. Keynote presentation.
199. Torsi, L. Solvay Colloquia, Belgium 7/02/2017. “Organic bio-electronics for ultra-sensitive bio-markers detection”. Invited presentation.
200. Torsi, L. SPIE Organic Photonics + Electronics, USA 06-10/08/2017. “Ultra-sensitive bio-markers detection with an electrolyte gated organic transistor”. Oral presentation.
201. Torsi, L. XXVI Congresso Nazionale Società chimica italiana divisione di chimica analitica, Italy 10-14/09/2017. “Printable organic bioelectronics for bioanalytical detections at the physical limit: is this feasible?”. Invited presentation.
202. Torsi, L.; Macchia, E.; Di Franco, C.; Mangiatordi, G.F.; Scamarcio, G.; Palazzo, G. Smart Sensing Workshop: Quantum Investigations in Living Systems, Italy 11-12/05/2017. “Shading light on biological interfaces: from quantum properties to electronic sensing”. Oral presentation.
203. Torsi, L.; Macchia, M.; Manoli, K.; Palazzo, G.; Lattanzi, G. SPIE Photonic West 2017, USA 31/01 – 02/02/2017. “Ultra-low detection limits and selectivity with organic bioelectronic sensors”. Keynote presentation.
204. Troisi, R.; Russo Krauss, I.; Napolitano, V.; Sica, F. 6th International Meeting on Quadruplex Nucleic Acids, Prague (Czech Republic) 31/05-3/06/2017. “Structural basis for the recognition of human α-thrombin by NU172, the only thrombin binding aptamer currently in phase II clinical trials”. Poster.
205. Trueba, M.; Betti, S.; Ferri, M.; Trasatti, S.P.; Cabrini, M.; Lo Conte, A. Joint EUROCORR 2017 & 20th ICC & Process Safe Congress, Prague (Czech Republic) 3-7/09/2017. “Effect of applied and residual stresses on the electrochemically induced repassivation of sensitized 5XXX series Al alloys in NaCl solutions”. Oral presentation.
206. Tuccitto, N.; 21st International Conference on SIMS 10-15/09/2017. “Novel approaches to data mining in molecular depth profiling: from the simulation to sophisticated data treatment”. Invited oral presentation.
207. Venditti, F.; Cuomo, F.; Ambrosone, L.; Ceglie, A.; Cinelli, G.; Lopez, F. XXVI Congresso Nazionale della Società Chimica Italiana, Paestum (SA) 10-14/09/2017. “Microstructured composite for Cr (VI) removal from polluted environment”. Oral presentation.
208. Vitiello, G; Luciani, G; Pezzella, A; Varcamonti, M.; Silvestri, B.; Costantini, A.; Branda, F. 5th International Conference on Multifunctional, Hybrid and Nanomaterials, Lisbona (Portugal) 6-10/03/2017. “Hybrid TiO2/DHICA-melanin materials: novel bioinspired nanosystems for

antimicrobial applications". Poster.

209. Vitiello, G.; Silvestri, B.; Costantini, A.; Pezzella, A.; Branda, F.; Natali Sora, I.; Luciani, G. VII Workshop Nazionale AICIng - Smart Materials for Technology: Preparation, Self-Assembly, Characterization, Modeling, Milano 12-13/06/2017. "Ceramic templated melanin nanostructures: a novel synthesis approach to bio-functional hybrid materials". Oral presentation.
210. Vitiello, G.; Silvestri, B.; Papari, G. P.; Rea, I.; De Stefano, A.; Andreone, A.; Aronne, A.; Luciani, G. VII Workshop Nazionale AICIng, Milano 12-13/06/2017. "On the morphological, structural and charge transfer properties of F-doped ZnO: a spectroscopic investigation". Poster.
211. Vizza, M.; Berretti, E.; Giaccherini, A.; Picciollo, E.; Passaponti, M.; Picca, R.A.; Cioffi, N.; Cavallini, M.; Innocenti, M. XII ECHEMS Meeting 2017 - Electrochemistry in… ingenious molecules, surfaces and devices. "E-ALD of MoSe2: a joint spectroscopic and electrochemical study". Poster.
212. Volpi, V.; Chiarantini, L.; Rovelli, A.; Bianchi, G.; Cicali, C.; Donati, A.; Benvenuti, M. Convegno tematico AIAR "Beni Culturali: grandi facilities, reti e networks di laboratori", Firenze 8-10/03/ 2017. "pXRF and archaeometallurgical analysis of silver coins from the 'Colline Metallifere district' (South Tuscany): preliminary results". Poster presentation.
213. Zanchi, C.; Lucotti, A.; Cancogni, D.; Fontana, F.; Trusso, S.; Ossi, P.M.; Tommasini, M. XVI International Conference on Chiroptical Spectroscopy, Rennes (France) 11-15/07/2017. "Nanostructured gold substrates functionalized with thiolated 5-Aza[5]helicene for SERS applications". Poster.
214. Akhunzada, M.J.; Catte, A.; Bhattacharjee, N.; Verbeek, D.S.; Kocer, A.; Brancato, G. Physiological role of ions in the brain: towards a comprehensive view by molecular simulation - CECAM workshop - Scuola Normale Superiore, Pisa May 21-23, 2018. "Predicting the effects of a de novo mutation in the Kv4.3 potassium channel". Poster.
215. Al Khatib, M.; Costa, J.; Baratto, M.C.; Basosi, R. Pogni, R. XXXVI Convegno Interregionale TUMA 2018, Pisa 4-5/10/2018. "Misure di rilassamento elettronico per la caratterizzazione di melanine naturali e sintetiche". Oral presentation.
216. Al Khatib, M.; Hairir, M.; Baratto M.C.; Basosi R.; Pogni R. XLVI Congresso di Chimica Fisica, Bologna 25-28/06/2018. "CW-Multifrequency and Q-band pulsed EPR for the characterization of natural and synthetic melanin-like pigments". Poster.
217. Al Khatib, M.; Harir, M.; Baratto M.C.; Basosi R.; Pogni R. International EPR School, Marsiglia (France) 3-7/06/2018. "CW-Multifrequency and Q-band pulsed EPR for the characterization of natural and synthetic melanin-like pigments". Oral presentation.
218. Avagnina, M.; Coffetti, D.; Coppola, L.; Fazio, M.G.; Guccione, M.; Liguori, F.R.; Virdia, E. Italian Concrete Days 2018, Lecco 13-16/06/2018. "Proposal for the conservative intervention of the reinforced concrete external surface of the MAXXI museum". Oral presentation.
219. Baglioni, P. 16th Conference of the International Association of Colloid and Interface Scientists (IACIS), Rotterdam (The Netherlands) 21-25 May 2018. Invited plenary lecture.
220. Baglioni, P. 2nd European Industry Days, Bruxelles (Belgium) 21-24/02/2018. Invited lecture.
221. Baglioni, P. 3rd Joint AIC-SILS Conference, Rome 28 June 2018. "Application of Neutrons and X-Rays to the Study of Materials for the Conservation of Cultural Heritage". Invited lecture.
222. Baglioni, P. 5TH international symposium on cultural heritage conservation and digitalization, Bejing (RPS) 12-15 September 2018. "New methods and materials for the conservation of Cultural Heritage"; Promotion of ECHOES Cluster. Invited lectures.
223. Baglioni, P. 7TH EuCheMS Chemistry Congress, Liverpool (UK) 26-30 August 2018. Invited lecture.
224. Baglioni, P. 82nd Prague meeting on Macromolecules; 24th Polymer Network group meeting, Prague, Czech Republic 15-19/06/2018. "Polymer hydrogel networks and complex fluid for the conservation of modern and contemporary art". Invited lecture.
225. Baglioni, P. Ansa.it: Nanorestart, La nanotecnologia salva le opere di Pollock e Picasso. http://www.ansa.it/europa/notizie/rubriche/speciali_elezioni2014/2018/02/27/nanorestart-nanotecnologia-salva-opere-di-pollock-e-picasso_c9579960-1e9c-4a86-a095-8768e02e2954.html. Communication.
226. Baglioni, P. 2018 European Year of Cultural Heritage, Royal Museum of Arts and History, Brussels (Belgium) 20 March 2018. "Nanorestart project and Echoes cluster". Invited lecture.
227. Baglioni, P. Israel-Italy Scientific Workshop on Conservation of Art, Tel Aviv (Israel) 15 March 2018. "Polymer hydrogel networks and complex fluid for the cleaning of modern and contemporary art". Invited lecture.
228. Baglioni, P. MacroBio Summer School 2018 Biomaterial Science in View of Digitalization, School Biomaterials, Berlin (Germany) 24-25 September 2018. ""Polymer Hydrogel Networks and Complex Fluids for the Conservation of Modern and Contemporary Art". Invited lecture.
229. Baglioni, P. Molecular Frontiers, Cambridge, MA (USA) 14-19/11/2018. Invited lecture.

230. Baglioni, P. Nanocathedral, Pisa 17/05/2018. “Innovation for Europe Cultural Heritage Protection and Conservation”. Invited lecture.
231. Baglioni, P. Nanosistemas, Madrid (Spain), Reina Sofia 6-8/06/2018. “Aplicacion en la eliminacion de Cintas adhesivas en suporte celulosico”. Invited lecture.
232. Baglioni, P. Nanotechnologies for conservation - Workshop at Academy of Fine Arts, Academy of Fine Arts, Krakow (Poland) 8-11 January 2018. “The use of highly retensive gels for the cleaning of artworks”; “Detergency, wetting and de-wetting”. Invited lecture.
233. Baglioni, P. Nanotechnologies for conservation - workshop at Pratt Institute, New York (USA) 12-16/02/2018. “Nanotechnologies for conservation of cultural heritage at Pratt Institute: A hands-on workshop available to midcareer conservators”. Training.
234. Baglioni, P. Resilient Cultural Heritage and Communities in Europe, Hungarian National Museum, Budapest (Hungary) 10-11 May 2018. “Nanorestart: Nanomaterials for the restoration of works of art”. Invited lecture.
235. Baglioni, P. Sistemas-nano: pesquisa e aplicacao para o patrimonio cultural, Fundação Casa de Rui Barbosa, Rio de Janeiro (Brazil) 10th April 2018. “A practical introduction to the use of a new generation of gels, emulsions and nano-fluids on cellulose based artworks”. Invited lecture.
236. Baglioni, P. Sistemas-nano: pesquisa e aplicacao para o patrimonio cultural, Pinacoteca Sao Paulo (Brazil) 12th April 2018. “Nano-ciência e sua contribuição para a conservação do Patrimônio Cultural: pedras, suporte de cobre e de celulose, pintura, sensores…”; “Introdução prática da aplicação de uma nova geração de gels, emulsões e nano-fluídos em obras de arte em suporte de celulose”. Invited lectures.
237. Baglioni, P. Workshop and training as dissemination activities of the Nanorestart Project, Rio de Janeiro (Brazil) 10-12/04/2018.
238. Baglioni, P. Workshop “Cleaning of modern oil paintings with nanomaterials and microemulsions”, Amsterdam (The Netherlands) 03-05/10/2018. “Nanomaterials and advanced solutions for the restoration of Cultural Heritage”. Invited lecture.
239. Balbi, A.; Tasinato, N.; Spada, L.; Puzzarini, C.; Barone, V. XXXIV European Congress on Molecular Spectroscopy, Coimbra (Portugal) 19-24/08/2018. “Structural, Spectroscopic and Energetic Properties of Creatinine Conformers by Quantum-chemical Calculations”. Poster.
240. Barone, V. 6th Workshop of the Italian Astrobiology Society, Napoli 29-31/10/2018. “From atoms to biomolecules in the space: the fascinating world of astrochemistry”. Oral presentation.
241. Barone, V. Accademia delle Scienze di Torino, Torino 01/02/2018. “Linguaggi comuni per sistemi complessi: la nuova frontiera di Arte e Scienza”. Oral presentation.
242. Barone, V. ASTRO-Winter Modeling "Advances in computational & experimental modelling: Application to Astrochemistry", Bologna 15-16/02/2018. “Virtual instruments for astrochemistry: from structure to reactivity”. Oral presentation.
243. Barone, V. II Italian Workshop on Astrochemistry, Follonica (GR) 13-16/06/2018. “STAR - Systems and Theories for Astrochemical Research”. Oral presentation.
244. Barone, V. La nuova frontiera di arte e scienza - Quattro istituzioni a confronto, Firenze 03/05/2018. “Linguaggi comuni per sistemi complessi: la nuova frontiera di Arte e Scienza”. Oral presentation.
245. Barone, V. Meeting Le due Culture - Cosmologia. L’uomo eterno Ulisse nell’infinità dei mondi, Ariano Irpino (AV) 05/09/2018. “Un affascinante viaggio tra le stelle: alla ricerca di molecole prebiotiche negli spazi siderali”. Oral presentation.
246. Barone, V. Molim Working Group 3 meeting:Ab-Initio Modelling of Molecular Processes Under Confinement, Madrid (Spain) 03-05/12/2018. “Virtual Instruments for Computational Spectroscopy in Gas and Condensed Phases”. Oral presentation.
247. Bartolozzi, I.; Baldareschi, E.; Mordini, A.; Basosi, R.; Parisi, M.L. VII Convegno della Associazione Rete Italiana LCA, Messina 12-13/06/2018. “Life Cycle Analysis of an innovative component for the sustainability in the building sector”. Oral presentation.
248. Basosi, R. Congr. Rete LCA, Messina 8/06/2018. “EU Policies for ENERGY Research: Horizon 2020 Work Program and role of LCA”. Plenary lecture.
249. Basosi, R. FEDERESCO, Roma 28/02/2018. “Ruolo dell’Efficienza Energetica nello sviluppo tecnologico della EU”. Oral presentation.
250. Basosi, R. GIURI, Bruxelles (Belgium) 12/09/2018. “Energy in EU: the new 2018-19 WP in H2020”. Oral presentation.
251. Basosi, R. Scuola Enerchem, Firenze 21/02/2018. “Energy Research on Renewable Energy in EU”. Invited lecture.
252. Basosi, R.; Capra, M. ENEA 24/10/2018. “Le politiche europee dell’Energia per la ricerca e l’innovazione: SET Plan e Mission Innovation”. Oral presentation.
253. Bergese, P. 7TH EuCheMS Chemistry Congress, Liverpool (UK) 26-30 August 2018. “Projecting

extracellular vesicles in two dimensions”. Talk.

254. Bergese, P. ISEV workshop "membranes and evs", Johns Hopkins University, Baltimore, Maryland, (USA) 24-25/03-2018. “Projecting extracellular vesicles in two dimensions”. Short list selection, talk.
255. Bergese, P. XI Congresso Nazionale AICIng, Università di Bologna – Complesso di S. Giovanni in Monte 9-12 Settembre 2018. “Surfaces from nanosized extracellular vesicles”. Invited talk.
256. Bhattacharjee, N.; Catte, A.; Akhunzada, M.J.; Verbeek, D.S.; Kocer, A.; Brancato, G. First Scientific Dutch Ataxia Symposium - Groningen, The Netherlands June 8, 2018. “Unravelling the molecular basis of Kv4.3 channelopathies: A molecular modeling study of the loss-of-function mutations causing spinocerebellar ataxia type 19/22”. Poster.
257. Bonini, M. 7th EUCHEMS Chemistry Congress, Liverpool (UK) 28/8/2018. “Clay nanotubes: towards functional composites”. Oral presentation.
258. Bonini, M. Nano Innovation 2018, Rome 12/9/2018, “Colloidi, Nanoscienze e Formulazioni: Sfide e Opportunità”. Oral presentation.
259. Bozgad, M.: ICCA 2018, Bucharest 27-30/06/2018. “Investigations of new analogs of SLC-0111”. Oral contribution.
260. Bruni, G. XL Congresso AICAT (Associazione Italiana di Calorimetria e Analisi Termica), Pisa 17-19/12/2018. “The role of DSC in the screening and characterization of cocrystals”. Invited Lecture.
261. Bua, S.: ICCA 2018, Bucharest 27-30/06/2018. “Bioisosteric replacement and stability study in plasma of Novel Ester-linked NSAID - Carbonic Anhydrase Inhibitor Hybrids”. Poster contribution.
262. Bua, S.: IMSC 2018, Firenze 26-31/08/2018. “Stability study in plasma of Novel Ester-linked NSAID - Carbonic Anhydrase Inhibitor Hybrids”. Poster contribution.
263. Bufalo, G.; Di Nezza, F.; Lopez, F.; Cuomo F.; Ambrosone, L. 46th Meeting of the Physical Chemisty Division of the Italian Chemistry Society, Bologna 25-28/06/2018. “Application of the principle of minimal wrecking and maximum separation for the reuse of solid leather waste”. Oral presentation.
264. Cabrini, M.; Lorenzi, S.; Pastore, T.; Bocchi, S.; D’Urso, G.; Giardini, C. Stress-Assisted Corrosion Damage V, Schloss Hernstein (Austria) 15-20/07/2018. “Electrochemical and environmental assisted cracking behavior of AA2024 T3 and AA7075 T6 welded by means of FSW”. Oral presentation.
265. Cabrini, M.; Lorenzi, S.; Pastore, T.; Pesenti Bucella, D. Stress-Assisted Corrosion Damage V, Schloss Hernstein (Austria) 15-20/07/2018. “Effect of Cyclic Loading on Hydrogen Diffusion in Low-Alloyed Carbon Steels”, Oral presentation.
266. Cabrini, M.; Lorenzi, S.; Pastore, T.; Pesenti Bucella, D. XXXVII Convegno Nazionale AIM, Bologna 12-14/09/2018. “Effetto del carico ciclico sulla diffusione di idrogeno in acciai basso-legati”. Oral presentation.
267. Cabrini, M.; Lorenzi, S.; Pastore, T.; Testa, C.; Manfredi, D.; Trevisan, F.; Calignano, F. 8th Aluminium Surface Science and Technology Symposium (ASST), Helsingør (Denmark) 27-31/05/2018. “Corrosion Resistance in chloride solution of the AlSi10Mg Alloy obtained by means of LPBF”. Oral presentation.
268. Cabrini, M.; Lorenzi, S.; Testa, C.; Pastore, T.; Manfredi, D.; Lorusso, M.; Calignano, F.; Fino, P. Electrochemical Methods in Corrosion Research (EMCR), Cambridge (UK) 22-27/07/2018. “Statistical approach for electrochemical evaluation of the effect of heat treatments on the corrosion resistance of AlSi10Mg alloy by laser powder bed fusion”. Oral presentation.
269. Caminati, G. 8th Annual World Congress of Nano Science and Technology, Potsdam (Germany) 24-26/10/2018. “Graphene Oxide/Silver Nanoparticles Platforms for the Early Diagnosis of Neurodegenerations”. Oral presentation.
270. Casiello, M.; Leonardi, A.A.; Picca, R.A.; Fusco, C.; D’Accolti, L.; Lo Faro, M.J.; Trusso, S.; Cotugno, P.; Sportelli, M.C.; Cioffi, N.; Nacci, A. E-MRS 2018, European Materials Research Society, 2018 E-MRS Spring Meeting. “Silicon Nanowires arrays decorated by Cu and Au Nanoparticles showing exceptional catalytic properties”. Poster presentation.
271. Catte, A.; Bhattacharjee, N.; Akhunzada M.J.; Verbeek, D.S.; Kocer, A.; Brancato , G Physiological role of ions in the brain: towards a comprehensive view by molecular simulation - CECAM workshop - Scuola Normale Superiore, Pisa May 21-23, 2018. “Modeling inherited and de novo mutations in a voltage-gated potassium channel”. Oral presentation.
272. Catte, A.; Bhattacharjee, N.; Jan Akhunzada, M.; Verbeek, D.S.; Kocer, A.; Brancato, G. Dutch Neuroscience Meeting 2018 - Lunteren, The Netherlandsv June 7, 2018. “Unravelling the molecular basis of Kv4.3 channelopathies: A molecular modeling study of the loss-of-function mutations causing spinocerebellar ataxia type 19/22”. Poster.
273. Catte, A.; Brancato, G. Meeting INFN BIOPHYS and PLEXNET 2018 - Castello Aldobrandesco, Arcidosso (GR) September 10-12, 2018. “Modeling inherited and de novo mutations in a voltage-gated potassium channel”. Oral presentation.
274. Cofelice, M.; Ceglie, A.; Cuomo, F.; Lopez, F. 46th Meeting of the Physical Chemisty Division of the Italian Chemistry Society, Bologna 25-28/06/2018. “Nanodispersions as edible coatings: impact on

fresh-cut fruit". Poster.

275. Consumi, M.; Jankowska, K.; Magnani, A. 21st International Conference on Secondary Mass Spectrometry, Krakow (Poland) 10-15/09/2018. "Time-of-Flight Second Ion Mass Spectrometry (ToF-SIMS); a promising tool for extracellular matrix ECM analysis". Oral presentation.
276. Coppola, L.; Coffetti, D.; Crotti, E. 12th International Conference on Superplasticizers and other Chemical Admixtures in Concrete ICSP 2018, Beijing (China) 28-31/10/2018. "CSA-based mortars manufactured with tartaric acid-based retarder". Oral presentation.
277. Coppola, L.; Coffetti, D.; Crotti, E. 15th International Conference on Recent Advances in Concrete Technology and Sustainability Issues 2018, Beijing (China) 31/10-02/11/2018. "One-part alkali-activated slag cement for conservation of existing structures". Oral presentation.
278. Coppola, L.; Coffetti, D.; Crotti, E. 1st FIB Conference on Sustainable Concrete: Materials and Structures, La Valletta (Malta) 27/11/2018. "A holistic approach to a sustainable future in concrete construction". Oral presentation.
279. Coppola, L.; Coffetti, D.; Crotti, E. 2nd International Workshop on Durability and Sustainability of Concrete Structures DSCS 2018, Moscow (Russia) 6-7/06/2018. "Environmentally friendly concretes manufactured with CSA cement". Oral presentation.
280. Coppola, L.; Coffetti, D.; Crotti, E. 2nd International Workshop on Durability and Sustainability of Concrete Structures DSCS 2018, Moscow (Russia) 6-7/06/2018. "Rheological and physical performances of mortars manufactured with plain and ultrafine fly ashes". Oral presentation.
281. Coppola, L.; Coffetti, D.; Crotti, E. 3rd European Geopolymer Network 2018, Faenza 30/11/2018. "Influence of naphthalene, polycarboxylates and lignosulfonates-based superplasticizers on fresh and hardened properties of alkali-activated slag mortars". Oral presentation.
282. Coppola, L.; Coffetti, D.; Crotti, E. 3rd European Geopolymer Network 2018, Faenza 30/11/2018 "Lightweight alkali-activated slag-based plaster for seismic retrofitting and thermal insulation of existing masonry buildings". Oral presentation.
283. Coppola, L.; Coffetti, D.; Crotti, E. ECI International Conference on Alkali Activated Materials and Geopolymers: Versatile Materials Offering High Performance and Low Emissions, Tomar (Portugal) 27/05-01/06/2018. "Influence of different types of superplasticizers on one-part alkali-activated slag mortars". Oral presentation.
284. Coppola, L.; Coffetti, D.; Crotti, E.; Forni, D.; Cadoni, E. 12th International Conference on the Mechanical and Physical Behaviour of Materials under Dynamic Loading DYMAT, Arcachon (France) 9-14/09/2018. "Fiber reinforced mortars based on free Portland-CSA binders under high stress rate". Poster.
285. Coppola, L.; Coffetti, D.; Crotti, E.; Nicoletti, A. Italian Concrete Days 2018, Lecco 13-16/06/2018. "The restoration and conservation of thin vault concrete structures – the example of the church at Longuelo (Bergamo)". Oral presentation.
286. Coppola, L.; Coffetti, D.; Crotti, E.; Torresan, I. Italian Concrete Days 2018, Lecco 13-16/06/2018. "Study of an innovative waterproofing admixture for self-repairing concrete with hydraulic seal". Oral presentation.
287. Cordaro, G.; Donazzi, A.; Pelosato, R.; Natali Sora, I.; Cristiani, C.; Dotelli, G. XX Congresso Nazionale di Catalisi & XX Congresso Nazionale della Divisione di Chimica Industriale (GIC DiChIn 2018) Milano, 2-5/09/2018. "Structural and electrochemical characterization of NdBa1-xCo2-yFeyO5+δ as cathode for intermediate temperature SOFCs". Oral presentation.
288. Cordaro, G.; Donazzi, A.; Pelosato, R.; Natali Sora, I.; Dotelli, G. Americas International Meeting On Electrochemistry and Solid State Science (AiMES 2018), Cancun (Mexico) 30/9 - 4/10 2018. "Structural and electrochemical evaluation of Iron doping and Barium deficiency in layered perovskite cathodes for IT-SOFCs: NdBa1-xCo2-yFeyO5+δ". Oral presentation.
289. Costa, J.; Baratto M.C.; Atrei, A.M.; Pogni, R. XXXVI Convegno Interregionale TUMA 2018, Pisa 4-5/10/2018. "Preparazione e caratterizzazione di laccasi immobilizzata in nanoparticelle magnetiche Fe3O4". Poster.
290. Cuomo, F.; Ceglie, A.; Miguel, M.; Lindman, B.; Lopez F. 16th Conference of the International Association of Colloid and Interface Scientists (IACIS) Rotterdam (The Netherlands) 21-25/05/2018. "In-vitro digestion of Curcumin loaded chitosan-coated liposomes". Poster.
291. Cuomo, F.; Ceglie, A.; Miguel, M.; Lindman, B.; Lopez F. 46th Meeting of the Physical Chemisty Division of the Italian Chemistry Society, Bologna 25-28/06/2018. "Polyelectrolyte capsules as carriers for hydrophilic and lipophilic molecules". Oral presentation.
292. Cuomo, F.; Lopez, A.; Ceglie, A. 7th Symposium on Polyelectrolytes, Coimbra (Portugal) 16-19/06/2018. "Liposomal formulation for polynucleotides delivery". Poster.
293. Dell'Aglio, M.; Valenza, G.; Palazzo, G.; Cioffi, N.; Picca, R.A.; De Giacomo, A. Advances nanoparticles generation & excitation by lasers in liquids - Angel 2018, Lyon (France) 3-7 June 2018.

"Characterization of Au and Ag nanoparticle produced by PLAL for considerations on their stability". Oral communication.

294. D'Errico, G.; Panzella, L.; d'Ischia, M.; Paduano, L. 32th Conference of the European Colloid and Interface Society (ECIS 2018), Ljubljana (Slovenia) 2-7/09/2018. "Bio-inspired functional polyphenolic materials: meso- and nanoscopic determinants of the antioxidant activity". Oral communication.
295. Fontana, F.; Zanchi, C.; Cancogni, D.; Tommasini, M.; Trusso, S. XI Congresso AICIng, Bologna 10-12/9/2018. "Functionalization of nanostructured gold substrates with chiral chromophores for SERS applications: The case of 5-Aza[5]helicene". Poster.
296. Fratini, E. SISN Advanced School 2018, San Giovanni in Valle Aurina, Bolzano Giugno 2018. "Investigation of block-copolymers nanostructure by SANS".
297. Giaccherini, A.; Baroni, T.; Russo, F.; Cioffi, N.; Capolupo, F.; Picca, R.A.; Montegrossi, G.; Di Benedetto, F.; Innocenti, M. Società Geologica Italiana (SGI) and Società Italiana di Mineralogia e Petrologia (SIMP), Catania 12-14 September 2018. "Electrochemical atomic layer deposition to grow a p-n junction with binary sulphides". Poster.
298. Guida, S.; Ferretta, A.; Serratì, S.; Cocco, T.; Maida, I.; Iacobazzi, R.M.; Porcelli, L.; Azzariti, A.; Tommasi, S.; Tamasi, G.; Rossi, C.; Pellacani, G.; Guida, G. 21st annual meeting of the European Society for Pigment Cell Research (ESPCR), Rennes (France) 24-27/09/2018. "New horizons in treatments of metastatic melanoma: the role of tomatine". Oral presentation.
299. Jankowska, K.; Brooker A.; Wright K. Face-2-Face meeting, Ghent (Belgium) 2-06/07/2018. "The fluorescent microscope study of initial bacterial attachment on the gram-positive and gram-negative bacteria model on to polymers films under three types of nutrient conditions". Oral presentation.
300. Jankowska, K.; Consumi M.; Magnani A.; Brooker A.; Wright K.; Rossi C. European Colloid and Interface Society 2018, Ljubljana (Slovenia) 2-6/09/2018. "The use of ATR-FTIR to study the mechanism of initial bacterial attachment and biofilm development on surfaces coated with different polymers". Poster presentation.
301. Jankowska, K.; Consumi, M.; Magnani, A.; Rossi, C. Biofilm 8, Aarhus (Denmark) 27-29/05/2018. "ATR-FTIR of Pseudomonas fluorescens from planktonic state to early biofilm formation under different nutrient condition". Poster presentation.
302. Jankowska, K.; Consumi, M.; Magnani, A.; Rossi, C. Face-2-Face meeting, Bioclean project, Birmingham (UK) 26-28/02/2018. "ATR-FTIR study of interaction between gram-negative bacterial model and three types of polymer under no nutrient conditions". Oral presentation.
303. Jankowska, K.; Consumi, M.; Magnani, A.; Rossi, C. International School of Physical Chemistry: Materials for Biomedical Applications, Venice 1-5/07/2018. "The ATR-FTIR study of bacterial EPS model with polymers surfaces prepared by spin-coating technique" Oral presentation and poster presentation.
304. Li Destri, G.; Tuccitto, N.; Amato, T.; Messina, G.M.L.; Marletta, G. XLVI Congresso Nazionale di Chimica Fisica, Bologna 25-28/06/2018. "Monitoring 2D material growth with competitive interfacial reactions". Oral presentation.
305. Li Destri, G.; Tuccitto, N.; Ruffino, R.; Messina, G.M.L.; Marletta, G. XLVI Congresso Nazionale di Chimica Fisica, Bologna 25-28/06/2018. "Polymer crystallization on substrates with controlled surface free energy and nano-curvature". Poster.
306. Lo Nostro, P.; Tatini, D.; Sarri, F.; Raudino, M. Ions in Solution: Biology, Energy, and Environment, Telluride, Colorado (USA) 16-21/07/2018. "How salts can influence the structuredness of organic solvents. The curious case of glycerol carbonate". Conference.
307. Loiselle, S. 2nd International Symposium on Watershed Geographic Sciences, Nanjing (China) 10/2018. "New tools and opportunities for watershed management". Session chairman and keynote.
308. Loiselle, S. Citizens Observatories for Water Management, Venice 9/2018. "Challenges and opportunities of citizen science water quality monitoring". Session chairman.
309. Loiselle, S. VIII Congreso Argentino de Limnología, Lujan (Argentina) 9/2018. "Integrated tools to limnology". Keynote.
310. Longhi, M.; Cova, C.; Pargoletti, E.; Coduri, M.; Santangelo, S.; Patanè, S.; Ditaranto, N.; Cioffi, N.; Facibeni, A.; Scavini, M. XXVII Congress of the Analytical Chemistry Division, Italian Chemical Society, Bologna 16-20 September 2018. "Surface characterization of non-noble metals embedded in N-doped carbon catalysts: the importance of hydrophilicity on oxygen reduction reaction activity". Oral communication.
311. Longhi, M.; Cova, C.; Pargoletti, E.; Coduri, M.; Santangelo, S.; Patanè, S.; Ditaranto, N.; Cioffi, N.; Facibeni, A.; Scavini, M. N&N 2018, Nanoscience & Nanotechnology INFN Meeting 2018. "Surface characterization of Pt-free catalysts: synergistic effects of active sites' nature and hidrophilicity on the oxygen reduction reaction activity". Invited oral communication.
312. Lorenzi, S. Electrochemical Methods in Corrosion Research (EMCR), Cambridge (UK) 22-27/07/2018.

"Electrochemical evaluations of the corrosion behaviour of carbon steel in innovative binders". Oral presentation.

313. Macchia, E.; Manoli, K.; Holzer, B.; Di Franco, C.; Ghittorelli, M.; Torricelli, F.; Alberga, D.; Mangiatordi, G. F.; Palazzo, G.; Scamarcio, G.; Torsi, L. Organic Bioelectronic Italy OrBItaly 2017, Italy 17-19/10/2018. "Single-molecule detection with a millimetre-sized transistor". Oral presentation.
314. Macchia, E.; Torsi, L.; Manoli, K.; Di Franco, C.; Scamarcio, G.; Zak, A.; Tenne, R. Winter School on Biophotonics and Bioelectronics, Hirschegg (Austria) 18-24 February 2018. "Insight into the charge transport of p-type/n-type blend materials for EG-OFET applications". Oral presentation.
315. Maranghi, S.; Cositore, F.; Basosi, R.; Busi, E. XII Convegno della Rete Italiana LCA, Messina 12-13/06/2018. "Energy saving in LT/MT transformers." Oral presentation.
316. Maranghi, S.; Parisi, M.L.; Sinicropi, A.; Basosi, R. 1st Enerchem School: Chemistry For The Energy Transition, Fiesole (FI) 20-24/02/2018. "Methodologies for the sustainability evaluation of innovative renewable energy technologies." Oral presentation.
317. Maranghi, S.; Sinicropi, A.; Basosi, R.; Parisi, M.L. 4th International Conference on Perovskite Solar Cells and Optoelectronics - PSCO, Lausanne (Switzerland) 30/09-02/10/2018. "Environmental profile of perovskite photovoltaic technology: harmonization of Life Cycle Assessment studies". Poster.
318. Maranghi, S.; Sinicropi, A.; Basosi, R.; Parisi, M.L. XLVI Congresso della Divisione di Chimica Fisica della Società Chimica Italiana (SCI), Bologna (BO) 28/06/2018. "Life Cycle Assessment of the Perovskite Photovoltaic Technology: Harmonization of Data". Poster.
319. Maranghi, S.; Sinicropi, A.; Basosi, R.; Parisi, M.L. XLVI Congresso della Divisione di Chimica Fisica della Società Chimica Italiana (SCI), Bologna 28/06/2018. "Life Cycle Assessment of the Perovskite Photovoltaic Technology: Harmonization of Data". Poster.
320. Martina, M.R. International Workshop on Plasmonics, Florence 6/06/2018. "Graphene Oxide-Functionalized SERS Substrates for a Simple Discrimination between Native and Fibrillar Lysozyme". Oral presentation.
321. Martina, M.R.; Lofrumento, C.; Banchelli, M.; Matteini, P.; Caminati, G. International Workshop on Plasmonics, Florence 6/06/2018. "Development of a Plasmonic Device based on Langmuir-Blodgett films of Ag Nanowires". Poster.
322. Mateos Cuadrado, H.; Palazzo, G.; Cioffi, N.; Robles, E.; Brooker, A. ECIS (European Colloid and Interface Society) 2018 conference, Ljubljana (Slovenia) 2-7 September 2018. "Influence of hard surface polymer coatings on biological soil removal". Poster.
323. Medda, L.; Lo Nostro, P.; Caminati, G. 32nd Conference of the European Colloid and Interface Society. Ljubljana (Slovenia) 2nd-7th September 2018. "Ion-specific effects on the Human Insulin fibrillation process". Poster presentation.
324. Mendolicchio, M.; Tasinato, N.; Licari, D.; Barone, V. XXXIV European Congress on Molecular Spectroscopy, Coimbra (Portugal) 19-24/08/2018. "The MSR Route to Accurate Equilibrium Molecular Structures through the Semi-Experimental Approach". Oral presentation.
325. Messina, G.M.L.; Bocchinfuso, G.; Mazzuca, C.; Palleschi, A.; Marletta, G. Congresso Nazionale Divisione Chimica Fisica – SCI 2018, Bologna 25-28/06/2018. "Organizing proteins by tailored nanostructures surfaces". Oral presentation.
326. Messina, G.M.L.; Marletta, G. BioEl International Winterschool on Bioelectronics 2018, Kirchberg in Tyrol (Austria) 11-16/03/2018. "Electrical properties of bifunctional PEDOT(PSS): Poly-L-Lysine thin films". Poster.
327. Milanese, C. Collegio Spallanzani (Pavia) 15/05/2018. "Vizi e virtù del (probabile?) vettore energetico del terzo millenio". Invited lecture.
328. Milanese, C. Institute for Energy Technology, Oslo (Norway) 29/06/2018. "Work in progress at the Pavia Hydrogen Lab: hydrogen and energy storage materials". Invited lecture.
329. Milanese, C.; Gaboardi, M.; Girella, A.; Magnani, G.; Pontiroli, D.; Riccò, M.; Fernandez-Alonso, F.; Marini, A. Future Energy EF 3 Conference, Sydney (Australia) 5-7/02/2018. "Effect of alkali metals on the hydrogen sorption properties of fullerene". Oral presentation.
330. Milanese, C.; Girella, A.; Aramini, M.; Ishida, K.; Bergemann, N.; Hillier, A.; Marini, A.; Dornheim, M.; Pistidda, C. 16th International Symposium on Metal-Hydrogen Systems (MH2018), Guangzhou (China) 28/10-2/11/2018. "Solving the mystery of the destabilized Ca(BH4)2-Mg2NiH4 system by µXES". Poster.
331. Milanese, C.; Girella, A.; Gioventù, M.; Cofrancesco, P.; Gaboardi, M.; Pontiroli, D.; Magnani, G.; Riccò, M.; Fernandez-Alonso, F.; Marini, A. 16th International Symposium on Metal-Hydrogen Systems (MH2018), Guangzhou (China) 28/10-2/11/2018. "Carbon based materials for solid state hydrogen storage and energy storage". Invited lecture.
332. Mohammadpourasl, S. Samset School, Advanced Materials for Sustainable Energy Technology, Lecce 11-15/06/2018. "The Future of Energy, Renewable or Nuclear Fusion". Round table discussion.

333. Mohammadpourasl, S.; Dessì, A.; Zani, L.; Reginato, G.; Basosi, R.; Sinicropi, A. Enerchem School, Chemistry for Energy Transition, Firenze 20-24/02/2018. “In silico design of near-IR D-A-π-A sensitizers for dye sensitized solar cells”. Poster.
334. Mohammadpourasl, S.; Dessì, A.; Zani, L.; Reginato, G.; Basosi, R.; Sinicropi, A. The 4th EMN Meeting, Computation and Theory, San Sebastian (Spain) 03-07/09/2018. “DFT modeling of redox potentials of full organic dyes for dye-sensitized solar cells”. Poster.
335. Mohammadpourasl, S.; Dessì, A.; Zani, L.; Reginato, G.; Basosi, R.; Sinicropi, A. TUMA 2018, congresso interregionale di chimica, Pisa 04-05/10/2018. “DFT modeling of redox potentials of full organic dyes for dye-sensitized solar cells”. Poster.
336. Monduzzi, M.; Piludu, M; Sogos, V.; Salis, A., ECIS 2018, Ljubljana. “Mesoporous Silica Nanoparticles for Smart Drug Depot Nanocarriers”. Invited key note.
337. Mosca, M; Ambrosone, L; Ceglie, A. XXXVII Congresso Nazionale di Chimica Fisica, Camogli (GE) 24-29/02/2018. “Antioxidant dispersion in biocompatibile oils”. Oral Presentation.
338. Murgia, S. 16th Conference of the International Association of Colloid and Interface Scientists (IACIS), Rotterdam (The Netherlands), 21-25/05/2018. “Cubic liquid crystalline nanoparticles as potential theranostic tools”. Oral presentation.
339. Murgia, S. Incontro Spettroscopia Analitica 2018, Cagliari, 5-8/06/2018. “Cubic liquid crystalline nanoparticles as potential theranostic tools”. Oral presentation.
340. Murgia, S. Nanomedicine Rome 2018, Roma 18-20/06/2018. “Bicontinuous cubic liquid crystalline dispersions as potential tools in nanomedicine”. Oral presentation.
341. Nasi, R.; Gadhi, T.A.; Freyria, F.S.; Ditaranto, N.; Esposito, S.; Hernandez, S.; Armandi, M.; Bonelli, B. ISA Cagliari 2018, Incontro di Spettroscopia Analitica 2018. “Surface chemical characterization of Mo doped TiO_2 nanoparticles for photocatalytic dye degradation”. Oral communication.
342. Natali Sora, I.; Luciani, G.; Pezzella, A.; Vitiello, G.; Silvestri, B. Atti del XI Congresso Nazionale dell’Associazione Italiana di Chimica per Ingegneria (AICIng 2018), Bologna 9-12/9/2018. “Nuove frontiere nella progettazione di dispositivi opto-elettronici: sistemi semiconduttori ibridi bio organo-inorganici”. Poster.
343. Paduano, L.; Russo Krauss, I.; Luchini, A.; Vitiello, G. 32th Conference of the European Colloid and Interface Society (ECIS 2018), Ljubljana (Slovenia) 2-7/09/2018. “Multimodal Iron-Oxide Nanoparticles: from Design to in vivo Applications”. Keynote.
344. Palazzo, G.; Mateos, H.; Cioffi, N.; Dell'Aglio, M.; Picca, R.A.; De Giacomo, A. 16th Conference of the International Association of Colloid and Interface Scientists (IACIS), Rotterdam (The Netherlands) 21-25 May 2018. “On the stability of gold nanoparticles synthesized by laser ablation and their interactions with phospholipid membranes”. Oral communication.
345. Pardini, A.; Bonechi, C.; Tamasi, G.; Magnani, A.; Rossi, C. ISEAC-40 40th International Conference on Environmental & Food Monitoring, Santiago de Compostela (Spain) 19-22/06/2018. “Chemical charactetrization and antioxidant properties of products and by-products from Olea Europaea L.”. Poster presentation.
346. Parisi, M.L. International School on Hybrid and Organic Photovoltaics (ISOPHOS), Castiglione della Pescaia (Italia) 2-6/09/2018. “Life Cycle Assessment of Hybrid and Organic Photovoltaics”. Oral presentation.
347. Perugini, L.; Cuomo, F.; Lopez F. 16th Conference of the International Association of Colloid and Interface Scientists (IACIS) Rotterdam (The Netherlands) 21-25/05/2018. “Effect of nanoemulsion stabilizers on solubility and the in-vitro digestion of curcumin”. Poster.
348. Picca, R.A.; Leonardi, A.; Lo Faro, M.J.; Calvano, C.D.; Fazio, B.; Trusso, S.; Ossi, P.M.; Neri, F.; D’Andrea, C.; Cioffi, N. E-MRS 2018, European Materials Research Society, 2018 E-MRS Spring Meeting. “Metal Nanoparticle-Decorated Si Nanowires as an Efficient Platform for Laser Desorption/Ionization Mass Spectrometry”. Poster.
349. Picca, R.A.; Lopetuso, R.; Torsi, L.; Innocenti, M.; Cioffi, N. ISA Cagliari 2018, Incontro di Spettroscopia Analitica 2018. “Spectroscopic characterization of electrosynthesized ZnO nanomaterials”. Poster.
350. Picca, R.A.; Macchia, E.; Manoli, K.; Di Franco, C.; Palazzo, G.; Cioffi, N.; Scamarcio, G.; Torsi, L. XXVII Congress of the Analytical Chemistry Division, Italian Chemical Society, Bologna 16-20 September 2018. “Environmental and operational stability of organic field effect transistors for biosensing applications”. Flash oral communication.
351. Picca, R.A.; Macchia, E.; Manoli, K.; Di Franco, C.; Tricase, A.; Cioffi, N.; Scamarcio, G.; Torsi, L. 73th International Workshop on Frontiers of Photonics, Plasmonics And Electronics With 2d Nanosystems – Erice 14-20th July 2018. “Investigation of the Stability of Organic Field Effect Transistors for Biosensing Applications”. Oral presentation.
352. Picca, R.A.; Manoli, K.; Sportelli, M.C.; Palazzo, G.; Torsi, L.; Cioffi, N. ISA Cagliari 2018, Incontro di Spettroscopia Analitica 2018. “Spectroscopic characterization of ZnO nanoparticles/biomolecule

active layers for applications in organic field effect transistor biosensors”. Poster presentation.

353. Pogni, R. I Workshop Gruppo Interdivisionale Biotecnologie, Bologna 23/02/2018. "Nanomaterials for Enzymatic Immobilization". Oral presentation.
354. Pogni, R.; Al Khatib, M.; Harir, M.; Costa, J.; Baratto, M.C.; Basosi, R. OxiZymes Conference 2018, Belfast (UK) 8-10/07/2018. “Characterization of natural melanin from Streptomyces cyaneofuscatus spp. And its comparison with the enzymatically synthesized melanin by tyrosine and laccase”. Poster.
355. Quarto, R.; Sportelli, M.C.; Picca, R.A.; Kranz, C.; Mizaikoff, B.; Tütüncü, E.; Valentini, A.; Cioffi, N. ISA Cagliari 2018, Incontro di Spettroscopia Analitica 2018. “Insights into the inhibition of P. fluorescens biofilm formation via AFM and ATR-IR characterizations”. Poster presentation.
356. Radeghieri, A. BBEV, Biogenesis and Biomarkers of Extracellular Vesicles, Padova 29-31 August 2018. “Exploring and exploiting the biophysical properties of EVs”. Invited talk.
357. Radeghieri, A. International Conference on Bioengineering and Cell therapy, Brescia 21 September 2018. “Extracellular vesicles in Regenerative Medicine”. Invited talk.
358. Rampino, S. Advances in computational & experimental modelling: application to astrochemistry. Bologna 15-16 febbraio 2018. “Computational modeling of gas-phase reactions in interstellar clouds, ASTRO-Winter Modeling”. Oral communication.
359. Rampino, S. Chimica Computazionale, Il pensiero computazionale – Percorso Formativo per i Docenti della Scuola Secondaria di Secondo Grado, Università di Pisa, Pisa 4 dicembre 2018. Invited oral.
360. Rampino, S. Emerging Technologies in Scientific Data Visualisation, Pisa 4-6 april 2018. “Immersive analysis of chemical bonding through virtual reality”. Invited oral.
361. Rampino, S. Invited seminar at Scuola Normale Superiore within the seminar cycle “Frontiere della Chimica”, Pisa 5 giugno 2018. “Probing charge-transfer effects in coordination chemistry through virtual reality”. Invited oral.
362. Rampino, S. La nuova frontiera di arte e scienza - Quattro istituzioni a confronto, Firenze 3 maggio 2018. “Virtualizzazione e sistemi interattivi per la tutela e la diagnostica dei beni culturali”. Invited oral.
363. Rampino, S. Problems in discrete dynamics: from biochemical systems to rare events, networks, clustering and related topics III Edition, Arcidosso 21-23 giugno 2018. “Analyzing the electron-charge rearrangement in chemical-bond formation through immersive virtual reality”. Invited oral.
364. Rampino, S. Second European Symposium on Chemical Bonding, Oviedo (Spain) 3-7 settembre 2018. “Combined Orbital-space/Real-space Immersive Analysis of Chemical Bonding through Virtual Reality”. Poster.
365. Riccardi, C.; Russo Krauss, I.; Musumeci, D.; Morvan, F.; Meyer, A.; Vasseur, J.J.; Paduano, L.; Montesarchio, D. E-WISPOC - 12th European-Winter School on Physical Organic Chemistry, Bressanone 28/01-2/02/2018. “Fluorescently-labeled thrombin binding aptamer conjugated to silica nanoparticles for efficient and reversible control of thrombin activity”. Poster.
366. Ridi, F. European Advanced Materials Congress 2018, Stockholm (Sweden) August 20-23, 2018. “Biologically relevant calcium-magnesium phosphates: from the physico-chemical study to the preparation of functional materials”. Invited oral presentation.
367. Ridi, F.; Gelli, R.; Gigli, L.; Scudero, M.; Bonini, M.; Baglioni, P. 2nd European Conference on Physical Chemistry 2017, Borgo (Corse) September 24-27, 2018. “Synthesis and characterization of immunologically relevant calcium and magnesium phosphate amorphous nanostructures and strategies for their stabilisation”. Poster.
368. Ridi, F.; Gelli, R.; Mati, L.; Baglioni, P. 2nd European Conference on Physical Chemistry 2017, Borgo (Corse) September 24-27, 2018. “Effect of cellulose ethers on the formation and properties of magnesium phosphate-based cements for biomedical applications”. Poster.
369. Ridi, F. 2nd European Conference on Physical Chemistry 2017, Borgo (Corse) September 24-27, 2018. “Interaction of phosphate-based additives with MgO/SiO2 cements”. Oral presentation.
370. Rosace, G.; Cardiano, P.; Urzì, C.; De Leo, F.; Galletta, M.; Ielo, I.; Plutino, M.R. Aegean International Textile and Advanced Engineering Conference (AITAE 2018) 5-7/09/2018 Mytilene (Lesvos, Greece). “Potential roles of fluorine-containing sol-gel coatings against adhesion to control microbial biofilm”. Oral presentation.
371. Rossi, F. Samset18 - School on Advanced Materials for Sustainable Energy Technologies, Lecce 11-15/06/2018. “Energy StorAge: toward a more sustainable and green world?”. Poster.
372. Rossi, F.; Parisi, M.L.; Maranghi, S.; Manfrida, G.; Basosi, R.; Sinicropi, A. 1st Enerchem school – Chemistry for the energy transition, Fiesole 20-24/02/2018. “Environmental impact analysis applied to Solar Pasteurization Systems”. Poster.
373. Russo Krauss, I.; Picariello, A.; Luchini, A.; Paduano, L. Nanomedicine 2018, Rome June 18th-20th 2018. “Functionalized superparamagnetic iron oxide nanoparticles as theranostic devices: from development to interaction with proteins”. Oral communication.

374. Salis, A. 15th ICSS, Cluj-Napoca (Romania) 17-22 April 2018. “Salty water: easy to do but difficult to understand. The Hofmeister series”. Plenary lecture.
375. Salis, A.; Nairi, V.; Piludu, M.; Sogos, V.; Vallet-Regì, M.; Monduzzi, M. XLVI Congresso Nazionale della Divisione di Chimica Fisica, Bologna 25-28 Giugno 2018. “Mesoporous silica nanoparticles functionalized with biopolymers: interactions with proteins and cell internalization”. Oral presentation.
376. Salvadori, A.; Fusè, M.; Mancini, G.; Rampino, S.; Barone, V. Quinto Congresso della Divisione di Chimica Teorica e Computazionale della Società Chimica Italiana DCTC 2018, Trieste 19-21 settembre 2018. “Combined Orbital- space/Real-space Analysis of Chemical Bonding through Virtual Reality”. Poster.
377. Sarcina, L.; García-Manrique, P.; Matos, M.; Ditaranto, N.; Cioffi, N.; Blanco, M.C.; Lopez, F. ISA Cagliari 2018, Incontro di Spettroscopia Analitica 2018. “Antimicrobial hybrid CuNPs-loaded nanovesicles: preparation and analytical characterization”. Poster.
378. Saturnino, C.; Sinicropi, M.S.; Iacopetta, D.; Ceramella, J.; Caruso, A.; Muià, N.; Longo, P.; Rosace, G.; Galletta, M.; Ielo, I.; Plutino M.R. Aegean International Textile and Advanced Engineering Conference (AITAE 2018) 5-7/09/2018 Mytilene (Lesvos, Greece). “N-Thiocarbazole-based gold nanoparticles: synthesis, characterization and anti-proliferative activity evaluation”. Oral presentation.
379. Sinicropi, A. International School on Hybrid and Organic Photovoltaics (ISOPHOS), Castiglione della Pescaia (Italia) 2-6/09/2018. “Computational modeling of processes and materials for solar energy conversion”. Oral presentation.
380. Sinicropi, A.; Maranghi, S.; Basosi, R.; Parisi, M.L. XXXVI Convegno Interregionale TUMA 2018, Pisa 4-5/10/2018. “Impronta ambientale del fotovoltaico a perovskite: armonizzazione di studi di Analisi del Ciclo di Vita”. Poster.
381. Spada, D.; Quinzeni, I.; Capsoni, D.; Bini, M. LXVI Congresso della Divisione di Chimica Fisica (SCI), Bologna 25-28/06/2018. “Investigation of the structural influence on the anodic performances of FeNb11O29”. Poster.
382. Sportelli, M.C.; Clemente, M.; Izzi, M.; Volpe, A.; Ancona, A.; Palazzo, G.; Cioffi, N. ISA Cagliari 2018, Incontro di Spettroscopia Analitica 2018. “Exceptionally stable silver nanoparticles synthesized by laser ablation in isopropyl alcohol”. Invited oral communication.
383. Sportelli, M.C.; Clemente, M.; Izzi, M.; Volpe, A.; Ancona, A.; Palazzo, G.; Cioffi, N. XXVII Congress of the Analytical Chemistry Division, Italian Chemical Society, Bologna 16-20 September 2018. “Spectroscopic characterization of exceptionally stable silver nanoparticles synthesized by laser ablation in isopropyl alcohol”. Poster.
384. Sportelli, M.C.; Izzi, M.; Volpe, A.; Clemente, M.; Picca, R.A.; Di Franco, C.; Palazzo, G.; Ancona, A.; Cioffi, N. N&N 2018, Nanoscience & Nanotechnology INFN Meeting 2018. “LASiS-generated nanoantimicrobials with exceptional stability at the colloidal state”. Invited oral communication.
385. Sportelli, M.C.; Quarto, R.; Picca, R.A.; Kranz, C.; Mizaikoff, B.; Tütüncü, E.; Valentini, A.; Cioffi, N. XXVII Congress of the Analytical Chemistry Division, Italian Chemical Society, Bologna 16-20 September 2018. “Insights into the inhibition of P. fluorescens biofilm formation via AFM and ATR-IR characterizations”. Flash oral communication.
386. Tadini-Buoninsegni, F.; Natile, G.; Arnesano, F. XXIV Congresso Nazionale della Società Italiana di Biofisica Pura e Applicata, Ancona 10-13/09/2018. “Interaction of anticancer drugs with P-type ATPases investigated by solid supported membrane technology”. Oral presentation.
387. Tamasi, G.; Pardini, A.; Bonechi, C.; Magnani, A.; Rossi, C. XXVII Congresso Divisione di Chimica Analitica, Società Chimica Italiana (SCI), Bologna 16-20/09/2018. “Bioactive molecules from tomato fruits and by-products”. Poster presentation.
388. Tamasi, G.; Pardini, A.; Bonechi, C.; Scazza, A.; Salvadori, C.; Lelli, S.; Lelli, A.; Magnani, A.; Rossi, C. ISEAC-40, International Conference on Environmental & Food Monitoring, Santiago de Compostela (Spain) 19-22/06/2018. “Tomato fruits and by-products as source of bioactive glycoalkaloids”. Oral presentation.
389. Tasinato, N. Modern Aspects of Computational Spectroscopy, Pisa 22-23/11/2018. “Synergisms between In Vitro and In Silico Infrared Spectroscopy”. Oral presentation (invited).
390. Tasinato, N.; Licari, D.; Spada, L.; Bloino, J.; Puzzarini, C.; Barone, V. II Italian Workshop on Astrochemistry, Follonica (GR) 13-16/06/2018. “Computational Tools for Astrochemistry”. Oral presentation (invited).
391. Tatini, D.; Lo Nostro, P.; Sarri, F.; Raudino, M.; Ambrosi, M. Final Meeting Project “Maximizing the EU shale gas potential by minimizing its environmental footprint”, Alicante (Spain) 11-12/06/2018. “Formulation of Hydraulic Fracturing Fluids”. Oral presentation.
392. Torsi, L. 73th International Workshop on Frontiers of Photonics, Plasmonics And Electronics With 2d Nanosystems – Erice 14-20th July 2018. “Ultra-Low Detection Limits and Selectivity with Organic Bio-

Electronic Sensors”. Invited presentation.

393. Torsi, L. Annual Meeting of the International Society of Electrochemistry, Italy 02-07/09/2018. “From the Frogs of Luigi Galvani to Bioelectronics: An Electrifying Journey Through a Blooming Field”. Keynote presentation.
394. Torsi, L. BioMolecularElectronics (BioMolectro), Spain 27-31/08/2018. “Sensing at the physical limit with solution processed bioelectronic transistors”. Keynote presentation.
395. Torsi, L. Emerging material technologies summit 2018, Vietnam 04-08/11/2018. “Molecule detection of markers with label-free bio-electronic sensor” Oral presentation.
396. Torsi, L. Gordon Research Conference - Hybrid Electronic & Photonic Materials and Phenomena, Hong kong 10-15/06/2018. “A Millimetre-Sized Transistor Selectively Detects at the Single-Protein Limit in Diluted Saliva". Invited presentation.
397. Torsi, L. ICOE 2018, France 18-22/06/2018. “Ultra-Low Detection Limits and Selectivity with Organic Bio-Electronic Sensors”. Invited speaker.
398. Torsi, L. Inaugurazione A.A. 2018-2019, Università di Torino 21/11/2018. “Towards the ultimate limit of detection with bioelectronic sensors”. Plenary presentation.
399. Torsi, L. InnoLAE 2018 (UK) 23-24/01/2018. “Label-free protein electronic detection with an electrolyte-gated organic field-effect transistor-based immunosensor”. Invited presentation.
400. Torsi, L. International Conference on Molecular Electronics, ElecMol, France 17-20/12/2018. “Single Molecule detection of Markers with a Label-free bio-electronic sensor”. Plenary presentation.
401. Torsi, L. LOPEC 2018, Germany 14-15/03/2018. “Ultra-sensitive biomarkers detection with printable electrolyte-gated FET”. Oral presentation.
402. Torsi, L. Materials and Technologies for Industrial Innovation, Italy 16-17/10/2018. “Printable bio-electronics: the reliable and scalable way for single molecule biosensing”. Oral presentation.
403. Torsi, L. Merck & Elsevier Young chemists symposium, Italy 19-21/11/2018. “Single molecule detection of markers with a label-free bio-electronic sensor”. Plenary presentation.
404. Torsi, L. MRS fall meeting, USA 25-30/11/2018. “Single-Molecule Detection with a Millimetre-Sized Transistor”. Oral presentation.
405. Torsi, L. MRS spring meeting, USA 02-06/04/2018. “Ultra-low detection limits and selectivity with organic bio-electronic sensors”. Oral presentation.
406. Torsi, L. Sensing the Future: The Future of Sensing Workshop, USA 06-07/12/2018. “Single molecule detection of markers with a label-free bio-electronic sensor”. Invited presentation.
407. Torsi, L. TCM2018 , Crete (Greece) 14-19/10/2018. “Single-molecule detection with a millimetre-sized transistor”. Invited presentation.
408. Torsi, L. Winterschool on Biophotonics and Bioelectronics, Austria 18-24/02/2018. “The toolbox for transistor biosensors”. Oral presentation.
409. Torsi, L. Workshop on Smell Sensing, Austria 17-18/04/2018. “Ultra-low detection limits and selectivity with organic bio-electronic sensors”. Oral presentation.
410. Torsi, L.; Macchia, E.; Manoli, K. XXVII Congresso della divisione di chimica analitica, Italy 16-20/09/2018. “Single molecule detection of markers in real bio-fluids with a label-free electronic sensor”. Oral presentation.
411. Trapani, A.; Mandracchia, D.; Tripodo, G.; Castellani, S.; Di Gioia, S.; Conese, M.; Ditaranto, N.; Cioffi, N.; Esteban Abade, M.A. Nanoinnovation, Rome 11-14 September 2018. “Solid lipid nanoparticles made of Gelucire® 50/13: a suitable delivery system for active substances in cell fish and in humans”. Oral communication.
412. Trapani, A.; Mandracchia, D.; Tripodo, G.; Di Gioia, S.; Conese, M.; Ditaranto, N.; Cioffi, N.; Esteban Abad, M.A. N&N 2018, Nanoscience & Nanotechnology INFN Meeting 2018. “Gelucire® 50/13-solid lipid nanoparticles: a colloidal carrier for hydrophilic active substances”. Invited oral communication.
413. Troisi, R.; Napolitano, V.; Russo Krauss, I.; Sica, F. 3rd Joint AIC (Associazione Italiana di Cristallografia) -SILS (Società Italiana Luce di Sincrotrone) Conference, Roma 25-28/06/2018. “Structural features of a duplex-quadruplex anti-thrombin aptamer: the highly effective NU172”. Oral communication.
414. Troisi, R.; Napolitano, V.; Russo Krauss, I.; Sica, F. Bionic 2018 – International Symposium - Biology of non-canonical nucleic acids: from humans to pathogens, Padova 26-28/09/2018. “Structural motifs determining the high anti-thrombin activity of NU172, an aptamer currently in Phase II clinical trials”. Poster.
415. Trovato, V.; Rosace, G.; Colleoni, C.; Pedrana, A.; Re, V.; Traversi, G.; Plutino, M.R.; Milone, C. 7th International Conference on Modern Circuits and Systems Technologies, MOCAST 2018, Thessaloniki (Greece) 7-9/05/2018. “Carbon nanotubes textile coating for the development of wearable sensors”. Oral presentation.
416. Tuccitto, N.; Bombace, A.; Torrisi, A.; Capizzi, G.; Licciardello, A. SIMS Europe, Muenster (Germania) 2018. “User-independent protocols for the analysis of complex ToF-SIMSdatasets without mass

binning, peak picking and peak integration”. Oral presentation.

417. Tuccitto, N.; Li Destri, G.; Messina, G.; Bombace, A.; Licciardello, A.; Marletta, G. Congresso Nazionale SCI-sez ChimicaFisica, Bologna 2018. “Molecular Communication: Fluorescent Quantum Dots as Molecular Bits”. Oral presentation.
418. Turkten, N.; Natali Sora, I.; Tomruk, A.; Bekbolet, M. 10th European meeting on Solar Chemistry and Photocatalysis: Environmental Applications (SPEA10), Almería (Spain) 4-8/06/2018. “Photocatalytic Degradation of Humic Acids Using LaFeO3”. Oral presentation.
419. Venditti, F.; Cuomo, F.; Ambrosone, L.; Cinelli, G.; Lopez. F. 46th Meeting of the Physical Chemisty Division of the Italian Chemistry Society, Bologna 25-28/06/2018. “Visible light activated C-doped titanium dioxide for water treatment: photodegradation of a textile dye”. Poster.
420. Vieira Pinto, S.M.; Tasinato, N.; Barone, V. XXXIV European Congress on Molecular Spectroscopy, Coimbra (Portugal) 19-24/08/2018. “Quantum Chemical Characterization of the Infrared Spectra of E- and Z-Ethanimine and its Isotopes”. Poster.
421. Vitiello, G. 2nd NapOsaka Meeting, Napoli 25/06/2018. “Hopanoids as key modulators of the membrane physico-chemical properties”. Oral communication.
422. Vitiello, G.; Luchini, A.; Radulescu, A.; Fragneto, G.; Paduano, L. XXIX Italian Neutron Scattering Conference INSC2018, Parma 4-6/07/2018. “Physico-chemical insights into Cardiolipin-containing Lipid Bilayers”. Oral presentation.
423. Vitiello, G.; Pezzella A.; Silvestri B.; Costantini A.; D’Errico G.; Luciani G.; Paduano, L. XLVI Congresso Divisione Chimica Fisica-SCI, Bologna 25-28/06/2018. “On the supramolecular organization of eumelanins obtained through TiO2-catalyzed oxidative polymerization”. Oral presentation.
424. Vitiello, G.; Silvestri, B.; Costantini, A.; Pezzella, A.; D’Ischia, M.; Luciani, G. 15th Eurasia Conference on Chemical Sciences, Roma 5-8/09/2018. “New frontiers in bio-sustainable multifunctional materials: ceramic templated eumelanin-like nanostructures”. Poster.
425. Vitiello, G.; Silvestri, B.; Costantini, A.; Pezzella, A.; D’Ischia, M.; Luciani, G. 4th International Conference on Bioinspired and Biobased Chemistry & Materials, Nice (France) 14-17/10/2018. “Ceramic templated melanin nanostructures: a biomimetic synthesis approach to bio-functional hybrid materials”. Poster.
426. Vitiello, G.; Silvestri, B.; Portarapillo, M.; Di Donato, P.; Piccolo, A.; Costantini, A.; Luciani, G.; Aronne, A. XI Congresso AICIng, Bologna 9-12/09/2018. “Nanoparticelle ibride organiche/inorganiche a base di acidi umici con proprietà antiossidanti”. Poster.
427. Vitiello, R.; Russo Krauss, I.; D’Errico, G.; Di Serio M. XX Congresso Nazionale di Catalisi - XX Congresso Nazionale della Divisione di Chimica Industriale, Milano 2-5/09/ 2018. “Synthesis and characterization of acrylate monomers used in the “Hydrophobic Alkali Swellable Emulsion (HASE)” synthesis”. Oral communication.
428. Baglioni, P. “APACHE: Materiais inteligentes de embalagem e expositores como ferramenta para a conservação preventiva do patrimônio cultural”, Sao Paulo (Brazil) 7/04/2019. Invited lecture and workshop.
429. Baglioni, P. “Frontiers of Silica Research”, Gotheborg (Svezia) 23-25/04/2019. Invited lecture.
430. Baglioni, P. “Heritage Science and Technology”, Institute de France, Paris (France) 12-15/02/2019. Invited lecture.
431. Baglioni, P. “Leonardo Da Vinci visits University College Dublin”, Dublino (Irlanda) 21-22/11/2019. Invited lecture.
432. Baglioni, P. “Molecular Frontiers”, Stoccolma (Svezia) 08-10/05/2019. Invited lecture.
433. Baglioni, P. “Nuove metodologie chimiche per la conservazione ed il restauro dei beni culturali”, Rome 18/10/2019. Invited lecture.
434. Baglioni, P. “Workshop Functional Materials for Cultural Heritage”, Matera 05-06/09/2019. Invited lecture.
435. Baglioni, P. “Workshop Advanced Materials and Nanotechnologies at the service of Cultural Heritage Conservation”, LACMA, Los Angeles County Museum of Art (USA) 09-03/09/2019. Invited lecture.
436. Baglioni, P. Ciclo di conferenze sui codici Mesoamericani, Harvard e Georgetown University (USA) 09-14/03/2019. Invited lectures.
437. Baglioni, P. Ciclo di conferenze sull’utilizzo dei prodotti Nanorestore® per la conservazione dei beni culturali, Tate Britain, London (UK) 20-22/01/2019. Invited lectures.
438. Baglioni, P. Ciclo di conferenze sull’utilizzo dei prodotti Nanorestore® per la conservazione dei beni culturali, Pratt Instisute, New York (USA) 04-09/02/2019. Invited lectures.
439. Baglioni, P. Ciclo di conferenze sulla conservazione dei beni culturali, Okinawa e Tokyo (Japan) 04-14/11/2019. Invited lectures.
440. Baglioni, P. Conference and Workshops on APACHE Project & Nano-Systems Research and Applications on Cultural Heritage and workshop on Apache at British Museum, London (UK) 03-

05/06/2019.

441. Baglioni, P. International agreement “The Belt and Road Cultural Heritage Global Alliance (BRCHGA)”, Xian (China) 11-15/10/2019.
442. Baglioni, P. Nanoinnovation 2019, Rome 11-14/06/2019. “Multifunctional materials based on chitosan for the chemisorption of degrading species in museum environments" and “Strengthening and deacidification of paper: a single-step treatment based on nanoparticles and cellulose nanocrystals". Invited lectures.
443. Barone, V. International Workshop: “Domesticated Landscapes. Incorporating nature in the Roman houses and villas – Pompeii, Herculaneum, and the Vesuvian region - Paesaggi domestici. L’esperienza della natura nelle case e nelle ville romane - Pompei, Ercolano e l’area vesuviana”. Pompei (NA) 26-27/04/2019. “Reale e virtuale per il patrimonio culturale - Nuovi ponti attraverso antiche frontiere”. Oral presentation.
444. Basosi, R; Capra, M. ENEA 6/02/2019. “Le politiche europee dell’Energia per la ricerca e l’innovazione sulle Smart Cities”. Oral presentation.
445. Bergese, P. evFOUNDRY - The Extracellular Vesicle Foundry, FET Seminars Series, Brussel (Belgium) 10th October 2019. Invited talk.
446. Bonini, M. UNISTEM 2019 – La Ricerca che ci cambia la Vita, Firenze 15/06/2019. “Il fascino magnetico dei materiali intelligenti”. Invited oral presentation.
447. Bonini, M. XLVII Congesso Divisione Chimica Fisica, Rome 4/7/2019. “Functional nanocomposites based on clay nanotubes”. Oral presentation.
448. Bonini, M. XXVI Congesso Nazionale Società Chimica Italiana, Rome (Italy) 12/9/2019. “Adsorption of Amino Acids and Glutamic Acid-Based Surfactants on Imogolite Clays”. Oral presentation.
449. Bonini, M. XXXIII ECIS Conference, Leuven (Belgium) 15/9/2019. “Macroporous gelatin hydrogels: structural and diffusive properties”. Poster presentation.
450. Brancato, G. The IDEA of a Centre Meeting, Collegio Volta, Pavia February 6-7, 2019. Unravelling the Molecular Basis of Inherited Channelopathies in a Voltage-Gated Potassium Channel. Oral presentation.
451. Bruni, G. CEEC-TAC5 (5th Central and Eastern European Conference on Thermal Analysis and Calorimetry) e MEDICTA2019 (14th Mediterranean Conference on Calorimetry and Thermal Analysis), Roma 27-30 Agosto 2019. “DSC applied to the study of an impossible system: probenecid-benzamide”. Oral presentation.
452. Cabrini, M. 3rd International Conference on 3D Printing Technology and Innovations, Rome 25-26/03/2019. “Corrosion behavior of metallic alloys obtained by additive manufacturing”. Oral presentation.
453. Cabrini, M.; Lorenzi, S.; Pastore, T.; Testa, C.; Andreatta, F.; Fedrizzi, L.; Manfredi, D.; Lorusso, M.; Lombardi, M.; Aversa, A. XIII Giornate Nazionali sulla Corrosione e Protezione dei Materiali, Palermo 3-5/07/2019. “Effetto della temperatura di trattamento termico post-processing sulla corrosione selettiva di leghe Al-Si prodotte per Laser Powder Bed Fusion”. Oral presentation.
454. Cabrini, M.; Lorenzi, S.; Pastore, T.; Testa, C.; Manfredi, D.; Lorusso, M.; Calignano, F.; Lombardi, M. XIII Giornate Nazionali sulla Corrosione e Protezione dei Materiali, Palermo 3-5/07/2019. “Comportamento alla corrosione di una lega Ti6Al4V per applicazione biomediche ottenuta tramite additive manufacturing”. Oral presentation.
455. Cabrini, M.; Lorenzi, S.; Pastore, T.; Testa, C.; Manfredi, D.; Lorusso, M.; Calignano, F.; Lombardi, M. XII INSTM Conference-XV AIMAT Conference, Ischia (NA) 21-24/07/2019. “Corrosion behavior of laser powder bed fusion Ti6Al4V alloy for biomedical purpose”. Oral presentation.
456. Caminati, G.; Medda, L.; Lucchesi, G.; Lofrumento, C.; Martina, M.R. 6th Nano Today Conference, Lisbon (Portugal) 16-20/06/2019. “Graphene oxide veiled ordered arrays of silver nanowires and nanostars for the early diagnosis of neurodegenerations”. Poster.
457. Castellano, A.; Rosace, G.; Trovato, V.; Iacono, G.; Malucelli, G. AUTEX2019 – 19th World Textile Conference on Textiles at the Crossroads, Ghent (Belgium) 11-15/06/2019. “A novel nitrogen-containing carboxyl- functionalized organophosphorus system for flame retardant finishing of cotton fabrics”. Oral presentation.
458. Cofelice, M.; Lopez, F.; Cuomo, F. 2nd Euro-Global Conference on Food Science and Technology, London (UK) 19 th -21 st September 2019. “Alginate encapsulating essential oil as edible coating to preserve the quality of fresh-cut apples”.
459. Coppola, L.; Coffetti, D.; Candamano, S.; Crea, F.; Crotti, E.; Iorfida, A.; Pastore, T. XII INSTM Conference – XV AIMAT Conference, Ischia (NA) 21-24/07/2019. “Performance and microstructure of one-part alkali activated slag cements: effect of alkali content”. Oral presentation.
460. Coppola, L.; Coffetti, D.; Crotti, E.; Dell’Aversano, R.; Gazzaniga, G. 9th International Conference on Structural Analysis and Advanced Materials ICSAAM 2019, Ischia (NA) 12-14/09/2019. “The influence

of heat and steam curing on the properties of one-part fly ash/slag alkali activated materials: preliminary results". Poster.

461. Coppola, L.; Coffetti, D.; Crotti, E.; Dell'Aversano, R.; Gazzaniga, G. 5th International Workshop The new boundaries of structural concrete NBSC 2019, Milano 19-20/09/2019. "Carbonation of sustainable Portland-free CSA-based mortars manufactured with lithium and sodium carbonates". Oral presentation.
462. Coppola, L.; Coffetti, D.; Crotti, E.; Gazzaniga, G. RILEM International Conference Strategies for Sustainable Concrete Structures, Lecco 5-7/09/2019. "A new approach to evaluate the sustainability of cementitious materials". Oral presentation.
463. Coppola, L.; Coffetti, D.; Crotti, E.; Marini, A.; Passoni, C. 5th International Workshop The new boundaries of structural concrete NBSC 2019, Milan 19-20/09/2019. "Lightweight alkali-activated slag plaster to improve the seismic performance and the energy efficiency of poor-quality masonry walls". Oral presentation.
464. Coppola, L.; Coffetti, D.; Crotti, E.; Pastore, T. XII INSTM Conference – XV AIMAT Conference, Ischia (NA) 21-24/07/2019. "An empathetic added sustainability index (EASI) for cementitious based construction materials". Oral presentation.
465. Coppola, L.; Coffetti, D.; Lorenzi, S. XIV AIMAT National Congress XI National Conference on Materials Science and Technology, Ischia (NA) 12-15/07/2019. "CSA-based ternary binders for sustainable mortars". Oral presentation.
466. Coppola, L.; Coffetti, D. XIV AIMAT National Congress XI National Conference on Materials Science and Technology, Ischia (NA) 12-15/07/2019. "One-part alkali activated slag for cement-free repair mortars for conservation, restoration and retrofitting of existing concrete structures". Oral presentation.
467. Curti, V.; Baldini, A.; Anselmi Tamburini, U.; Bini, M. XVI ECerS Conference, Turin 16-20 June 2019. "New functional properties of high entropy oxides". Poster presentation.
468. D'Errico, G. 9th International Colloids Conference, Sitges (Spain) 16-19/06/2019 "Branched surfactants: An effective strategy for the design of high concentration/low viscosity surfactant formulations". Oral communication.
469. D'Errico, G. 9th International Colloids Conference, Sitges, Spain 16-19/06/2019. "Not just a fluidizing effect: omega-3 phospholipids induce formation of non-lamellar phases in biomembranes". Oral communication.
470. D'Errico, G. International Conference on Reproduction, Endocrinology and Development (ICRED 2019), Vadodara, Gujarat (India) 19-21/01/2019. "Physico-chemical and analytical tools for the monitoring of oxidative stress in biosentinel gonads". Oral communication.
471. D'Errico, G.; Murgia, S.; Paduano, L. 33th Conference of the European Colloid and Interface Society (ECIS 2020), Leuven (Belgio) 8-13/09/2019. "Branched surfactants: An effective strategy for the design of high concentration/low viscosity surfactant formulations". Oral communication.
472. D'Errico, G.; Russo Krauss, I.; Paduano, L. XLVII Congresso Nazionale della Divisione di Chimica Fisica della Società Chimica Italiana (SCI), Roma (Italy) 1-4/07/2019. "Not just a fluidizing effect: omega-3 phospholipids induce formation of non-lamellar phases in biomembranes". Oral communication.
473. Ferrara, N.; Bonciani, D.; Baratto, M.C.; Torsello, L.; Basosi, R.; Parisi, M.L. European Geothermal Congress EGC 2019, The Hague (The Netherlands) 11-14/07/2019. "Investigation of atmospheric emission profiles for the minimization of the environmental footprint of geothermoelectric production: an LCA approach". Poster.
474. Fontana, F.; Tommasini, M.; Zanchi, C.; Ossi, P.M.; Trusso, S.; Rizzo, S. 21st European Symposium on Organic Chemistry, Vienna (Austria) 14-18/07/2019. "Synthesis and characterization of SERS-active heteroaromatic molecules". Poster.
475. Fratini, E. Current and Future Development of Neutron Scattering Techniques for Time-Resolved Studies, Oak Ridge (TN–USA) October 2019. "Structure and water dynamics in porous systems by neutron scattering".
476. Gelli, R.; Tempesti, P.; Bonini, M.; Ridi, F.; Baglioni, P. 14th International Symposium on Macrocyclic and Supramolecular Chemistry, June 2-6, 2019 Lecce. "Biologically-Relevant Amorphous Magnesium-Calcium Phosphate Nanoparticles: Effect of pH, Mg2+ and Complex Fluids on the Formation and Crystallization Processes". Oral presentation.
477. Laurati, M.; Moreno-Guerra, J.A.; Martinez-Borquez, A.; Romero-Sanchez, I.; Stiakakis, E.; Tassieri, M. 2nd Workshop on Matter Out-of-Equilibrium, San Luis Potosí (Mexico) 23-27/11/2019. "Nanoscale viscoelasticity of soft solids by Rheo-AFM". Invited oral presentation.
478. Laurati, M.; Romero-Sanchez, I.; Stiakakis, E. 5th International Soft Matter Conference, Edinburgh (UK) 03-07/06/2019. "Reentrant transitions of adaptive dsDNA colloids". Oral presentation.
479. Lo Nostro, P. 12th International Conference on the History of Chemistry, Maastricht (The

Netherlands) 28/07-02/08/2019. “The Hofmeister series. A tantalizing yet unsolved problem in Physical Chemistry”. Oral presentation.

480. Lo Nostro, P.; Ninham, B.W. Bubble & Drop 2019, Sofia (Bulgaria) 24-28/06/2019. “Some Peculiar Properties of Degassed Liquids”. Oral presentation.
481. Lo Nostro, P.; Tatini, D.; Carnerup, A.; Ninham, B.W. 33rd ECIS Conference, Leuven (Belgium) 8-13/09/2019. “Green stimuli-responsive viscoelastic formulations”. Oral presentation.
482. Lo Nostro, P.; Tatini, D.; Sarri, F.; Raudino, M.; Ambrosi, M. 15th International Conference on Properties and Phase Equilibria for Products and Process Design (PPEPPD 2019), University of British Columbia, Vancouver (Canada) 12-16/05/2019. “Stimuli-Responsive Green Viscoelastic Formulations”. Oral presentation.
483. Lucchesi, G.; Lofrumento, C.; Martina, M.R.; Caminati, G. Conventional and High-Energy Spectroscopies Surfaces analysis, Florence 2-6/12/2019. “Surface characterization of SERS-active substrates for the early diagnosis of neurodegenerations”.
484. Lupi, J.; Salta, Z.; Tasinato, N.; Barone, V. Young researchers meet molecular spectroscopy, Pisa 4-5/04/2019. “Quantum Mechanical Strategies for Reactivity and Kinetics of Atmospheric Reaction Pathways”. Oral presentation.
485. Marini, A. Aula Magna del Broletto, Pavia 2/12/2019. “Risorse energetiche e sostenibilità ambientale. La transizione energetica”. Invited lecture for the students of Liceo Scientifico Taramelli and Liceo Classico Foscolo.
486. Milanese, C. International Conference on Materials Research and Nanotechnology, Roma June 10-12 2019. "Carbon based Materials for Solid State Hydrogen Storage and Energy Storage". Invited lecture
487. Milanese, C.; Girella, A.; Cofrancesco, P.; Gaboardi, M.; Pontiroli, D.; Magnani, G.; Riccò, M.; Marini, A. E-MRS 2019 Fall Meeting, Warsaw (Poland) 16-19/09/2019. “Innovative Carbon-based Materials for Hydrogen and Energy Storage”. Oral presentation.
488. Milanese, C.; Pontiroli, D.; Scaravonati, S.; Magnani, G.; Fornasini, L.; Bertoni, G.; Ridi, F.; Verucchi, R.; Mantovani, L.; Malcevschi, A.; Riccò, M. E-MRS 2019 Fall Meeting, Warsaw (Poland) 16-19/09/2019. “Super-Activated Biochar from Poultry Litter for Electrodes in Supercapacitors”. Poster presentation.
489. Muzzi, B.; Caminati, G. 6th Nano Today Conference, Lisbon (Portugal) 16-20/06/2019. “Leadfree perovskite solar cells coupled to plasmonic nanoarrays”. Oral presentation.
490. Parisi, M.L. Relatore al “Workshop BIPV - Progetto PV-IMPACT” per coordinamento gruppo sostenibilità, NOI Tech Park, Bolzano 16 Dicembre 2019. Relatore.
491. Pastore, T.; Cabrini, M.; Lorenzi, S.; Della Longa, L. XIII Giornate Nazionali sulla Corrosione e Protezione dei Materiali, Palermo 3-5/07/2019. “Valutazione della velocità di corrosione di ancoraggi per barriere autostradali”. Oral presentation.
492. Pelosato, R.; Carrara, V.; Natali Sora, I. 3rd International Conference on Nanotechnology Based Innovative Applications for the Environment (NINE) – Napoli 14-17/04/2019. “Enhanced photocatalytic degradation of ibuprofen in aqueous solution under visible-light irradiation: effects of LaFeO3 and Cu/LaFeO3”. Oral presentation.
493. Pižl, M.; Fusè, M.; Tasinato, N.; Vlček, A.; Barone, V.; Záliš, S. Young researchers meet molecular spectroscopy, Pisa 4-5/04/2019. “Time-resolved Vibrational Spectra of Ru and Re Diimine Complexes: Anharmonic Calculations”. Oral presentation.
494. Radeghieri, A. ISEV 2019 Kyoto (Japan) 25th-28th April 2019. “Different ATT isoforms are associated to EVs from ATT type II deficient patients”. Oral presentation.
495. Rampino, S. Invited lecture at Scuola Normale Superiore within the cycle “Chimica e storia: l’affermazione dell’atomismo” of the program “Accademia dei Lincei e Normale per la scuola”, Pisa 3 aprile 2019. “Aggiungi un posto a tavola: relatività e periodicità nei nuovi arrivati Copernicio, Flerovio e Oganesson”. Invited oral.
496. Rampino, S. Invited seminar at École nationale supérieure de chimie de Paris – Chimie ParisTech, Paris (France) 15 maggio 2019. “Combined orbital-space/real-space analysis of electron-charge rearrangement upon chemical bonding: from theory to vir-tual reality”. Invited oral.
497. Rampino, S. Invited seminar at Scuola Normale Superiore within the seminar cycle “Frontiere della Chimica”, Pisa 1 aprile 2019. “Relativity and the Periodic Table: The Chemical Character of Copernicium, Flerovium and Oganesson”. Invited oral.
498. Ridi, F.; Gelli, R.; Bonini, M.; Baglioni, P. 33rd Conference of the European Colloid and Interface Society (ECIS), Leuven (Belgium) September 8-13, 2019. “Calcium-magnesium phosphates: from the physico-chemical study to the preparation of functional materials”. Oral presentation.
499. Ridi, F.; Gelli, R.; Bonini, M.; Baglioni, P. XLVII National meeting of Physical Chemistry Division 2019, Rome July 1-4, 2019. “Calcium-magnesium phosphates: from the physico-chemical study to the preparation of functional materials”. Oral presentation.

500. Rizzo, S.; Mussini, P.R.; Arnaboldi, S.; Longhi, M.; Fontana, F.; Cirilli, R.; Forni, A. 5th Smart Materials and Surfaces - SMS Conference, Lisbona (Portugal) 23-25/10/2019. "Inherently Chiral Ionic Liquids with Axial, Helical and Central Stereogenicity for Highly Efficient Enantioselective Sensors". Oral presentation.
501. Rizzo, S.; Mussini, P.R.; Arnaboldi, S.; Longhi, M.; Fontana, F.; Cirilli, R.; Forni, A. XXXIX Convegno Nazionale della Divisione di Chimica Organica della Società Chimica Italiana, CDCO 2019, Torino 8-12/9/2019. "High Enantioselection Performances of Inherently Chiral Ionic Liquids with Axial, Helical and Central Stereogenicity". Oral presentation.
502. Rosace, G.; Cardiano, P.; Urzì, C.; De Leo, F.; Galletta, M.; Ielo I.; Plutino, M.R. VIII Workshop Nazionale AICIng., Lipari (ME) 27-29/06/2019. "Promising fluorine-containing sol-gel coatings to prevent microbial biofilm settlement and adhesion". Poster presentation.
503. Rossi, F. AVOGADRO COLLOQUIA 2019, Elements of the Periodic Table for Energy, Rome, CNR, Sala Marconi 17th-18th December, 2019. "Environmental profile of manufacturing and use phases of different types of batteries".
504. Salis, A. Biological Surfaces and Interfaces: the Mechanistic View, Sant Feliu de Guixols (Spain) 30 June-5 July 2019. "Specific effects of electrolytes at biointerfaces". Invited key note.
505. Salis, A. Sardinia Goes Nano, Sassari 24 May 2019. "Nanobiointerfaces: Cell Internalization of Functional Nanomterials". Oral presentation.
506. Salvadori, A.; Fusè, M.; Mancini, G.; Rampino, S.; Barone, V. Winter Modeling 2019, Napoli 14 febbraio 2019. "Diving into chemical bonding: an immersive analysis of the electron charge rearrangement through virtual reality". Invited oral.
507. Savi, P.; Cirielli, D.; Di Summa, D.; Ruscica, G.; Natali Sora, I. 2019 IEEE 5th International forum on Research and Technology for Society and Industry (RTSI), Firenze 9-12/09/2019. "Analysis of shielding effectiveness of cement composites filled with pyrolyzed biochar". Oral presentation.
508. Spada, D.; Quinzeni, I.; Capsoni, D.; Bini, M. EMRS Spring 2019, Nice (France) May 27 to 31, 2019. "The amazing electrochemical potential of FeNb11O29 as anode for LIBs". Oral presentation.
509. Spada, D.; Quinzeni, I.; Capsoni, D.; Mozzati, M.C.; Albini, B.; Galinetto, P.; Bini, M. XVI ECerS Conference, Turin 16-20 June 2019. "Interesting structural and magnetic features of the shear structure FeNb11O29". Poster presentation.
510. Testa, C.; Cabrini, M.; Lorenzi, S.; Carugo, F.; Pastore, T.; Brevi, F.; Biamino, S.; Fino, P.; Manfredi, D.; Marchese, G.; Calignano, F.; Scenini, F. XII INSTM Conference-XV AIMAT Conference, Ischia (NA) 21-24/07/2019. "AMCRA project: Additive Manufacturing of valves in Alloy 625 for Oil&Gas service". Poster.
511. Tonelli, M.; Ridi, F.; Giorgi, R.; Baglioni, P. XLVII National meeting of Physical Chemistry Division 2019, Rome July 1-4, 2019. "Halloysite nanotubes as nano-carriers in cementitious materials". Poster.
512. Torsi, L. 2nd edition of the European Biosensor Symposium, Florence 18-20/02/2019. "Single molecule detection of markers with a label-free bio-electronic sensor". Plenary presentation.
513. Trovato, V.; Rosace, G.; Piperopoulos, E.; Colleoni, C.; Castellano, A.; Milone, C.; Plutino, M.R. VIII Workshop Nazionale AICIng. Lipari (ME) 27-29/06/2019. "Sol-gel based halochromic coatings for the development of wearable pH sensors". Poster presentation.
514. Trovato, V.; Teblum, E.; Kostikov, Y.; Pedrana, A.; Re, V.; Nessim, G.D.; Rosace, G. AUTEX2019 – 19th World Textile Conference on Textiles at the Crossroads, Ghent, Belgium. 11-15/06/2019, "Designing of carbon nanotubes/cotton fabric composite for e-textiles: effect of carbon nanotubes- length on electroconductive properties". Oral presentation.
515. Vitiello, G.; Luciani, G.; Silvestri, B.; Nuzzo, A.; D'Errico, G.; Paduano, L.; Aronne, A.; Piccolo, A. The 6th Nano Today Conference, Lisbon (Portugal) 16-20/06/2019. "Bio-sustainable design of multifunctional humic acids-based nanohybrids: from the ceramic-templated synthesis to technological applications". Oral communication.
516. Vieira Pinto, S.M.; Tasinato, N.; Barone, V.; Amadei, A.; Zanetti-Polzi, L.; Daidone, I. Young researchers meet molecular spectroscopy, Pisa 4-5/04/2019. "In silico Infrared Spectroscopy of Protein Side Chains". Oral presentation.
517. Avelar, M.; Ienco, A.; Parisi, M.L.; Olivucci, M.; Santucci, A.; Basosi, R.; Sinicropi, A. 2nd Congress of the interdivisional group on Chemistry for renewable energy of the Italian Chemical Society – SCI Enerchem, Padova 12-14/02/2020. "MD and QM/MM investigation of Bacteriorhodospin/TiO2 system".
518. Baglioni, P. "Research and Applications on Cultural Heritage", Napoli 21/01/2020. Invited lecture.
519. Baglioni, P. "Science ABC" c/o Università La Sapienza, Roma 19/02/2020. Invited plenary lecture.
520. Baglioni, P. Corso su conservazione con prodotti Nanorestore e presentazione del progetto EU Apache, New York (USA) 13-18/01/2020. Invited lecture.
521. Baglioni, P. Corso teorico-pratico su nanomateriali per la conservazione, Parigi (Francia) 12-

14/02/2020. Invited lecture.

522. Brancato, G. Ion Channels Mini-Symposium, University of Twente (The Neatherlands), 23 January 2020. “Understanding the effect of pathogenic mutations on the structure and function of the voltage-gated potassium channel Kv4.3”. Relatore.
523. Coppola, C.; Muñoz-García, A.B.; Basosi, R.; Infantino, R.; Reginato, G.; Sinicropi, A.; Pavone, M. 2nd Congress of the interdivisional group on Chemistry for renewable energy of the Italian Chemical Society – SCI Enerchem, Padova 12-14/02/2020. “Understanding interfacial charge transfer between the lead halide perovskite and novel phenothiazine-based organic hole transport materials”.
524. Dessì, A.; Bilancia, S.; Sinicropi, A.; Vesce, l.; Di Carlo, A.; Calamante, M.; Zani, L.; Mordinia, A.; Reginato, G. 2nd Congress of the interdivisional group on Chemistry for renewable energy of the Italian Chemical Society – SCI Enerchem, Padova 12-14/02/2020. “New organic sensitizers with improved spectral properties for application in greenhouse-integrated Dye-Sensitized Solar Cells”.
525. Maranghi, S.; Parisi, M.L.; Basosi, R.; Sinicropi, A. 2nd Congress of the interdivisional group on Chemistry for renewable energy of the Italian Chemical Society – SCI Enerchem, Padova 12-14/02/2020. “Life Cycle Assessment of Perovskite Solar Cells technology: environmental profile harmonization of the manufacturing process”.
526. Marchianò, V.; Salvador, M.; Moyano, A.; Yáñez, S.; Piñeiro, Y.; Rivas, J.; Martínez-García, J.C.; Blanco-López, M.C.; Rivas, M.; Cioffi, N.; Ditaranto, N. Nanomaterials Applied to Life Sciences NALS 2020, 29-31 January 2020, Madrid (Spain). “Magnetic hyperthermia-induced ionic release for anti-biofilm action”. Oral communication.
527. Milanese, C. Collegio Borromeo, Pavia 23/04/2020. “Idrogeno: energia del futuro?” Invited Zoom webinar.
528. Parisi, M.L. Relatore per il Webinar “How to simplify Life Cycle Assessment in deep geothermal projects with the novel GEOENVI tool”, 27 Aprile 2020. Relatore.
529. Parisi, M.L. Two days Geothermal Brussels events, Bruxelles (Belgium) 4-5 Febbraio 2020. Invited lecture.
530. Parisi, M.L. Webinar "How to simplify Life Cycle Assessment in deep geothermal projects with the novel GEOENVI tool", 27 Aprile 2020. Invited lecture.
531. Rossi, F.; Parisi, M.L.; Maranghi, S.; Sinicropi, A.; Basosi, R. 2nd Congress of the interdivisional group on Chemistry for renewable energy of the Italian Chemical Society – SCI Enerchem, Padova 12-14/02/2020. “Comparative Life Cycle Assessment of Solar Home Systems”.

Publishing Activity

- Alessandro De Giacomo - Editor of *Spectroschimica Acta B: Atomic Spectroscopy.*
- Debora Berti - Editorial board member of *Journal of Colloid and Interface Science.*
- Debora Berti - Editorial board member of *Advances in Colloid and Interface Science.*
- Luisa Torsi - Associate Editor of *ACS Omega.*
- Maria Chiara Sportelli - Editorial board member of *Antibiotics.*
- Nicola Cioffi - Editor of *Analytica Chimica Acta*, Elsevier, section «Sensors and Bioselective Reagents».
- Nicola Cioffi - Editorial board member of *Sensors Letters, Applied Sciences.*
- Nicoletta Ditaranto - Editorial board member of *Antibiotics.*
- Piero Baglioni – Editor of *Physical Chemistry Chemical Physics.*
- Piero Baglioni – Editor of *The European Physical Journal E.*
- Piero Baglioni – Advisory board member of *Langmuir.*
- Piero Baglioni – Advisory board member of *Soft Matter.*
- Piero Baglioni – Advisory board member of *Colloids and Surfaces A.*

Guests Seminars

- Prof. Erhan Piskin - Hacettepe University, Turkey, 23/01/2017. “Tissue Engineering in Some Selected Maxillofacial Applications”.
- Dr. Farzaneh Moghtader - Hacettepe University, Turkey, 23/01/2017. “Phage-Based Fluorescent Biosensor Prototypes to Specifically Detect Enteric Bacteria”.
- Dr. Taku Ogura, Research and Development Headquarters LION Corporation, Japan; Research Institute for Science and Technology, Tokyo University of Science, 10/02/2017. “Scattering and spectroscopic study on the hydration and phase behavior of surfactant solutions (micelle, vescicles and other structures)”.
- Prof. Efrat Lifshitz, Russell Berrie Nanotechnology Institute Technion, Israel, 28/04/2017. “Excitons in colloidal quantum dots”.
- Dr. Andreas Lesch, École Polytechnique Fédérale de Lausanne (EPFL) – Energypolis Laboratoire d'Electrochimie Physique et Analytique (LEPA), Switzerland, 19/05/2017 “Bioanalytical imaging and diagnostics with inkjet printed electrochemical sensing platforms”.
- Dr. Karima Lasri, University of Central Florida (USA), 15/06/2017. “Lithium-ion batteries: Science and Technologies”.
- Prof. Kara - University of Central FLorida (USA), 15/06/2017. “Organic materials/metal surfaces Interface Characteristics: Role of van der Waals interactions”.
- Dr. Marco Laurati, Soft Matter Laboratory División de Ciencias e Ingenierías, Universidad de Guanajuato, Campus León, Mexico, 14/07/2017. “Non-equilibrium states of colloidal systems studied by quantitative confocal microscopy”.
- Prof. Giuseppe Spoto, Dipartimento di Scienze Chimiche – Università di Catania, 06/09/2017. “Isothermal amplification of nucleic acids in droplet microfluidic devices”.
- Dr. Abel Jerez, P&G Services Company, Strombeek-Bever, Belgium, 30/10/2017., “Advanced rheology methods for soft matter systems: LAOS and DWS”.
- Prof. Paolo Samorì, ISIS, Universit de Strasbourg & CNRS, France, 30/10/2017. “When molecular science meets 2-D materials: orchestrating multiple functions”.
- Dr. Anne-Françoise Mingotaud, Lab. des Interactions Moléculaires et Réactivité Chimique et Photochimique University of Toulouse, France, 15/11/2017. “Controling polymeric self-assemblies for biomedical applications: examples of photodynamic therapy and MRI”.
- Dr. Walter Broeckx, P&G Services Company Strombeek-Bever, Belgium, 16/11/2017. “Multivariate data analysis and chemometrics”.
- Dr. Taku Ogura, Research and Development Headquarters LION Corporation, Japan; Research Institute for Science and Technology, Tokyo University of Science, 21/11/2017. “Industrial Applications of Interfacial Science Techniques for Household products”.
- Prof. Ayse Karakeçili, Ankara University, 08/05/2018. “Tissue engineering scaffolds: from 3D porous structures to hydrogels”.
- Prof.ssa Angela Agostiano, Università di Bari e Presidente Società Chimica Italiana, 24/05/2018. “Colloidal nanoparticles: hot topics of current research in material chemistry with great potential for innovation in biomedical, energy and environmental sectors”.
- Prof. Paolo Samorì, Institut de Sciences et d’Ingénierie Supramoléculaires, Université de Strasbourg & CNRS, 30/05/2018. “Advances in Polymer Matrix-CNT nanocomposite: to make outstanding CNT Properties Accessible”.
- Prof. Klaus D. Jandt. Chair of Materials Science - Otto Schott Institute of Materials Research (OSIM) - Friedrich Schiller University of Jena, 30/05/2018. “Polymer-based Nanoparticle Libraries for Targeted Anti-inflammatory Strategies”.
- Dr.ssa Izabela Firkovska Boden, Otto Schott Institute of Materials Research (OSIM) – Friedrich Schiller University of Jena, 30/05/2018, “Simplistic Approach toward Advanced Bio- and Thermal Management Materials”.
- Prof. Paolo Samorì, Institut de Science et d'Ingénierie Supramoléculaires, Université de Strasbourg & CNRS, 24/10/2018. “Internet of functions in tailored-made 0D to 3D multicomponent nanostructures: from high-performance sensors to multiresponsive hybrid nanostructures”.
- Prof. Paolo Samorì, Institut de Sciences et d’Ingénierie Supramoléculaires, Université de Strasbourg & CNRS, 30/10/2018. “Nanomaterials properties tuned by their environment:integrating supramolecular concepts into sensing devices”.
- Prof. Eckart Ruehl, Freie Universität Berlin, 16/01/2019. “Local Structural and Dynamical Properties of Variable Size Matter”.

- Dr. Sara Malekkhaiat Häffner, Department of Pharmacy, University of Copenhagen, 30/01/2019. “Membrane interactions of nanoparticles as carriers of antimicrobial peptides”.
- Prof. Antonello Merlino, Department of Chemistry, University of Naples, 27/03/2019. “Ferritins as nanoplatforms for delivery of anticancer metallodrugs: structure and cytotoxicity”.
- Prof. To Ngai, Department of Chemistry - The Chinese University of Hong Kong, 23/07/2019. “Colloidal Particles at Interfaces: from fundamentals to Applications”.
- Prof.ssa Francesca Baldelli Bombelli, Dipartimento di Chimica, Materiali e Ing. Chimica Politecnico di Milano, 31/10/2019. “Functional hybrid Au-protein supraparticles for nanodelivery”.
- Dr. Antonio Benedetto, “Rita Levi Montalcini” Principal Invistigator – Department of Sciences, University of Roma Tre, 18/02/2020. “Ionic liquids and bio-systems: from model biomolecules to living cells”.

Theses (undergraduate, master and PhD)

U.O. Bari

Bachelor in Chemistry (Laurea triennale)

- Centobelli, T.: “Sintesi elettrochimica-termica e caratterizzazione analitica di ZnO nanostrutturato” (2017).
- Marra, S.: “Studio degli effetti del plasma atmosferico sull’enzima Tirosinasi da Agaricus Bisporus” (2017).
- Tursellino, L.: “Stainless steel-assisted synthesis of gold nanocolloids” (2017).
- Di Corato, G.: “Sintesi e caratterizzazione di compositi nano-strutturati di impiego nell’imballaggio e conservazione degli alimenti” (2019).

Bachelor in Materials Science (Laurea triennale)

- Clemente, M.: “Sintesi LASiS di nanocolloidi antimicrobici per potenziali applicazioni nel food packaging” (2017).
- Minervini, F.: “Stainless steel-assisted synthesis of gold nanocolloids” (2017).
- Blasi, F.: “Studio sulla interazione delle vescicole fosfolipidiche unilamellari con le nanoparticelle di oro” (2018).
- Santeramo, F.: “Deposizione IBS e caratterizzazione spettroscopica e morfologica di nanoantimicrobici multicomponenti” (2018).
- Conte, F.M.: “Sintesi e Caratterizzazione di Nanoparticelle di Rame e loro Applicazione a Materiali dell’Industria Automobilistica” (2020).
- Lettini, R.: “Sintesi e caratterizzazione di nanoparticelle di ossido di zinco per la modifica di consolidanti di manufatti lapidei” (2020).

Master in Chemistry (Laurea magistrale)

- Lapenna, A.: “Esposizione degli enzimi a Plasmi Freddi a pressione atmosferica: effetti sulla Tirosinasi e sulla Glucosio Ossidasi I” (2017).
- Spagnulo, V.: “Nanoantimicrobici a base di argento per potenziali usi nel food packaging” (2018).
- Tricase, A.: “Caratterizzazione analitica di biosensori Electrolyte-Gated Organic Field-Effect Transistors” (2019).

Master in Materials Science and Technology (Laurea magistrale)

- Izzi, M.: “Sviluppo di nanocompositi innovativi per il food packaging” (2017).
- Lopetuso, R.: “Caratterizzazione spettroscopica di film sottili elettrodepositati per applicazioni nel settore dell’energia” (2017).
- Quarto, R.: “Development of second generation nanoantimicrobials: Insights into the bioactivity mechanisms through a comprehensive spectroscopic analysis” (2017).
- Sarcina, L.: “Inclusion of electro-synthesized Cu nanoparticles in vescicular and magnetic nano-systems for antibacterial applications” (2017).

Master in Pharmaceutical Chemistry and Technology (Laurea magistrale)

- Marchianò, V.: “Electrodecoration and characterization of iron oxide nanoparticles with bioactive nanophases for targeted antimicrobial materials” (2019).
- Sportella, M.: “Electrodecoration and characterization of superparamagnetic iron oxide nanoparticles with bioactive synergistic nanocopper for targeted antimicrobial materials” (2020).

Master in Pharmaceutical Sciences (Laurea magistrale)

- Cimarusti, C.: “Sintesi di un tiolo a catena corta per la realizzazione di sam misti atti a migliorare la sensibilità di un biosensore” (2020).

PhD in Chemical and Molecular Sciences

- Macchia, E.: “Flexible bioelectronic Field Effect Transistors as analytical biosensors” (2017).
- Tiwari, A.: “OTFT biosensor fabrication and analytical testing” (2017).
- Mateos Cuadrado, E.: “Surfactant-polymer interaction at the liquid-solid interface” (2020).

U.O. Bergamo

Bachelor in Ingegneria delle tecnologie della salute (Laurea triennale)

- Bertulessi, L.: “Studio di protesi vascolari destinate a trattamenti emodialitici” (2018).
- Spandri, M.: “Prototipazione e caratterizzazione di membrane in fibroina e poliuretano per la produzione di protesi vascolari per emodialisi” (2019).

Bachelor in Ingegneria edile (Laurea triennale)

- Bresciani, R.: “Studio dell’influenza della maturazione umida sulle prestazioni di malte a base di cemento solfoalluminoso” (2018).
- De Angelis, V.: “Proprietà di autopulizia di pitture additivate con ferrite per applicazioni indoor” (2018).
- Quartararo, D.: “L’influenza di acceleranti di presa e indurimento sulle proprietà di miscele ternarie a base di CSA, SCM e gesso” (2018).
- Raimondi, C.: “Studio sperimentale nel settore delle pitture murali autopulenti” (2018).
- Trianni, V.: “La carbonatazione nei leganti alternativi al cemento Portland: studio sull’influenza di filler basaltici” (2018).
- Viganò, G.: “Schiume ceramiche modificate per la degradazione di microinquinanti nelle acque” (2018).
- Baldassarre, D.: “Studio sperimentale di miscele a base di calce per la conservazione di beni culturali” (2019).
- Cornelli, M.E.; Mazzucchetti, V.: “La durabilità ai cicli di gelo/disgelo e all’attacco solfatico di malte ad attivazione alcalina” (2019).
- Dozio, O.: “Studio sperimentale di inibitori di corrosione migranti per calcestruzzi in ambienti ricchi di cloruri” (2019).

- Rottoli, D.: “Glicoli etilenici e metilcellulose come aggiunte anti-ritiro in sistemi ad attivazione alcalina” (2019).
- Sonzogni, R.; Gerosa, L.; Damiani, A.: “Il settore del cemento e le potenzialità dei leganti eco-sostenibili” (2019).
- Tomasoni, P.: “Studio sperimentale di additivi anti-ritiro per intonaci totalmente privi di cemento Portland” (2019).

Master in Mechanical Engineering (Laurea magistrale)

- Zucchi, I.: “Realizzazione, caratterizzazione e verifica di durabilità di superfici di rame superidrofobiche” (2017).
- Barcella, F.: “Valutazione della resistenza a corrosione della lega Ti6Al4V ottenuta per LPBF per applicazioni biomedicali” (2018).
- Maurizio, L.: “Stress corrosion cracking di giunti di leghe di alluminio saldati con tecnologia friction stir welding” (2018).
- Pesenti, D.: “Caratterizzazione corrosionistica e di meccanica della frattura della lega AlSi10Mg ottenuta per LPBF” (2018).

Master in Building Engineering (Laurea magistrale)

- Baroni, I.; Mazzoleni, A.: “Intonaci privi di cemento a base di leganti ad attivazione alcalina, termoisolanti, per il recupero energetico e strutturale di edifici in muratura” (2018).
- Caltran, M.: “Miscele di leganti sostenibili a base di cementi solfoalluminosi per la realizzazione di malte Portland cement-free rinforzate con fibre in acciaio e polimeriche per il ripristino e l’adeguamento sismico del costruito” (2018).
- Chioda, F.; Licini, M.: “L’impiego di aggregati artificiali provenienti dal settore siderurgico nella produzione di calcestruzzi a basso impatto ambientale” (2018).
- Furneri, V.: “L’impiego delle ceneri volanti ultrafini per la realizzazione di malte durevoli e a basso impatto ambientale” (2018).
- Moioli, M.: “Studio di additivi superfluidificanti innovativi per conglomerati a base di loppa attivata alcalinamente” (2018).
- Prometti, C.; Sonzogni, M.: “Realizzazione di schiume ceramiche con fotocatalizzatori e loro applicazione al trattamento di reflui acquosi” (2018).
- Bassetti, V.: “La durabilità di malte ad attivazione alcalina in ambienti aggressivi” (2019).
- Muzzupappa, E.; Ruscio, D.: “Studio di intonaci strutturali ecosostenibili totalmente privi di cemento Portland per edifici in muratura e pietra” (2019).
- Surini, E.: “Studio di additivi per la riduzione del ritiro in malte a base di loppa attivata alcalinamente” (2019).

Master in Tecnologie e processi della filiera tessile (1° livello)

- Sangaletti, M.: “La formaldeide nell’industria tessile” (2019).

PhD in Engineering and Applied Science

- De la Fuente Garcia, E.: “Visible light photocatalyst for water purification and self-cleaning coatings” (2018).
- Coffetti, D.: “Alternative binders as milestone of 3R strategy for sustainable construction materials” (2019).
- Pesenti Bucella, D.: “Cathodic protection and hydrogen embrittlement” (2019).

U.O. Bologna

Bachelor in Industrial Chemistry (Laurea triennale)
- Gaja, D.: “Caratterizzazione cinetica di β-glucosidasi” (2017).
- Nota, M.: “Valorizzazione di materiali lignocellulosici (Arundo donax) mediante pretrattamento alcalino e digestione enzimatica” (2018).
- Peduto, P.: “Metodi sostenibili per la produzione di idrolizzati cheratinici da scarti industriali” (2018).

Master in Industrial Chemistry or Molecular and Industrial Biotechnologies (Laurea magistrale)
- Caramia, S.: “Purification and preliminary structural characterization by NMR spectroscopy of “HoLaMa” DNA Polymerase” (2017).
- Crescenzi, M.: “Applicazione di tecniche molecolari innovative per l’autenticità alimentare” (2017).
- D’Alessio, F.: “Stimolazione della crescita e variazioni del proteoma di Deinococcus radiodurans indotte dallo ione Mn2+” (2017).
- Baldin, A.: “Purificazione e caratterizzazione cinetica della tirosin fosfatasi di Mycobacterium tuberculosis sovraespressa in Escherichia coli” (2018).
- Castaldo, A.: “Purification and characterization of the stability of the “HoLaMa” DNA polymerase, free or engaged in complex with nucleic acids” (2018).
- Pettinari, V.: “Applicazioni di metodi molecolari e di fingerprinting dei composti volatili per analisi di autenticità in spezie ed erbe aromatiche” (2018).
- Santoro, S.: “Analisi fenotipiche e molecolari della fioritura in due varietà di canapa (Cannabis sativa L.) con diverso fotoperiodismo” (2018).
- Tomaselli, F.: “Caratterizzazione cinetica in regime di steady-state e di pre-steady-state della lattato deidrogenasi di muscolo di coniglio” (2018).

U.O. Brescia

Bachelor in Biotechnology (Laurea triennale)
- Arceri, D.: “An Exploratory Study Of Nanomechanical Properties Of Extracellular Vesicles And Their Potential Applications” (2018).
- Consoli, G.:” Profiling Of Extracellular Vesicles By Fourier-Transform Infrared Spectroscopy” (2018).
- Zaghen, S.: Manipulation And Analysis Of Extracellular Vesicles By Lateral Flow Chromatography” (2018).

Ph.D. in Technology for Health
- Zendrini, A.: “Exploring and exploiting extracellular vesicles with nanotechnology” (2018).
- Busatto, S.: “Novel routes for manipulating and engineering extracellular vesicles” (2019).

Post-Doc
- Paolini, L.: “evFOUNDRY – The Extracellular Vesicle Foundry”

U.O. Cagliari

Bachelor in Chemistry (Laurea triennale)

- Granitzio, G.: “Un nuovo sistema per l’adsorbimento e la determinazione del cadmio costituito da silice mesoporosa (SBA-15) funzionalizzata con composti macrociclici” (2017).

Master in Chemical Sciences (Laurea magistrale o a ciclo unico)

- Licheri, L.: “Produzione di biodiesel mediante biocatalisi a partire da oli di scarto” (2018).
- Tocco, D.: “Caratterizzazione di ADH@MOF (alcol deidrogenasi immobilizzata su metal organic framework): effetto del pH, della temperatura e della concentrazione di etanolo sulla stabilità e l’attività enzimatica” (ERASMUS+, 2018).
- Zanda, D.: “Silice Mesoporosa ordinata (SBA-15) funzionalizzata con trietilentetrammina per l’adsorbimento di ioni Cu2+ e Zn2+ in soluzione acquosa” (2018).

Master in Chemistry and Pharmaceutical Technologies (Laurea magistrale)

- Furcas, L.: “Caratterizzazione chimico-fisica di liposomi a gradiente di pH per il rilascio controllato di un farmaco” (2017).
- Secci, S.: “Nanoparticelle lipidiche con struttura cubica bicontinua ibridizzate con nanoparticelle d’oro” (2017).

PhD in Chemical Sciences and Technologies

- Nairi, V.: “Functional ordered mesoporous silica in nanomedicine: target and drug delivery systems” (XXX ciclo, Doctor Europaeus, 2018).
- Pitzalis, F.: “Immobilization of enzymes on SBA-15 and ZIF-8 for biocatalytic applications” (XXX ciclo, 2018).

U.O. Campobasso

Bachelor in Food Sciences and Technology (Laurea triennale)

- Sacco, L.: “Impiego di ossido di titanio dopato per la rimozione di sostanze fenoliche da acque di vegetazione” (2017).
- Zurlo, S.: “Coatings edibili nello sviluppo di prodotti “ready-to-eat” (2017).
- Zollo, K.: “Impiego di sistemi nanoemulsivi per l’assorbimento di sostanze bioattive” (2018).

Master in Biology (Laurea magistrale)

- Gizzarelli, M.: “Rigenerazione cellulare mediante l’utilizzo di nanosistemi” (2017).

Master in Food Sciences and Technology (Laurea magistrale)

- Iacovino, S.: “Caratterizzazione Chimico Fisica della mucillagine di Chia e applicazioni nell’industria alimentare” (2019).
- Sacco, L.: “Emulsioni di olio di oliva arricchite con estratto di vino: ruolo dei polifenoli nella stabilità ossidativa” (2019).

- Zurlo, S.: “Studio di nanovettori per la protezione e veicolazione di sostanze bioattive” (2019).

PhD in Agriculture, Technology and Biotechnology

- Perugini, L.: “Use of Colloidal systems for food applications” (2018).
- Cofelice, M.: “Alginate-based nanodispersions to assemble edible coatings and films for food applications” (2020).

PhD in Biology and Environmental Technology

- Di Nezza, F.: “Setup of nanodevices and their applications” (2017).

U.O. Catania

Bachelor in Chemistry (Laurea triennale)

- De Grazia, A.: “Processi di ricristallizazione di film sottili polimerici” (2017).
- Finocchiaro, G.: “Selective anchoring of proteins to bioactive surfaces” (2017).
- Gullo, M.: “Metodologie di funzionalizzazione enzimatica di superfici polimeriche” (2017).
- Milazzo, C.: “Processi di interazione di peptidi funzionalizzati con nucleotidi su superfici di oro” (2017).
- Strazzanti, P.: “Nanoconfinamento di laminina: il ruolo dell’energia libera di superficie” (2017).
- Amore, R.: “Metodologie di ancoraggio di un sistema anticorpo-calix” (2018).
- Bonaccorso, G.: “Proprietà elettriche di film nanostrutturati di politiofene” (2018).
- Calì, F.: “Preparazione e stabilizzazione di monostrati di coordinazione all’interfaccia aria/acqua” (2018).
- Consoli, A.: “Proprietà meccaniche di macromolecole biologiche” (2018).
- Contarino, G: “Metodi avanzati di trattamento dati per la valutazione dei risultati nei laboratori” (2018).
- Contino, T.: “Preparazione e caratterizzazione di superfici a bagnabilità e nano-curvatura controllata” (2018).
- Garra, E.: “Processi di riconoscimento di glicoproteine da monostrati di lectine funzionalizzare” (2018).
- Mangano, M.: “Monostrati di coordinazione all'interfaccia acqua-aria” (2018).
- Ragonese, P.: “Sintesi e caratterizzazione di nanoparticelle di carbonio a partire da acido citrico” (2018).

Master in Materials Chemistry (Laurea magistrale)

- Sipala, M.D.: “Sintesi di nanoparticelle di carbonio fluorescent come messaggeri nella comunicazione molecolare2 (2017).
- Amato, T.: “Preparazione e caratterizzazione di materiali bidimensionali di coordinazione” (2018).
- Carciola, F.: “Caratterizzazione di polimeri elettro-attivi per l’elettronica molecolare” (2018).
- Fichera, L.: “Modelli matematici per la comunicazione molecolare” (2018).

- Livio, P.A.: “Modifiche non convenzionali di nanostruttura e conducibilità di film sottili di semiconduttori polimerici” (2018).
- Ruffino, R.: “Superfici nano-curve e auto-organizzazione di polimeri semicristallini” (2018).
- Scuderi, I.L.: “Assemblaggio di film molecolari per applicazioni in elettronica molecolare” (2018).

U.O. Firenze

Bachelor in Biotechnologies (Laurea triennale)

- Pini, M.: “Prove biologiche di nanoparticelle metalliche sintetizzate da estratti di mirtillo” (2018).
- Sautariello, G.: “Nanoformulazioni lipidiche per il delivery di fito-ormoni: verso una preparazione totalmente eco-sostenibile” (2018).

Bachelor in Chemistry (Laurea triennale)

- Bassu, G.: “Sintesi e caratterizzazione di film di ossidi di metalli mistiper vetri riflettenti nel vicino infrarosso - Synthesis and characterization of mixed metal oxides films for reflective glasses in the near infrared” (2017).
- Casale, M.: “Caratterizzazione chimico-fisica di pectina da materiali di riciclo - Physical-chemical characterization of pectin from recycled materials” (2017).
- Lombardi, M.: “Rimozione dei residui di pulimentatura da ZAMAK mediante lavaggio a ultrasuoni e relativo studio della corrosione - Removal of polishing residues from ZAMAK using ultrasonic cleaning and corrosion study of the metal surface” (2017).
- Massi, M.: “Frazionamento e caratterizzazione di polisaccaridi da Punica granatum L. - Fractionation and characterization of polysaccharides from Punica granatum L.” (2017).
- Mastromartino, V.: “Interazioni intermolecolari in nanostrutture auto-assemblate - Intermolecular interactions in self-assembled nanostructures” (2017).
- Moretti, C.: “Synthesis and characterization of nanoporous alumina membranes” (2017).
- Perdichizzi, A.: “Studio dell'effetto di alluminati su cementi a base di silicato di magnesio” (2017).
- Perini, I.: “Self-assembly di tensioattivi derivati dalla vitamina C - Self-assembly of surfactants derived from vitamin C” (2017).
- Tinti, V.: “Effetto dello ione specifico sull’aggregazione dell’Insulina in fibrille amiloidi - Specific ion effect on the aggregation of Insulin in amyloid fibrils” (2017).
- Uva, L.: “Sintesi e caratterizzazione di alcool polivinilico funzionalizzato con amminoacidi” (2017).
- Benassai, S.: “Studio di proprietà chimico-fisiche di alogenati in soluzione acquosa - Study about chemical-physical proprieties of halogenates in aqueous solution” (2018).
- Ciardi, D.: “Studio delle proprietà diffusive di idrogel di gelatina macroporosi” (2018).

- Ciofalo, C.: “Self-assembly di un anfifilo piperidinico - Self-assembly of a piperidine amphiphile” (2018).
- Cipollesci, L.: “Diagrammi di fase di miscele binarie di composti alifatici a catena lunga - Phase diagrams of binary mixtures of long chain aliphatic compounds” (2018).
- Dini, T.: “Preparazione e caratterizzazione di idrogel a base di alcol polivinilico e sodio esametafosfato” (2018).
- Esposito, S.: “Embedding di nanoparticelle di ossidi di metalli misti in matrici polimeriche per superfici NIR riflettenti - Embedding of mixed metal oxides nanoparticles in polymeric matrices for NIR reflecting surfaces (2018).
- Minimi, A.: “Preparazione e caratterizzazione di cementi ossei a base di fosfato di magnesio per ingegneria tissutale ossea” (2018).
- Panzanelli, F.: “Proprieta’ chimico-fisiche di tio-e seleno-acilgliceroli - Physico-chemical properties of thio-and seleno-acylglycerols” (2018).
- Salvestrini, S.: “Studio chimico-fisico di fosfati amorfi di calcio e magnesio rilevanti nei sistemi biologici.” (2018).
- Sarti, M.: “Development and physico-chemical characterization of castor oil based sponges for hydrocarbons recovery” (2018).
- Berni, S.: “Synthesis and characterisation of "duplex" nanoporous alumina membranes” (2019).
- Boni, T.: “Effetto dello ione specifico su sistemi viscoelastici stimulus-responsive - Specific ion effect on stimulus-responsive viscoelastic systems” (2019).
- Mert, A.: “Comportamento di soluzioni di alogenati ed effetto dello ione specifico - Behavior of halate solutions and specific ion effect” (2019).
- Pecori, G.: “Production and physical-chemical characterization of char obtained from ligno-cellulosic biomass” (2019).
- Venturi, A.: “Studio del degrado superficiale di modelli di frutti in cera - Study on the surface degradation of wax fruit models” (2019).
- Lucarini, I.: “Proprietà in bulk di soluzioni acquose di alogenati di sodio - Bulk properties of sodium halates aqueous solutions” (2020).
- Orsillo, E.: “Effetto dello ione specifico sulle variazioni conformazionali della Bovine Serum Acbumin - Specific ion effect on the confomartional changes of Bovine Serum Albunim” (2020).

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

- Baracani, M.: “Nuove Formulazioni da fonti rinnovabili per il trattamento della carta” (2018).
- Cianci, C.: “Indagini diagnostiche per la conservazione dei modelli botanici polimaterici della manifattura Brendel” (2018).
- Spallina, L.: “Il Palazzo Nazionale di Città del Messico: degrado delle superfici e rimozione di graffiti” (2018).
- Bonechi, P.: “Caratterizzazione dei materiali impiegati come supporti di affreschi strappati” (2019).
- Borri, F.: “Caratterizzazione chimica delle superfici di monumenti in cemento appartenenti al patrimonio culturale del XX secolo” (2019).

- Gabrielli, L.: “Soluzione enzimatica caricata su gel ad alta ritenzione per la rimozione di amido” (2019).
- Marrini, M.: “Consolidamento di materiale cartaceo e caratterizzazione delle proprietà fisico-meccaniche” (2019).
- Palombo, M.: “Valutazione dello stato di conservazione degli affreschi della chiesa di Santa Maria Maggiore in Sant’Elia Fiumerapido (FR)” (2019).
- Pertica, A.: “Il dipinto murale di Capogrossi nel Cinema Airone a Roma: rimozione selettiva di ridipinture tramite microemulsioni confinate in gel” (2019).
- Santi, L.: “Negativi fotografici in acetato di cellulosa: caratterizzazione chimico-fisica ed organogel per la loro pulitura” (2020).

Master in Biotechnology (Laurea magistrale)

- Clemente, I.: “Nanovettori biocompatibili come carrier per fitormoni verso piante recalcitranti alla radicazione” (2017).
- Benassai, E.: “Sintesi e caratterizzazione di nanoparticelle di rame a partire da estratti di bacche e saggi di attività antimicrobica” (2018).

Master in Chemical Sciences (Laurea magistrale)

- Bani, A.: “Synthesis of mesoporous silicas funzionalized with CaO as heterogeneous catalysts for Biodiesel synthesis” (2017).
- Caselli, L.: "Fasi liquido cristalline lipidiche contenenti nanoparticelle inorganiche" (2017).
- Cerretani, C.: “Nanocluster di argento stabilizzati da DNA: sintesi e caratterizzazione fotofisica - DNA-stabilized silver nanoclusters: synthesis and photophysical characterization” (2017).
- Ciapetti, A.: "Comportamento di Fase e Caratterizzazione Strutturale di Nuovi Surfattanti Contenenti CO" (2017).
- Crocini, A.: “Sintesi e caratterizzazione di nanomateriali per tessuti con nuove funzionalità. - Syntesis and characterization of nanomaterials for textiles with new functionalities” (2017).
- Gigli, L.: “Sintesi, caratterizzazione e strategie per la stabilizzazione di nanostrutture amorfe di fosfato di calcio e magnesio rilevanti per il sistema immunitario” (2017).
- Guaragnone, T.: "Caratterizzazione chimico-fisica del dewetting di film polimerici da superfici di interesse storico-artistico" (2017).
- Lucchesi, G.: “Preparazione e caratterizzazione chimico-fisica di materiali innovativi per lo stoccaggio di idrogeno” (2017).
- Magnani, C.: "Vescicole ibride da lipidi e copolimeri: una nuova famiglia di vettori e modelli per applicazioni biomediche" (2017).
- Mati, L.: “Effetto di additivi polisaccaridici sulla formazione e sulle proprietà di cementi ossei a base” (2017).
- Picone, A.: "Studio di proprietà strutturali di modelli di membrana mediante microfluidica" (2017).
- Rinaldi, E.: “Commercial plastics functionalization with silver nanoparticles for antimicrobial purpose” (2017).
- Tili, F.: “Synthesis and physico-chemical characterization of polymeric sponges containing spent coffee for the removal of heavy metal ions from water” (2017).

- Barletti, B.: “Interazione della Trodusquemine con membrane lipiche contenenti domini rafts. - Troduquemine interaction with raft-containing lipid membranes In corso” (2018).
- Becheri, G.: "Proprietà colloidali di vescicole extracellulari" (2018).
- Bernardi, S.: “Sviluppo di film nanostrutturati IR-riflettenti su vetro -Development of nano-structured IR-reflective coatings on glass” (2018).
- Corvi, G.: “Functionalization of polystyrene with gold-based metal nanostructures” (2018).
- Muzzi, B.: “Preparazione e caratterizzazione di celle solari a perovskite a base di magnesio - Preparation and characterization of magnesium perovskite solar cells” (2018).
- Orazzini, S.: "Proprietà strutturali e viscoelastiche di mesofasi non-lamellari: effetto dell'inclusione di nanoparticelle magnetiche" (2018).
- Salvi, M.: “Physico-chemical characterization of dispersants for lubricant oils” (2018).
- Simonelli, M.: “Effetto dei gas disciolti su alcune proprietà chimico-fisiche dei liquidi - Effect of dissolved gases on some physico-chemical properties of liquids” (2018).
- Sordi, G.: “Studio a livello molecolare dell’attivazione della Ca-ATPasi del reticolo sarcoplasmatico” (2018).
- Tempestini, E.: "Sistemi ibridi autoorganizzati di copolimeri a blocchi e nanoparticelle responsive" (2018).
- Tramonti, V.: “Piattaforma ibrida a base di nanoparticelle metalliche e ossido di grafene per la diagnostica della neurodegenerazione - Graphene based nano-hybrid platforms for early diagnosis of neurodegeneration” (2018).
- Balestri, A.: "Bistrati ibridi lipidici e copolimerici su supporto solido" (2019).
- Brandi, F.: "Sintesi di un Sistema Catalitico Avanzato per la Valorizzazione Sostenibile di Biomasse" (2018). Lignocellulosiche in Condizioni di Flusso Continuo" (2019).
- Cardellini, J.: "Interazione di nanoparticelle d'oro con membrane biomimetiche: Self-Assembly su bistrati lipidici" (2019).
- Casale, M.: “Castor oil-based polyurethane sponges as sorbents for organic pollutants” (2019).
- Conti, S.: “Sintesi e caratterizzazione di copolimeri polisolfobetaina-polietilenglicole e film compositi contenenti silice nanoporosa” (2019).
- Cuccoli, E.: “Caratterizzazione di stampati 3D di ABS e successive metallizzazione” (2019).
- Loliva, D.: “Formulation and physico-chemical characterization of shaving soaps” (2019).
- Maltoni, P.: "Interazione di mesofasi lipidiche lamellari e non-lamellari con nanoparticelle inorganiche" (2019).
- Mazzoncini, V.: “Influenza della componente abrasiva sulle proprietà di una formulazione per dentifricio - The effect of the abrasive component on toothpaste formulation properties” (2019).
- Mugnaini, G.: “Stampa 3D di formulazioni polimeriche a base di pullulano” (2019).
- Nincheri, A.: “Sintesi e caratterizzazione chimico-fisica di polimeri biodegradabili a base di pva e leucina” (2019).

- Perini, I.: “Preparazione e caratterizzazione di alloisiti come nano-contenitori per agenti antifouling” (2019).
- Pucci, E.: “Chemical-physical characterization of doughs with ancient grain flour and water” (2019).
- Riccitelli, T.: "Celle solari organiche fabbricate via slot-die coating" (2019).
- Tinti, V.: "Indagine chimico-fisica di mesofasi lipidiche ternarie: proprietà strutturali e diffusive" (2019).
- Ciardi, D.: “Effetto dello ione specifico in formulazioni viscoelastiche stimulus-responsive - Specific ion effect in viscoelastic stimulus-responsive formulations” (2020).
- Lombardi, M.: “Analisi delle proprietà termiche e meccaniche di film biodegradabili di polivinil alcool plasticizzati con glicerolo e sorbitolo per applicazioni di packaging - Thermal and Mechanical properties of poly(vinyl alcohol) films plasticised with glycerol and sorbitol for packaging applications” (2020).

Master in Food Science and Technology (Laurea magistrale)

- Pancrazzi, F.: “Physico-chemical characterisation of ice cream formulations with different compositions” (2017).
- Vallone, V.: " Use of capped-nanoclays as controlled release systems for food applications" (2017).
- Frassineti, S.: “On the influence of intestinal conditions and different doses of enzymatic supplements on single and combined food ingredients” (2018).
- Rinaldi, M.: “Physico-chemical characterisation of homemade ice cream formulations containing structuring agents of different nature” (2019).

Master in Pharmacy (Laurea magistrale)

- Filippini, C.: “Ibridi molecolari come potenziali inibitori delle anidrasi carboniche in grado di revertire la chemoresistenza mediata dalla glicoproteina P” (2017).
- Gracci, G.: “Inibitori della glicoproteina P e delle Anidrasi Carbonica a struttura ibrida: una nuova strategia per revertire la MDR” (2017).
- Pellecchi, M.: “Studio di stabilità plasmatica di inibitori ibridi dei sistemi enzimatici anidrasi carbonica e ciclossigenasi mediante analisi LC-MS/MS” (2017).
- Caponi, F.: “Applicazione della spettrometria di massa nello studio di stabilità plasmatica di inibitori ibridi dei sistemi enzimatici anidrasi carbonica e ciclossigenasi” (2018).
- Petreni, A.: “Design, sintesi e valutazione biologico-strutturale di derivati ibridi stabilizzanti del G-quadruplex e inibitori delle Anidrasi Carboniche IX/XII come potenziali agenti antitumorali” (2018).
- Picchioni, I.: “Progettazione, sintesi e valutazione biologica preliminare di nuovi inibitori dell’anidrasi carbonica” (2018).
- Maach, S.: “Progettazione, sintesi e valutazione biologica preliminare di nuovi ligandi del recettore nicotinico e di nuovi attivatori dell’anidrasi carbonica” (2019).

Master in Pharmaceutical Chemistry and Technology (Laurea magistrale)

- Chiaramonte, N.: “Chimica esplorativa per la sintesi di derivati benzilpiperazinici come potenziali inibitori delle anidrasi carboniche” (2017).

- Schillaci, D.: “Applicazione dell’algoritmo Linear equations deconvolution analysis (LEDA) in Ion Trap Mass Spectrometry (IT-MS): risoluzione di miscele isomeriche di inibitori ibridi dei sistemi enzimatici anidrasi carbonica e ciclossigenasi” (2017).

Master in Sciences and Materials for the Conservation and Restoration (Laurea magistrale)

- Campo, G.: “Studio di protettivi nanocompositi a base di TiO2 per materiali lapidei: valutazione del contributo delle nanoparticelle all’efficacia protettiva” (2017).
- Casini, A.: “Rimozione di patine di corrosione del Ferro da arte contemporanea mediante sistemi ‘peelable’ a base di PVA” (2017).
- Guarducci, A.: “Studio degli effetti della pulitura su superfici plastiche di interesse artistico a base di PVC, PET e Acetato di Cellulosa” (2017).
- Marini, G.: “Formulazioni ottenute da fonti rinnovabili per il trattamento conservativo della carta” (2017).
- Alterini, M.: “Processi di rimozione di film polimerici da superfici artistiche a diversa bagnabilità mediante l’utilizzo di fluidi nanostrutturati” (2018).
- Xiaoling, W.: “Sintesi di nanoparticelle di silice mesoporosa e loro applicazioni nell’arte moderna e contemporanea” (2018).
- Carlino, M.: “Il ruolo dei tensioattivi nella rimozione di materiali filmogeni mediante fluidi nanostrutturati” (2019).

PhD in Chemical Sciences

- Andriulo, F.: “Nanotechnologies for the restoration of alum-treated archaeological wood” (2017).
- Lucchesi, G.: “Effetto plasmonico in metamateriali nanostrutturati: dalle celle solari a perovskite ai nanosensori per la diagnostica di malattie neurodegenerative - Plasmonic enhancement in nanostructured metamaterials: from perovskite-based solar cells to early diagnosis of neurodegenerative disease” (XXXV cycle).
- Pianorsi, M.D.: “Study of parchment degradation and assessment of new nanotechnologies for the long-term protection of manuscripts” (2017).
- Tonelli, M.: “Investigation of the structural properties of magnesium silicate hydrate cements and assessment of strategies for their development” (2017).
- Tovar, J.: “Nuove Prospettive nella sintesi e funzionalizzazione di materiali mesoporosi e nanostrutturati di silicio e loro applicazione nella catalisi” (2018).
- Camerini, R.: “Nanocomposites for the consolidation of stone: novel formulations and a kinetic study” (2019).
- Ferrari, P.: “Organic solvents confined in poly (ethyl methacrylate) based organogels for the removal of unwanted materials from works of art” (2019).
- Sarri, F.: “Studio delle proprietà fisico-chimiche di dispersioni polimeriche in sistemi ibridi: effetto delle condizioni ambientali e della natura dei solute - Study of physico-chemical properties of polymeric dispersion in hybrid systems: effect of ambient conditions and nature of solutes” (2019).
- Tatini, D.: “Formulazioni a basso impatto ambientale per formazioni europee di gas da argille - Lower Environmental Impact Formulations for European Shale Gas Plants” (2019).
- Gelli, R.: “Biologically relevant phosphate-based nanostructures: interactions with Soft Matter and biomedical applications” (2020).

PhD in Pharmaceutical Chemistry

- Bua, S.: “Synthesis and in vitro kinetic evaluation of new modulators of the metalloenzymes Carbonic Anhydrases: The tail approach for the obtainment of Low molecular weight hybrids for biomedical purposes” (2017-2019).
- Angeli, A.: “Synthesis, characterization, biological assays and development of new enzyme modulators for the treatment of human pathologies” (2016-2018).
- Nocentini, A.: “Modeling and structure-based approaches in the design, synthesis and biological evaluation of ligands targeting the metalloenzymes carbonic anhydrases” (2014-2017).

Postdoc Fellowship

- Nocentini, A.: “Sintesi e studio strutturale di derivati ad azione antitumorale mediante modulazione di target di natura nucleica (Q-DNA, Q-RNA) ed enzimatica (CAIX e CAXII)” (2017-2018).
- Bozdag, M.: “Inibitori di enzimi presenti nei tumori ipossici” (2018-2019).
- Nocentini, A.: “Design, sintesi e caratterizzazione biologico-strutturale di ligandi multipotenti inibitori di anidrasi carboniche per sviluppo di farmaci per il trattamento del glaucoma” (2018-2019).

U.O. Napoli

Bachelor in Chemical Engineering (Laurea triennale)

- Rinaldi, A.: “Progettazione bio-ispirata di antimicrobici nanostrutturati” (2017).
- Di Luca, C.: “Da scarto a risorsa: valorizzazione di scarti organici in preziosi bio-nano-materiali” (2019).
- Ferone, A.: “Nanoparticelle a base lipidica per applicazioni biomediche” (2019).

Bachelor in Chemistry (Laurea triennale)

- Pellegrino, M.: “Sviluppo di una formulazione a basso impatto ambientale per la detergenza industriale” (2019).

Bachelor in Industrial Chemistry (Laurea triennale)

- Caianiello, C.: “Effetto di elettroliti sul processo di micellizzazione di tensioattivi N,N-dimetil-alchilammino-N-ossidi” (2017).
- Carbone, S.: “Sintesi e caratterizzazione di nanoparticelle antimicrobiche TiO2-melanina in presenza di poli vinil alcol (PVA)” (2017).
- Caruso, C.: “Sintesi e caratterizzazione di nanoparticelle ibride a base di TiO2 e acidi umici da biomasse” (2017).
- D’Avino, C.: “Caratterizzazione chimico-fisica di una miscela acquosa di tensioattivi costituita da dodecil-etossi-solfato di sodio e decil-N-ossido” (2017).
- D’Avino, M.: “Il processo di invecchiamento di bitumi in presenza di agenti antiossidanti: uno studio di risonanza paramagnetica elettronica” (2017).
- Ferraro, E.: “Costruzione del diagramma di fase ternario di una miscela di tensioattivi costituita d N,N-dimetil-propil-eptanammina-N-ossido e dodecil-etossi-solfato di sodio” (2017).
- Savoia, S.: “Ottimizzazione di una formulazione anticorrosiva e detergente” (2017).

- Di Leva, D.: "Sintesi e caratterizzazione di nanostrutture ibride a base di TiO2, grafene ed eumelanina" (2018).
- Giglio, M.: "La rigenerazione dei bitumi: uno studio EPR" (2018).
- Giordano, I.: "Effetto del pH sul processo di micellizzazione di tensioattivi anfoteri" (2018).
- Ingenito, L.: "Organizzazione supramolecolare di melanina da 5,6-diidrossindolo (DHI) in presenza di TiO2: uno studio EPR" (2018).
- Maresca, M.: "Effetto del pH sul raggio idrodinamico delle micelle formate da tensioattivi N,N-dimetilalchilammino ossidi" (2018).
- Ruocco, M.: "Effetto del Glicerolo e dell'isopropanolo sulla micellizzazione e sulla gelificazione di miscele di polossameri" (2018).
- Sgamato, M.: "Polimerizzazione della dopamina in presenza di diversi Sali di zinco" (2018).
- Adaldo, G.: "Caratterizzazione di sistemi liposomiali diversamente funzionalizzati per applicazioni biomediche" (2019).
- Galario, M.A.: "Studio, mediante risonanza elettronica paramagnetica, dell'effetto di agenti rigeneranti sull'invecchiamento dei bitumi" (2019).
- Longobardi, V.: "Determinazione mediante EPR spin-trapping di Specie Reattive dell'Ossigeno (ROS) prodotte da nanoparticelle di ossidi metallici" (2019).
- Migliaro, G.: "Effetto del pH sul raggio idrodinamico delle micelle di N,N-dimetildecil-1-ammino ossido" (2019).
- Zimbaldi, G.: "Influenza delle condizioni chimico-fisiche sul processo di auto-aggregazione della proteina dolce MNEI" (2019).

Master in Chemical Engineering (Laurea magistrale)

- De Simone, C.: "Progettazione di sistemi antiossidanti per la valorizzazione di scarti del comparto agro-alimentare" (2018).
- Greco, I.: "Bioinspired design of high contrast photoacustic nanoprobes" (2018).
- Pota, G.: "Progettazione di nanostrutture biocompatibili ed ecosostenibili per imaging fotoacustico" (2019).

Master in Chemical Science (Laurea magistrale)

- Picariello, A.: "Towards the development of aptamer-functionalized SPIONs for biomedical applications" (2017).
- Basile, I.: "Role of different catechols in the coating process of ZnO nanoparticles: structural features and functionalization kinetics" (2017).

Master in Science and Technology of Industrial Chemistry (Laurea magistrale)

- Fernandez, F.: "Miscele catanioniche di tensioattivi salt-free: effetto dell'asimmetria delle catene alchiliche sul proceso di aggregazione" (2017).
- Pasqua, V.: "Sintesi sol-gel e caratterizzazione di materiali ibridi a base di biossido di titanio per applicazioni catalitiche" (2017).
- Quinterno, M.: "Formulazione e caratterizzazione di sistemi nanostrutturati a base di idrogeli polimerici termosensibili contenenti nanoparticelle mesoporose di silice e acido ialuronico per applicazioni biomedicali" (2017).
- Rossano, C.: "Synthesis of associative polymers in aqueous emulsion" (2017).

- Russo, V.: “Formulazioni acqua-tensioattivo thickener-free: caratterizzazione strutturale e reologica” (2017).
- Bonifazi, M.M.: “Sviluppo di materiali ibridi a base di biossido di titanio per la stabilizzazione superficiale di specie reattive dell’ossigeno” (2018).
- Di Gennaro, M. “Idrogeli termoreversibili contenenti liposomi come formulazioni dermatologiche senza alcoli” (2018).
- Cavasso, D.: “Studio del comportamento di fase dell’idrossipropilcellulosa in solventi misti ed interazioni con nanostrutture lipidiche” (2019).
- Gallucci, N.: “Sintesi e caratterizzazione chimico-fisica di nanoparticelle di CeO2 redox attive stabilizzate mediante ricoprimento anfifilico” (2019).
- Musone, G.: “La conversione industriale del glucosio in sorbitolo: L’importanza dei coefficienti di diffusione del sistema glucosio/sorbitolo/acqua nella descrizione del processo” (2019).
- Salzano, C.: “Studio del processo dell’evoluzione temporale di formulati contenenti tensioattivi cationici di ammonio quaternario” (2019).
- Savignano, L.: “Caratterizzazione strutturale e dinamica di miscele acquose di tensioattivi mono- e bi-codati come sistemi modello di tensioattivi di-esterei parzialmente idrolizzati” (2019).
- Scermino, L.: “Effetto del pH sulla micellizzazione di tensioattivi zwitterionici N,N-dimetilalchil-ammino ossidi a catena lineare e ramificata” (2019).

PhD in Chemical and Molecular Sciences

- De Santis, A.: “Effect of polyunsaturated fatty acids on the structure and dynamics of lipid bilayers and on their interaction with peptides” (2018).
- Perfetti, M.: “Increasing the Deposition Efficiency of Perfume Ingredients in Liquid Detergents.” (2018).
- Fabozzi, A.: “Design, formulation and characterization of anhydrous/highly concentrated surfactant mixtures” (2019).

U.O. Pavia

Bachelor in Biological Sciences (Laurea triennale)

- Paganelli, G.: “Curcumina, estrazione del principio attivo e tecniche molecolari cristallografiche" (2020).

Bachelor in Biotechnologies (Laurea triennale)

- Gilardenghi, J.C.: "Analisi Termica (TG-DSC): fondamenti, strumentazione ed esempi pratici" (2019).

Bachelor in Chemistry (Laurea triennale)

- Lecchi, A.: “Ematite come anodo in batterie al litio: sintesi e prestazioni elettrochimiche” (2017).
- Preda, G.: “Rilascio di farmaci anionici mediato da nanoparticelle di LDH (Layered Double Hydroxides)” (2017).
- Romani, L.: “Studio dell’influenza del tipo di plastificante sull’invecchiamento di film a base di PVC flessibile” (2017).

- Colombi, S.: “Sintesi e Caratterizzazione di un ossido perovskitico per celle fotovoltaiche: la ferrite di bismuto BiFeO3” (2018).
- Davino, S.: “Materiali bidimensionali per batterie a ioni litio e sodio” (2018).
- Fantozzi, E.: “Gli Smart Memory Polymers (SMPs): una versatile categoria di materiali” (2018).
- Foini, L.: “Materiali polimerici a memoria di forma: recenti sviluppi per la loro attivazione e applicazione” (2018).
- Morina, R.: “Fattori che influenzano la solubilità dei cocristalli tra principi attivi farmaceutici e coformers” (2018).
- Rosa, C.: “Ruolo di Ti e Mo nell’ottimizzazione dell’ossido elettrocromico WO3 per Smart Windows” (2018).
- Tartaglione, A.: “Nanomateriali catodici e anodici per applicazioni in batterie al litio ottenuti mediante Solution Combustion Synthesis (SCS)” (2018).
- Zubani, M.: “Leghe ad alta entropia, potenziali candidati in ambienti corrosivi” (2018).
- Cozzolino, G.: “Metodi di indagine dei materiali catodici: Na0.67Fe0.425Mn0.425Mg0.15O2 ed Na[Ti0.03(Ni0.6Co0.2Mn0.2)0.97]O2 per batterie al sodio ad alta prestazione” (2019).
- Franco, C.: "Leghe a memoria di forma e loro applicazioni in campo biomedico" (2019).
- Gamba, S.: "Materiali per la transizione di fase per lo stoccaggio di energia: meccanismo ed esempi applicativi" (2019).
- Lovati, G.: "Meccanochimica: esempi di sintesi in chimica inorganica e organica" (2019).
- Mirani, D.: "Ossidi ad alta entropia: dal disordine strutturale alla proprietà funzionali" (2019).
- Nodari, D.: "Materiali catodici innovativi per batterie agli ioni sodio: NaNi0.5Mn0.5O2 e NaNi0.33Co0.33Mn0.33O2" (2019).
- Salinelli, M.: "Influenza della energia meccanica sulle reazioni allo stato solido. Fattori sperimentali e casi di studio" (2019).
- Suppini, S.: "I Ferrati: preparazione per via chimica ed elettrochimica. Applicazioni in campo ambientale" (2019).

Master in Chemistry (Laurea magistrale)

- Gioventù, M.: “Preparazione e caratterizzazione chimico-fisica di materiali innovativi a base boroidruri per lo stoccaggio di idrogeno allo stato solido” (2017).
- Spada, D.: “FeNb11O29, emergente materiale anodico per batterie al litio ad alte prestazioni” (2018).
- Curti, V.: “Ossidi ad alta entropia (HEO) come materiali ceramici avanzati con enormi potenzialità” (2019).
- Gazzola, G.: “ZnFe2O4 puro e sostituito: un materiale dalle enormi potenzialità in ambito biomedico” (2019).
- Leccardi, F.: “NaMn0.5Ni0.5O2 puro e drogato (Ti, V e Cu) per il miglioramento delle prestazioni elettrochimiche” (2019).
- Nuti, M.: “Effetto delle sostituzioni in Na0.44Mn0.5Fe0.5O2 come catodo per batterie a ioni sodio” (2019).

- Ruffo, A.: “Nanoferriti di gadolinio come materiali innovativi per la cura non invasiva delle neoplasie” (2019).
- Ambrosetti, M.: "Sintesi e caratterizzazione di elettroliti solidi e liquidi per batterie al sodio" (2020).

Master in Pharmaceutical chemistry and technology (Laurea magistrale)

- Camussi, I.: “Generazione di ossigeno singoletto mediante g-C3N4 e sue applicazioni in sintesi organica” (2018).
- Monteforte, F.: “Intercalazione di farmaci poco solubili all’interno di idrossidi a doppio strato (LDH)” (2018).
- Schembri, D.: “Funzionalizzazione e caratterizzazione chimico-fisica di nanotubi di halloysite come possibile eccipiente di una forma farmaceutica solida” (2018).
- Chierici, R.: “Preparazione di nanotubi di halloysite funzionalizzati come eccipienti di forme farmaceutiche solide (insulina e tetraciclina cloridrato)” (2019).
- Flamini, L.: “Preparazione e caratterizzazione chimico-fisica di nanotubi di halloysite funzionalizzati come eccipienti per farmaci antistaminici” (2019).
- Nardini, M.: "Nuovi eccipienti per farmaci contro il dolore severo in Arnold chiari e siringomielia: preparazione e caratterizzazione chimico-fisica del composito tramadolo-nanotubi di halloysite" (2019).
- Belloni, G.: “Progettazione e caratterizzazione chimico-fisica di formulazioni innovative no smoking” (2020).
- Marino, S.: “Progettazione e caratterizzazione chimico-fisica di sistemi innovativi termosensibili per il rilascio di molecole bioattive" (2020).
- Montagna, I.: “Formulazioni innovative per la veicolazione orale di farmaci peptidici: preparazione e caratterizzazione chimico-fisica" (2020).
- Paternieri, M.: “Preparazione e caratterizzazione termoanalitica di sistemi farmaceutici a rilascio modificato a base di acidi grassi” (2020).

Master in Advanced Biotechnologies (Laurea magistrale)

- Guagliano, M.: “Layered double hydroxides: una strategia efficace, innovativa e sicura per il rilascio di farmaci poco solubili” (2019).
- Stancampiano, S.: “Convalida di metodi analitici chimici e microbiologici nell’ambito di un technology transfer di un prodotto farmaceutico” (2019).

Master in Pharmacy (Laurea magistrale)

- Pattonieri, U.: “Vaccini orali estratti da colture agricole” (2019).
- Yosef, G.G.: “Nanotubi di halloysite per il trasporto e il rilascio controllato di principi attivi” (2019).
- Sopa, A.D.: “Nanotubi di halloysite per la veicolazione di antibiotici” (2020).
- Tedesco, C. “Attività antibatterica di sistemi termosensibili a base di polimeri e acidi grassi" (2020).

U.O. Scuola Normale Superiore Pisa

Master in Materials and Nanotechnology (Laurea magistrale)

- Sagresti, L. “Structure and dynamics of a dye-labeled lipid in a model membrane bilayer: a computational study” (2019).

PhD in Methods and Models for Molecular Sciences

- Akhunzada, M. “Understanding molecular phenomena and mechanisms occurring in the lipid membranes through molecular dynamics simulations” (2019).

U.O. Siena

Bachelor in Chemical Sciences (Laurea triennale)

- Brcina, H.: “Rilevamento di attività antropica nel sito archeologico di Carlappiano (LI)” (2017).
- d’Ettorre, A.: "Modellazione dell’acido caffeico e del diidrossindolo su TiO2: valutazione mediante DFT del loro ruolo come sensibilizzatori per celle fotovoltaiche DSSC di tipo II" (2017).
- Filippeschi, O.: “Indagine su campioni di etanolo contaminato prodotto in un impianto di distillazione” (2017).
- Guerrini, M.: “Caratterizzazione delle componenti inorganiche di suoli ad uso agricolo nell’area del Monte Amiata” (2017).
- Leti, R.: “Studio della calcite (CaCO3) come agente di decontaminazione di As nelle acque” (2017).
- Obissi, O.B.: “Analisi delle proprietà strutturali e dinamiche di derivati stilbenici, da misure di risonanza magnetica nucleare in una e due dimensioni” (2017).
- Tiburtini, G.A.: “Analisi LCA (Life Cycle Assessment) di processi di smaltimento della frazione organica dei rifiuti: confronto fra compostaggio industriale e compostaggio domestico” (2017).
- Baglieri, A.: “Ottimizzazione di metodi di estrazione e quantificazione del solanesolo da matrici vegetali” (2018).
- Bisozzi, F.: “Analisi della stabilità dei glicoalcaloidi α-tomatina e deidrotomatina in relazione a stress termici dei preparati ottenuti da Solanum lycopersicum, L.” (2018).
- Boldrini, A.: “Valutazione dei profili ambientali di sistemi di conversione di energia solare basati su Biosensibilizzatori” (2018).
- Bonfrate, S.: “Studio di complessi del Cu con aza-crown ethers sostituiti attraverso metodi ab-initio” (2018).
- Cangeloni, L.: “Decontaminazione di acque contenenti As attraverso la co-precipitazione con CaCO3” (2018).
- Charaf, R.: “Proton-coupled electron transfer at TiO2 interfaces” (2018).
- Favilli, G.: “Sistemi di drug delivery per il targeting tumorale” (2018).
- Ferri, E.: “Caratterizzazione chimico fisica di liposomi rivestiti con polisaccaridi” (2018).
- Marisi, G.: “Analisi chimico-fisica delle frazioni argillosa e sabbiosa di suolo contaminato con arsenico” (2018).

- Morandi, M.: “Studio UV e NMR sulla reazione tra acido caffeico e DPPH” (2018).
- Pratelli, T.: “Studio NMR di birre artigianali e industriali: caratterizzazione qualitativa e quantitativa” (2018).
- Scartoni, A.: “Studio di provenienza di ceramiche antiche attraverso spettroscopia XRF” (2018).
- Pesci, M.: “Green metrics for the environmental sustainability analysis of innovative solar cells based on fully organic sensitizers” (2019).
- La Capra, M.: “Study on the mechanical decomposition of ldpe and bio-plastic bags in sea wate” (2020).

Master in Health Biology (Laurea magistrale)

- Rocca Semeraro, L.R.: “Positività all’alcolemia negli incidenti stradali nel 2017 a Siena e ruolo dei differenti metodi d’indagine diagnostica” (2017).

Master in Chemistry (Laurea magistrale)

- Jodeiri Iran, K.:" Synthesis and physicochemical characterization of functionalized magnetic nanoparticles for enzyme immobilization" (2017).
- Pashaei, R: “Analysis methods for microplastics in Urmia Lake, Iran” (2017).
- Rostom, H.G.K.A.: “Synthesis and characterization of liposomes containing nutraceutical compounds: tyrosol, hydroxytyrosol and oleuropein” (2017).
- Coppola, C.: “Design of novel organic hole transport materials for efficient perovskite solar cells” (2018).
- Danzi, M.: “Characterization of nutraceutical components in flours from cereals and legumes” (2018).
- Lazar, E.: “Analysis of capsaicin-protein recognition processes and capsaicin dynamics, by spectroscopic studies” (2018).
- Nasirzadehroshenin, F.: “Identification and quantification of microplastics in sediments of the Elsa River, Italy” (2018).
- Chakraborty, A.: “In vitro dissolution studies of poorly-water soluble drug fenofibrate incorporated in amorphous solid dispersion formulations and self-nano emulsifying drug delivery system (SNEDDS)” (2019).
- Pòta, L.S.: “Spectroscopic characterization of functionalised benzofulvene molecules for decontamination of heavy metals” (2019).
- Pourmozafari, A.: “Spatial analysis of microplastic pollution in Tuscan rivers” (2019).
- Saleh, V.: “Chemometric analysis of process variables and products in fluid catalytic cracking” (2019).
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- Ferrara, N.: "Study of the geothermal resource for the investigation of suitable technological solutions aimed at the minimization of the environmental impact in energy production, aided by LCA analysis" (2017, XXXIII ciclo).
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RESEARCH PROJECTS

1A – Amorphous Magnesium-Calcium-Phosphate nanoparticles: effect of pH, Mg^{2+} and complex fluids on their formation and crystallization

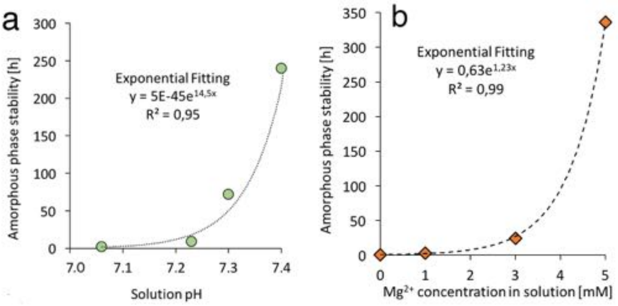
R. Gelli, M. Tonelli, M. Bonini, F. Ridi, P. Baglioni

Aims

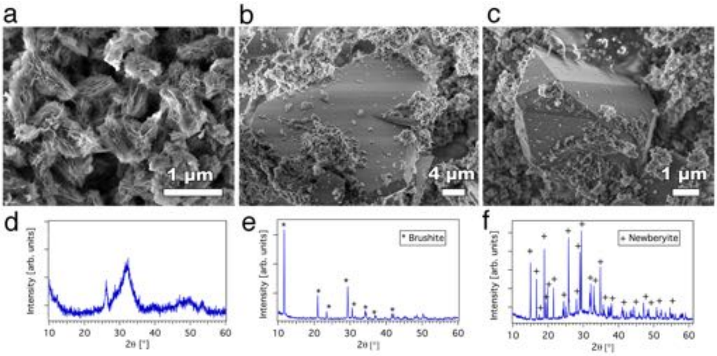
Recent investigations showed that the secretion of calcium and phosphate ions from humans' distal small intestine into the lumen leads to the formation of Amorphous Magnesium-substituted Calcium Phosphate nanostructures (AMCPs), which trap macromolecules, such as antigens and bacterial peptidoglycan, and transport them to the immune cells of the intestinal tissue [1]. The formation mechanism and the factors affecting AMCPs' stability are thus relevant topics, as a deeper understanding would clarify the role of these newly-discovered particles and the potential pathological implications.

Results

The investigation aimed at elucidating the role of pH and Mg^{2+} concentration on the structural properties and the stability of synthetic analogues of endogenous AMCP particles, so to investigate how an alteration in these parameters may affect the fate of the nanostructures, and potentially their role in the organism. [2] We performed the synthesis of the particles at physiological temperature by readapting a protocol from the literature, consisting in the co-precipitation of Ca^{2+} and Mg^{2+} from phosphate buffers, using an excess of magnesium and phosphorous with respect to calcium to favor the formation of AMCP. The effect of subtle pH differences (in the physiological range) was explored, by using different H2PO4-/HPO42- molar ratios, but keeping constant the total phosphate concentration. Precipitates were characterized with a multi-technique approach in terms of morphology, crystallinity, chemical composition and porosity, obtaining AMCPs with features matching those found in the gut. The stability of the prepared particles was then tested by re-dispersing them in aqueous phosphate buffers at different concentrations, pHs, and at different Mg^{2+} concentrations. We found that subtle differences in these three parameters strongly affect the lifetime of the amorphous phase and the nature of the newly-formed crystalline material. In particular the crystallization time of the particles show an exponential trend both with the pH and the Mg^{2+} concentration.



The nature of the formed crystalline material is also affected by these parameters. The concentration of Mg^{2+} not only affects the lifetime of the amorphous phase, but also the type of crystalline phase to which AMCP converts. These results can be explained in terms of the calcium phosphates solubility and of the effect of magnesium ions on the calcium phosphates crystallization rate. Due to these effects, at low Mg^{2+} concentration we observe the conversion of AMCP to poorly crystalline hydroxyapatite. When Mg^{2+} concentration in solution increases, brushite is the phase that finally precipitates. When $[Mg^{2+}] = 5$ mM, AMCP particles are extremely stable and $Mg^{2+}$is so abundant in solution that a magnesium phosphate, MgHPO4_3H2O, is the first crystalline phase that precipitates.



In the attempt of making a step towards the in vivo conditions, we synthesized AMCPs in a commercial simulated intestinal fluid, which contains sodium taurocholate and lecithin [3]. The influence of their self-assembly on the formation of AMCPs was investigated, as well as their effect on the particles' nanostructure and stability. We found out that the presence of lecithin and taurocholate prolongs the lifetime of the amorphous phase, delaying the conversion to a crystalline phase. The morphology of AMCPs in the two synthetic media is also different, as the particles forming in the SIF are smaller and less aggregated than in water. We also observed that AMCPs are able to incorporate the organic molecules present in the fluid in a time-dependent manner, as shown by means of both FT-IR spectroscopy and thermal analysis. We also studied the formation of AMCP in the presence of proteins, such as the Moringa protein, having well-known nutraceutics properties, with the aim to produce a composite combining the beneficial properties of Moringa with the effects of AMCP on the immune system. Finally, the investigation of AMCP formed in the presence of hydrogel-forming mucins, abundant in the intestine, is still an ongoing study.

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1A – Azahelicenes in SERS and fluorescence spectroscopy

F. Fontana, B. Bertolotti, R. Pelosato, I. Natali Sora,
M. Tommasini (Politecnico di Milano)

Aims

A significant current research activity aims at developing efficient probes of molecular structure, suitable for drug detection, where sensitivity to specific chiral targets is desired, usually at low concentrations. The quest for simpler and more cost effective devices for therapeutic drug monitoring prompted us to try to exploit the interesting optical properties of azahelicenes. Nanostructured gold thin films can be fabricated by controlled pulsed laser deposition (PLD) to realize surfaces with uniform morphology and optimized plasmon resonance, to be employed as plasmonic substrates in Surface Enhanced Raman Scattering (SERS) spectroscopy. By binding onto these surfaces a thin layer of an azahelicene derivative, its interaction with the drug to monitor would give rise to easily detectable changes in the spectroscopic properties of the helicene, thus overcoming any problem of low detectability of the drug itself.

Results

The scope of the work was at first to test the feasibility of covalently bonding a helicene moiety to a nanostructured gold surface and to verify the chemical stability and spectroscopic activity of such functionalized surfaces. To this purpose, we employed the easily accessible azahelicene (1), which, however, is not enantiomerically stable in solution at r.t., and we endowed it with the appropriate sulfur-containing functionality for anchoring the substituted azahelicene moiety to gold surfaces (2). 5-aza[5]helicene (1) was treated with 6-bromo-1-pentene in the presence of TTMSS and AIBN in toluene at 80°C so as to introduce a chain terminating with a double bond. This latter is then reacted with thioacetic acid to introduce a thioester functionality (2) (Fig.1), which can be removed in situ in the presence of the nanostructured gold surface by basic treatment.

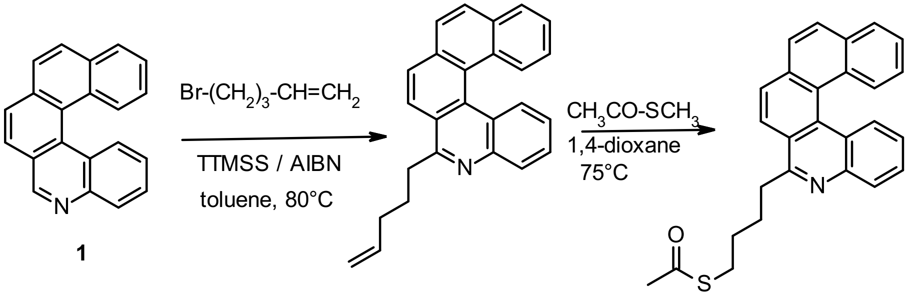

Fig. 1. Introduction of a thioester functionality onto 5-aza[5]helicene.

The intensities of the recorded SERS signals were uniform across the substrate, and a remarkable reproducibility of the SERS peaks was observed for the three different functionalization methods. In addition 5-(6-(5-aza[5]helicenyl))pentane-1-thiol on gold shows sharp lines at 436, 659, 675, 863, 1038, 1204 cm^{-1}. These are useful features of the SERS spectra produced by the helicene-functionalized gold substrates that would facilitate detecting spectroscopic changes in the helicene signals upon effective interaction with a given drug.

In addition to SERS, we have also investigated the fluorescence behavior of the helicene-functionalized plasmonic substrates. As shown in Fig. 2, by adopting a second experimental set up, with exciting laser radiation at 458 nm, we can collect the fluorescence originating from the helicene mono-layer anchored on the gold surface, while no SERS peaks are observed. This happens because the 458 nm excitation lies far away from the plasmon resonance of the gold substrates.

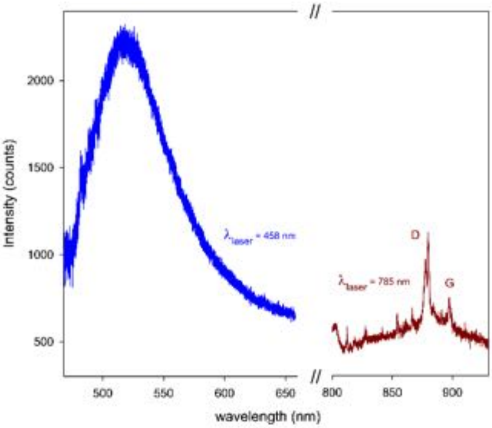

Fig. 2. Comparison of fluorescence (blue line) and SERS (brown line) spectra of functionalized gold substrate, depending upon the excitation line used to illuminate the substrate. Fluorescence and SERS spectra are reported on a common intensity scale, in order to compare the relative strength of the two phenomena.

With these results in hand, ongoing research is now aimed at realizing these surfaces with enantiomerically stable 5-aza[6]helicene, in order to realize a device which can discriminate chiral substances. Varying the length of the spacer chain should moreover enhance the SERS activity (shorter chain) or the fluorescence (longer chain). Varying the structure of the helicene could make it more fit to interact with the functional groups of specific drugs

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1A – Breaking Bad Biofilms - Innovative Analysis and Design Rules for Next-Generation Antifouling Interfaces, ITN-MSCA Project Number: GA-2018-813439, 2019-2022

N. Ditaranto, R.A. Picca, G. Palazzo, N. Cioffi

Aims

Biofilms, i.e. communities of micro-organisms that attach and grow on a solid surface, cause about 80% of infections in humans and disinfectants rarely succeed in destroying them. They cost European economy billions of euro annually. The BREAK BIOFILMS Training Network aims to solve this issue by training the next generation leaders. They will understand the (bio)physicochemical mechanisms of biofilm formation, be able to produce technology for detecting and identifying biofilm formation with extreme sensitivity and develop next generation biocides for preventing and destroying biofilms in industrial and biomedical areas. This integrated strategy from biofilm detection to destruction that builds on key innovations from the partner labs, is globally distinctive and promises significant progress. The network brings together world leaders in sensors, cell imaging, microbiology, interfacial engineering and nanoformulation from 6 universities, 9 companies, a research centre, and a Business and Innovation Centre. Thus, it is ideal to provide technical, industrial and business training to 15 ESRs and support the missions of the industry partners who will provide deep insights into the most pressing and impactful challenges. The graduates will be ideally placed to enter and support existing European industry across a number of different sectors (biomedical, food, antimicrobials). However, they will also be capable of creating new businesses thanks to a combination of in depth training in entrepreneurship and direct experience of establishing and running a virtual company as part of the training network. Beyond the trained researchers, this project will produce technologies that will enhance the productivity of European industry, create intellectual property with a strong probability of commercialization and improve the health and well-being of European citizens by minimizing infection rates and the inappropriate use of ineffective biocides that is leading to resistance.

Results

Copper, silver and, more recently, zinc oxide nanophases, are electrosynthesized or produced by physical techniques such as laser ablation or ion beam sputtering. They are used as nano-reservoirs able to exert a controlled release of bioactive metal ions. It was shown that this release is controlled thanks to nanoparticles (NPs) structure, stabilized and/or incorporated in various polymeric matrices. These materials exhibit antimicrobial properties against a wide variety of microorganisms, even antibiotic-resistant ones. This bioactivity can be modulated simply by tuning NPs loading, or by modifying nanoparticle structure. All nanomaterials, both colloidal and composite ones, are being characterized both morphologically and spectroscopically. Furthermore, systematic correlation between biological activity and controlled metal ion release has also been demonstrated. An interpretation of the controlled release process was proposed, representing a standard for industrial literature more than ten years after its publication, still receiving several dozen citations every year. We also monitored *in situ* the anti-biofilm properties of antibacterial nanocomposites through the integrated use of ATR-IR spectroscopy and AFM microscopy.

The analytical characterization of these materials also involved experiments (i.e. electron microscopy, Single Particle-Inductively Coupled Plasma-MS, etc.) aimed at excluding the release of potentially toxic nanophases in contact media. The development of nanomaterials is extremely interesting for a number of technological applications, such as the production of antimicrobial food packaging, the development of antibacterial coatings for biomedical equipment, the fabrication of textile products or non-woven fabric matrices, polyurethane foams and leathers/leatherettes of industrial importance, conservation of cultural heritage stones, etc.

The scientific, technological and industrial relevance of the activity is testified by several publications and grants received for the research activities. In fact, the budget for this research unit in the referenced period is more than 1 million €. Among the most recent project activities: a four-year H2020-MSCA-ITN-2018 Break Biofilms project is started in 2019, specifically dedicated to monitoring and fighting biofilms and antibiotic-resistant microorganisms. Other national projects have been positively evaluated and the relevant grant agreements are presently under definition.

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1A – Comparative Life Cycle Assessment study on environmental impact of oil production from micro-algae and terrestrial oilseed crops

E. Busi, S. Jez, D. Spinelli,
A. Fierro (University of Naples Federico II), R. Basosi

Aims

Attributional LCA is applied to satisfy two goals: i) to evaluate the environmental hot spots in site-specific production chain of biodiesel from terrestrial oil seeds and micro-algae feedstock; ii) to evaluate quantitatively, utilizing primary data, if the first generation of bio-fuels is environmentally unfavorable respect to the third generation. Furthermore, the study explored the possibility to enhance the environmental performances of micro-algae oil through the application of renewable energies

Results

This analysis has used average primary data of two crops (rapeseed and sunflower) grown in the years 2012-2014, using traditional farm practices, in experimental plots located in Campania Region (Southern Italy). The total cultivated area consists of 5 ha of flat land with sandy-loam soil texture. The algae cultivation stage has the largest electricity requirement for air and nutrient pumping into the raceway pond, water pumping due to evaporation lost and pumping algae slurry for harvesting stage.
For these reasons, two alternative energetic scenarios have been evaluated besides the base case of Italian electricity mix (scenario1): use of photovoltaic technology (scenario 2) and use of biogas produced from micro-algae cake (scenario 3).
In Fig.1 it is reported the comparison of the three scenarios calculated with ReCiPe Midpoint Method for micro-algae oil production with different energy sources:

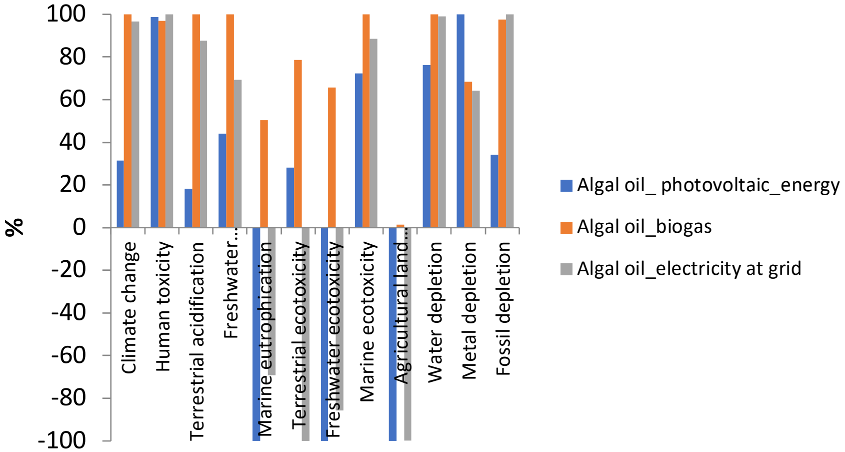

Fig. 1 - Comparison among electricity from biogas, photovoltaics, italian electric mix).

The scenario with photovoltaic energy seems to be the most environmentally convenient in almost all the impact categories while the scenarios with biogas and conventional electricity are similar in five categories even if biogas is the worst. The difference between biogas and conventional electricity increases in the impact categories where the influence of the credits from the avoided product “soybean meal”, highly affects the results.

A decrease of about 68% in Climate Change and 66% in Fossil Depletion can be calculated if the energy source “Italian mix” is substituted by photovoltaic system. Also in the context of sensitivity analysis, another key parameter appears to be the avoided product. In fact the huge amount of residual biomass in the micro-algae oil production, which was considered as substitute of soybean meal, strongly affects many impact categories.

For this reason scenario 3, where the biomass was used to produce biogas was penalized. Therefore, the convenience of using the residual cake for biogas production or as animal feed was evaluated moving the residual cake out of the system boundaries, as compost for 1 and 2. In Fig. 2 the results of the comparison with ReCiPe Method are shown. It is evident that with these last assumptions the biogas scenario improves its position in the trend.

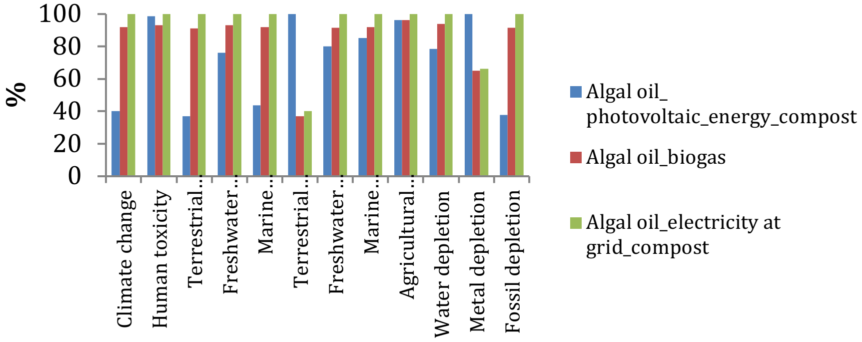

Fig. 2 -Comparison of three scenarios for micro-algae oil production with different destination of residues for Scenarios 1 and 2

Despite their high potential as sustainable energy feedstock, micro-algae are not yet competitive with the traditional oil crops in both economic feasibility and environmental impact. The main achievement of this study is to have a confirmation of these findings by an LCA analysis based on primary data coming from a case study of an integrated biorefinery. A further important result is that the use of renewable technologies as photovoltaics and biogas self-production could increase the competitiveness of micro-algae oil reducing its demand of non-renewable energy sources.

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1A – Controlled deposition of gold NPs on plastic surfaces

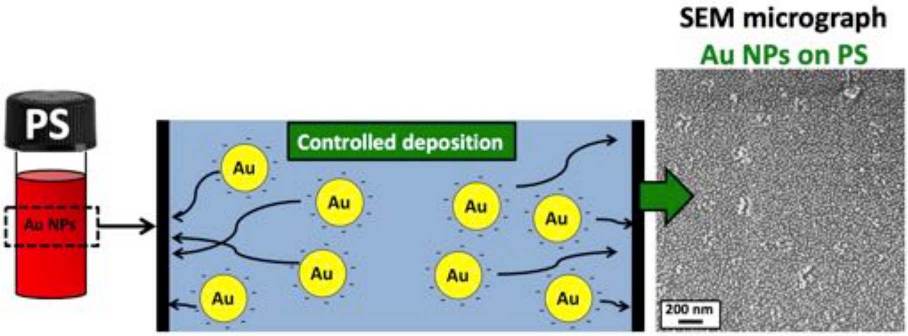
G. Ferraro, E. Fratini, P. Baglioni, V.L. Rossi, A. Sanesi**
*(*BioMérieux Italia S.p.A., Bagno a Ripoli, Italy)*

Aims

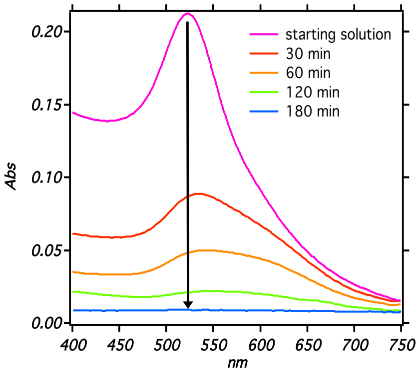
The controlled deposition of gold nanostructures on disposable plastic surfaces is a big challenge in different fields, for the production of optoelectronic devices, solid phases for biomedical or analytical applications. In an immunological assay, gold nanoparticles (NPs) can increase the efficiency of the antibodies bound to the solid phase, due to the interaction of the -SH fragment of the antibodies with the metal.

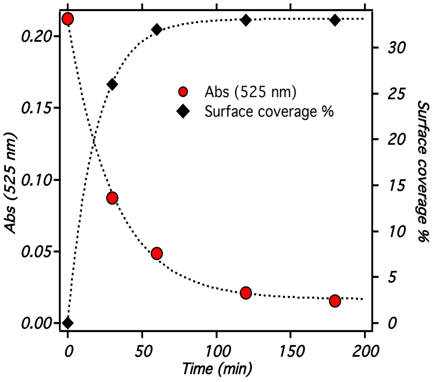
Results

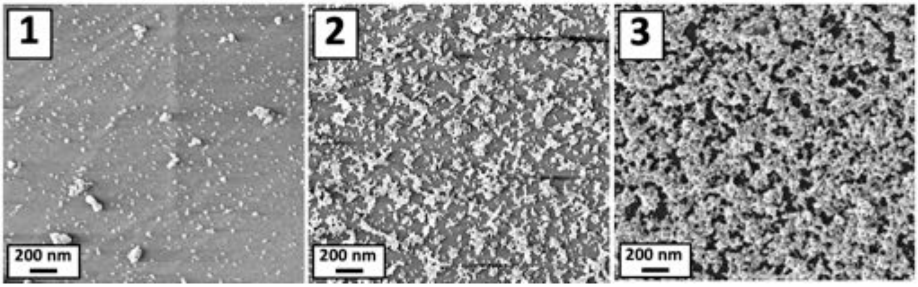
The migration of gold NPs from the solution to the plastic surface is induced and controlled changing the incubation conditions. In this approach, citrate-capped gold NPs interact directly with the plastic surface and no binding molecules or polymers are necessary to anchor the nanoparticles to the plastic surface.



The entire process can be optimized in terms of incubation time, temperature of the coating step and starting concentration of the gold NPs dispersion to tune the coverage degree of the treated substrate.







Moreover, changing the size of gold nanostructures, it is also possible to obtain surfaces with different morphologies and gold concentration.

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1A – Eco-friendly alkali activated materials for conservation of cultural heritage and repair of modern reinforced concrete buildings and infrastructures

L. Coppola[1,2], D. Coffetti[1], E. Crotti[1], G. Gazzaniga[1], M. Cabrini[1], S. Lorenzi[1], A. Felici[3], T. Pastore[1]
[1]Department of Engineering and Applied Sciences – University of Bergamo – Italy;
[2]Material and Construction Institute – SUPSI – Lugano (CH);
[3]Opificio delle Pietre Dure, MiBACT; FirenzE – Italy)

Aims:

In recent years, the international scientific community has been exponentially concerned with alkali-activated materials (AAMs). It is now apparent that it is possible to use AAMs for both the realization of new artistic works and restoration and conservation of cultural heritage. Indeed, the inorganic nature of AAMs allows it to be widely used for the preservation of brick and natural stones. In this context, their use is quite vast and disparate: production of artificial stone substitution, filling of gaps, adhesives, bonding agents for repair mortars, surface consolidations. Moreover, just over one hundred years after the first use of reinforced concrete, it is increasingly common to be faced with repair and conservation of modern reinforced concrete buildings and infrastructures, which - because of their historical, artistic and architectural value - must be understood as monumental goods to be protected and preserved and where aspects such as color and texture are fundamental as structural and durability requirements. In modern reinforced concrete structures, restoration and conservation have to take into account, in addition to the traditional elastic and mechanical issues, also the respect of aesthetic instances such as color and texture. Finally, in order to reduce the environmental impact produced by cementitious materials, repair works need mortars and concretes made by environmentally-friendly binders based on AAMs capable to reduce both CO_2 emissions and consumption of non-renewable environmental resources.

The first aim of this experimental research is to formulate AAM mortar with elasto-mechanical characteristics comparable to those of natural-hydraulic mortars, often used in the field of restoration. AAM mortars applicable to spatula based on ground granulated blast furnace slag and alkaline powder activators (sodium metasilicate, potassium hydroxide and sodium carbonate) with the addition of additives - modified cellulose, starches, calcium oxide and fibers - for improving the rheological and physical characteristics were produced. Mixtures of two silica aggregates of different nature were used, with mass ratios of 3: 1 and 2: 1 with respect to the binder. Bulk density, entrapped air, set and hardening time, compressive and flexural strength, elastic modulus, adhesion, and capillary absorption were measured. Finally, using the three-dimensional CreaForm GO! SCAN20 scanner and the 3D FormLabs printer, epoxy resin was created of several decorative elements and then a direct silicone cast for the use of decorative elements in AAM mortars.

The second aim of this research is to evaluate, through an engineering-conservative approach, the possibility of using a AAM binder for the production of pre-mixed thixotropic mortar that complies with the requirements of UNI EN 1504-3 and those imposed on cultural property with the aim of providing a mixture that ensures adequate physical and elastic performances and is compatible with the traditional aggregates and pigments used on site to achieve the desired aesthetic yield. The experimental work envisaged the study of two precursors, metakaolin and blast furnace slag, suitably activated with calcium hydroxide and various solutions based on sodium and potassium silicates and hydroxides. All the mortars produced have been subjected to fresh and hardened tests. In addition, the influence of adding additives - modified calcium oxide, starch and cellulose - and glass fibers was studied on the performance of the AAM compounds. Finally, the possible use of powder and filler activators and colored aggregates was evaluated in order to achieve the desired texture and color.

Results:

From the analysis of the experimental data, it can be stated that AAM mortars can be used in the field of cultural heritage for conservation and repair with environmental benefits such as use of secondary raw materials, reduction of CO_2 emissions and reduction of energy consumption for the production of binders. Furthermore, it has been demonstrated that, by using appropriate pigments and colored aggregates, it is possible to attain the aesthetic yield and the desired texture. Finally, the proof of decorative elements with casting technology inside molds has not shown any problem in terms of elastic-mechanical, physical and aesthetic characteristics, showing higher properties than conventional gypsum even with low humidity environments.

In the field of repair of modern reinforced concrete structures, from the analysis of the experimental data it is clear that slag-based binder allows to achieve the desired elastic and physical performance, whereas metakaolin is not suitable for this type of application except as a minor part in blends. In spite of the fact that the manifold composite has a very large dimensional contractions, thanks to the reduced elastic modulus, good tensile strength and the use of adequate shrinkage reducing admixtures, there are no detachments or cracks due to the application on different types of support. As for the possible leaching of alkaline ions, at present there is no efflorescence or release of pollutants on the original media.

At present, geo-polymeric mortars based on blast furnace slag seems to be an excellent alternative to the use of cement in the recovery of both cultural heritage and modern reinforced concrete architectures of historical-artistic relevance.

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1A – Energy saving in LT/MT transformers

S. Maranghi, R. Basosi, E. Busi

Aims

In Europe, the number of Medium Voltage/Low Voltage (MV/LV) transformers in 2005 amounted to over 4.5 million. Over 430000 units (for a total output of 79 GVA) are installed on the distribution network in Italy. Market estimates foresee up to 2020, an annual growth rate of around 2% and a replacement rate that will reach 4%. The MV/LV transformer is then, given the annual sales volumes, subject to Directive 2009/125/EC (Eco-design): in May 2014 the implementing entered into force, which defines the minimum efficiency requirements that, starting from 2015, the MV/LV transformers placed on the market should have. This allows to estimate a saving of 16.2 TWh per year by 2020.

After 1 July 2015 it will not be possible to place on the market transformers not fulfilling the minimum requirements. Energy savings become important particularly for the reduction of the environmental burdens of grid and buildings. Power Transformer losses represent approx. 2.5% of total EU energy consumption. By 2020, savings of approximately 16 TWh/year would be achievable with the new regulation. The innovation in this project consists in realizing the continuous magnetic core (TANC) by wrapping a strip of amorphous magnetic material directly around the primary and secondary windings, creating a process similar to matassing in the textile sector. In this work, these innovative production process and product are analyzed by a comparative LCA (Life Cycle Assessment) assuming the conventional transformer as a reference.

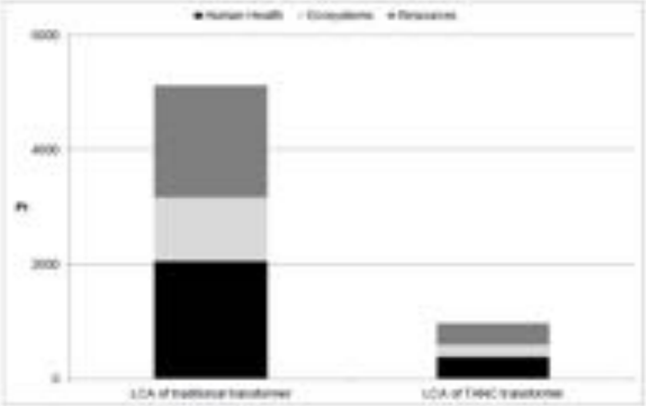
Results

The main differences between the two production processes are related to the first three steps of the manufacturing phase and to the nature of the primary raw materials, i.e. steel. In the innovative transformer, the steel that is employed in the core fabrication is an amorphous steel. Whereas, in the traditional electrical transformer the core is manufactured with an “oriented grain steel”. The amorphous steel does not require many treatments, therefore, the energy and raw materials consumption during the fabrication of the core is considerably lower, the wastes produced during the process are eliminated and the transport is made by freight. Furthermore, for TANC transformer, it is assumed a complete automation. This could lead to a significant increase the number of transformers built per day, going from the current 18 pieces/day (for the traditional transformer) to 50 pieces/day. The use phase is the same for both systems and the main difference between them is only the electricity transformation yield. In order to model the use phase some scenarios were performed, considering the information and data concerning a traditional transformer, adapting them to the innovative TANC system.

As reported in literature, the use phase and the energy losses of the transformer during its life time are the main environmental and economic issues that must be taken into account for a comprehensive LCA analysis. Generally, these losses are of two types: i) losses in the loading phase and ii) no-load losses, with the latter clearly higher than the first ones. Therefore, the transformer efficiency can be calculated as follows:

$\eta = (P \times \cos\phi \times \xi) / (P \times \cos\phi \times \xi + Po + Pc \times \xi^2)$

where η as efficiency, P as transformer power in kVA,ξ as applied load percentage, Po as “no load” losses in kW, Pc as load losses in kW Energy saving of a TANC transformer respect to a conventional one comes from its higher efficiency, with regard to no-load losses, which can be estimated as 0.6 kWh. Assuming 25 years as the transformer life-time, the estimated energy saving is relevant: 0.6 kWh x 24 hours/day x 365 days/year x 25 years = 131400 kWh. The differences between the environmental impacts related to the production phase of the electrical transformer are minimal (less than 1% for all the LCIA methods). The innovative TANC transformer does not show appreciable advantages in the production phase, despite the absence of waste during processing and the different kind of transportation. In contrast, considering the efficiencies and assuming a life time of 25 years for both transformers, the difference in electricity losses during the use phase is remarkable. The results and the comparison between the two whole life cycles, calculated with ReCiPe Endpoint method are shown in Figure.



The environmental benefit achievable due to the very good performances of the innovative TANC transformer could be the key issue for the improvement of future Italian and European electricity network and can contribute to the achievement of the energy efficiency goals in EU.

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1A – Environmental impact analysis applied to solar pasteurization systems

F. Rossi, M.L. Parisi, S. Maranghi,
G. Manfrida, R. Basosi, A. Sinicropi

Aims

Solar Pasteurization is a thermal process to disinfect water from pathogens using solar radiation in a cheap, reliable and sustainable way. Indeed, if water is warmed up to 85°C, bacteria are killed or inactivated almost instantly (Burch and Thomas, 1998). Two types of Solar Pasteurization systems are available in the market (Duff and Hodgson, 2002): Natural Circulation Systems (NCSs) and Thermostatic Valve Systems (TVSs). In this work, the eco-profiles of a specific NCS (modelled by Dainelli et al. (2017) and Manfrida et al. (2017)) and a TVS (tested by Carielo da Silva et al. (2016), Carielo et al. (2017)) have been compared considering several installation sites. In NCSs heat is collected thanks to a Solar Collectors (SCs) array and the consequent thermal dilatation of water allows a natural motion of the fluid. Thanks to the design of the piping system, water continues flowing through a recirculation system that brings the flow back to the SCs; for such reason temperature increases step by step until the desired temperature (85°C) is reached. In that moment the thermal dilatation of the fluid allows an exceeding volume to overtop in a discharge pipe bringing the disinfected water outside to a treated water reservoir. Because of the communicating vessels principle, the same amount of raw water enters inside the plant: first the inlet flow is warmed up by the treated fluid thanks to a regenerative heat exchanger; than it mixes with the recirculating water flow. This is very important because water would otherwise reach boiling conditions and the system would stop working. TVSs are based on the same disinfection principle but the control of outlet temperature is managed thanks to electronic systems called thermostatic valves (TVs). Even if this system seems simpler, it is less reliable than the NCS because TVs, such as any electronic device, are susceptible to failures and require electricity (which could be produced by photovoltaic). As the scope of Solar Pasteurization is to produce water in a sustainable way, Life Cycle Assessment (LCA) has been applied in order to estimate the environmental gain derived by solar energy and to point out which Pasteurization system is more sustainable. Furthermore, exergo-environmetal analysis has been performed to assess the environmental impact related to the exergy destructions inside the components of the NCS. Finally, some qualitative considerations related to their effectiveness in several socioeconomic conditions have been be done.

Results

The results of the LCA analysis show that the specific impact of the NCS per liter of treated water (0.30 mPt/l) is generally lower than the burden of the TVS (0.83 mPt/l) thanks to its higher productivity. The contribution of solar energy is significative to mitigate the environmental impact of this system; indeed, the environmental footprint of equivalent Pasteurization plants burning fossil fuels is estimated at least to 1.2 mPt/l. The exergo-environmental analysis allows the evaluation of the total environmental impact of the NCS. Nevertheless, the SCs represent a major contribution (45%) to the single score impact value. Furthermore, according to the results of the exergo-environmental analysis, most of the impact related to the exergy destructions is are due to the heat exchange irreversibility occurring inside them. The large-scale diffusion of NCSs would be very useful in countries, such as Somalia, where the problem of drinking water availability is particularly dangerous. These results and the description of the applied methodology.

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1A – ESPResSo - Efficient Structures and Processes for Reliable perovskite Solar modules

S. Maranghi, M.L. Parisi, C. Coppola, R. Basosi, A. Sinicropi

Aims

Perovskite solar cell (PSC) technology has significant potential to revolutionise the photovoltaics industry in Europe due to high efficiencies and the potential for short energy payback periods in comparison to other established PV technologies making them truly. The challenge is now to transfer this unprecedented progress from its cell level into a scalable, stable, low-cost technology on module level.

Therefore, the ESPResSo project will overcome the limitations of current state of the art devices by bringing the novel emerging hybrid organic-inorganic PSC technology to its next maturity level. Specifically, ESPResSo targets alternative cost effective materials, novel cell concepts and architectures, and advanced processing know-how and equipment to overcome the limitations of current state of the art technology.

Results

High performing cell architectures

High performance cell architectures will be pursued by controlling the formulation and crystal structure of the active perovskite material, and by additionally minimizing recombination losses in the perovskite absorber or at the interfaces with the selective contacts.

Low-cost materials

ESPResSo will also focus on (i) Hole Transport Layer (HTL), (ii) Electron Transport Layer (ETL) (iii) Alternative electrodes. alternative organic HTLs will be tested making use of new low-cost formulations of Spiro-family or conjugated polymers such as P3HT and PTAA, connecting the device performance to polymer characteristics such as its Molecular Weight (MW), after having recently demonstrated that a strong correlation exists between PSC performance and MW.

Similarly, organic (PEIE, fullerenes) and inorganic ETL materials (TiOx, SnOx, ZnO, AZO) will be evaluated as solution-processed or sputtered interface layers.

Carbon-based electrodes (including graphene and carbon nanotube hybrid structures) will be considered to replace the standard expensive Au electrode, while also improved device stability is expected.

Advanced atomistic, electrical and optical modelling

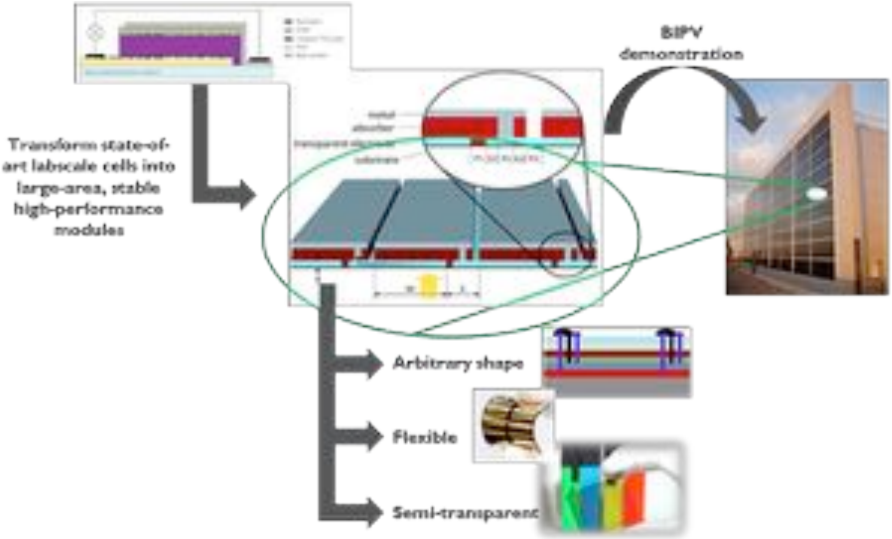
Advanced characterisation of these perovskite layers, including determination of optical constants with ellipsometry, photo- and electroluminescence, LBIC and Suns-Voc, on single films or in archetypical full device configurations will be carried out to identify the relationship between its optoelectronic properties and this variety of conditions and compositions.

Transition from lab-scale to large area processing

The development of advanced, stable and sustainable material for high PV performance, the use of advanced architectures for high performance modules and the definition and optimization of advanced processes for large-area solar module will thus continuously feed the development of advanced technology for stable, efficient and long-lived large area modules.

Sustainability

Continuous assessment of LCoE, carbon-footprint, energy-payback time, ecological impact and environmental toxicology, in the LCA frame (lead partner CSGI) will be done based on detailed data inventories for many components and fabrication process steps of innovative hybrid PV modules (glass-based and flexible substrate-based) to be employed as background processes for perovskite manufacturing processes.



Project ESPResSo outline

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1A – Immobilization of Trametes versicolor Laccase on modified magnetic Fe3O4 nanoparticles

J. Costa, M.C. Baratto, A.M. Atrei, R. Pogni

Aims

Use of enzyme in many biotechnological processes is a solution for environmentally friendly industry, they are eco-compatible, biodegradable and non-toxic to environment keeping the cornerstones of Green Chemistry. Laccase is a multicopper enzyme that use molecular oxygen as a co-substrate to oxide various compounds by a radical-catalyzed reaction mechanism. Although laccase is a very promising tool for industrial purposes, there are some disadvantages in its application considering a high production cost and low stability during storage.

The immobilization of Laccase represents a solution of this problem, because it's a convenient method for increasing enzymatic activity, operation stability and enabling enzyme reuse.

Magnetic Fe3O4 nanoparticles have been receiving an increasing attention in the field of immobilized enzymes due to their advantages: easy preparation, strong magnetic response, small size and easy separation from the reaction solution.

Results

Laccase from Trametes versicolor was immobilized on magnetic Fe3O4 nanoparticles. The nanoparticles were prepared by chemical co-precipitation of Fe3+ and Fe2+ ions. Then, the surface of nanoparticles was modified by the amino residual of APTES ((3-Aminopropyl) triethoxysilane) because the hydroxyl group of magnetic nanoparticles are able to react with the oxoethyl side chain in APTES. To extend the spacer and facilitate the covalent attachment of laccase, the amino group on the nanoparticles were linked with aldehyde groups by glutaraldehyde. On one hand, using glutaraldehyde as the arm of the spacer, the laccase has a better dispersion in the microenvironment, which allows more proteins to be attached to the carrier, and on the other hand, the higher mobility of the enzyme in the space, could facilitate the reaction with the substrate, resulting in the increase of the activity recovery.

Chemical-physical characterization of the magnetic nanoparticles was carried out using AFM (Atomic Force Microscopy), FTIR (Fourier Transform Infrared Spectroscopy), DLS (Dynamic Light Shattering), TGA (Thermogravimetric analysis) and Z-potential analysis. The activity of free and immobilized laccase was assayed by following the formation of the dye 2-amino-3-oxo-3H-phenoxazine-8-sulfonic acid.

Laccase was successfully immobilized on magnetic Fe3O4 nanoparticles, a yield of immobilization of about 75% was observed and the immobilized laccase was able to retain 100% of activity after 30 consecutive cycles of reactions.

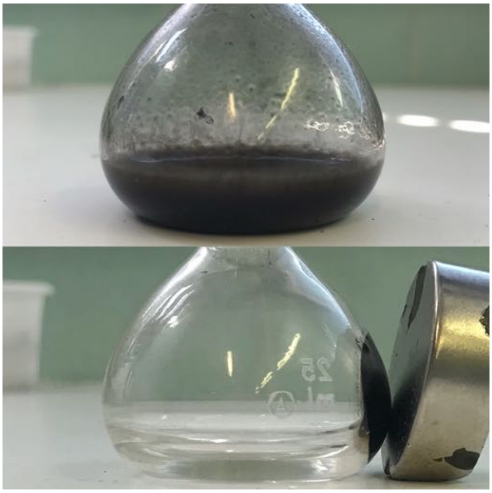

Fig.1: Separation of nanoparticles from solution with a magnet

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1A – Innovative carbon-based nanostructures for hydrogen and energy storage energy systems

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Aims

Ideation and preparation of novel carbon-based nanostructures and composites for solid-state H_2 storage; evaluation of their sorption properties; determination of the thermodynamic and kinetics characteristics of the sorption reactions. Preparation of carbon based materials for energy storage.

Results

Thanks to our intensive work in the last 2 years, we were able to demonstrate to the scientific community that alkali-cluster intercalated fullerides really constitute a novel class of materials for hydrogen storage, thanks to their proved capability to uptake reversibly high amounts of hydrogen via a complex chemisorption mechanism. We optimized the synthesis of Li, Na, and mixed Li-Na clusters intercalated fullerides, belonging to the families $Na_xLi_{12-x}C_{60}$ ($0 \le x \le 12$; we were the first group to explore these stoichiometries) and $Na_xLi_{6-x}C_{60}$ ($0 \le x \le 6$) by solid state methods, obtaining high purity and good reversibility.

The structural properties of the materials were clarified by means of in-situ neutron diffraction and the analysis of the Pair Distribution Function (PDF) obtained from high-energy synchrotron diffraction. The mechanism of hydrogenation was unveiled by Muon Spin Relaxation spectroscopy (µSR), a very powerful technique “able to see hydrogen” in the structures. Thanks to these two methods, we were able, for the first time in literature, to explain the chemisorptions mechanism leading to the hydrogenation of fullerene in these structure: Li atoms help the dissociation of the hydrogen molecules on the C structures, acting as catalyst and destabilizing agent, but then capture some hydrogen in the formation of LiH. Na atoms act as a more powerful catalyst and do not hydrogenate by themselves, but are able to decrease the dehydrogenation working temperature of the C structure. Thanks to our work, we demonstrate the importance to prepare mixed stoichiometries richer in the Li side to obtain good kinetic and thermodynamic properties. By coupled manometric - calorimetric analyses and thermogravimetric measurements, we proved that in these composites C_{60} covalently binds more than 5 wt% H_2 at moderate temperature and pressure, reaching properties similar to those of Mg hydride, the first generation material for hydrogen storage.

We also identified some strategies to further improve the absorption performance in this class of materials. For example, we succeeded to catalyze Li-fullerides with Ni, Pt and Pd nanoparticles, whose known activity towards hydrogen dissociation allows to increase the H_2 absorption up to 5.9 wt% H_2 and the absorption rate of about 35 % with respect to the pure undoped compounds.

Finally, we demonstrated that the Li decorated compounds have very good properties concerning ammonia storage, a very hot topic in new fuels and energy vectors transportation and use.

Due to the high price of fullerene, we are exploring new cheaper C structures. In particular, we were able to prepare a novel hierarchically-porous super-activated carbon, with specific surface area exceeding 3000 m^2/g, starting from biochar derived by the pyrolysis of chicken-manure. The chemical activation process, realized with KOH solutions, was efficient in removing all impurities, stabilizing a highly porous structure with local graphene-like morphology. This compound demonstrated to behave as an excellent electrode material for high-performance supercapacitors, reaching high specific capacitance up to 230 F/g; the laboratory scales realized devices supply high current density of 10 A/g without using any conducting additives and display high power density and reliability, operating both with KOH and Na_2SO_4 eco-friendly electrolyte aqueous solution. The availability, the biocompatibility and the inexpensiveness of the starting materials, together with the low environment impact of the electrolyte, suggest possible large-scale applications for such devices, for example in the field of transportation or in renewable energy-grids, but also in the field of bio-medicine.

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1A – Inorganic materials for the consolidation of bone remains

E. Carretti, A. Salvatore
In collaboration with M. Lari and D. Caramelli

Aims

Bones recovered from archaeological excavations are not simply objects of historical and archaeological interest. They can be also considered as a true “Biological Archive” that should be accessible for long-term studies, in fact, ancient human bones are a fundamental resource to understand the uses of past human societies.

Since the twentieth century the products that have been largely used for the consolidation of bone remains are mainly composed by natural and synthetic polymers (vinyl and acrylic polymers, cellulose derivatives, etc.). Unfortunately, the extensive application of these products has many drawbacks mainly due to their low chemical stability that results in simultaneous depolymerization and crosslinking reactions that partially compromise their performances. Furthermore, shrinking phenomena can occur inducing mechanical stresses into the matrix on which they are applied (that can result in formation of local detachments). Finally the aging reactions of these polymeric materials also result in a strong decrease of their solubility that reduces the reversibility of the treatment (that is a mandatory requirement especially when the consolidation performances are completely or partially compromised) up to the 50%. In addition to these problems the presence of these materials can limit future analysis such as radiocarbon dating, isotope analysis and the access to the residual genetic heritage.

Then, at today, the set up of innovative conservation strategies and products for the conservation of of bone remains is crucial to warrantee the fruition of the relics and, most important, to maintain the long-term access to the biological information recorded in the bones. The approach that is purposed in this study is based on inorganic materials characterised by a high physical and chemical compatibility with the treated support. In particular, diammonium hydrogen phosphate, a chemical precursor of hydroxyapatite (HAP, the main mineral component of bones) has been used to restore a continuous 3D crystalline network of HAP in bone relics affected by degradation and decohesion phenomena.

Results

The consolidating effect of the HAP has been evaluated also after a pre-treatment with Ca(OH)2 nanoparticles. The in-situ precipitation of hydroxyapatite with or without pre-treatment with Ca(OH)2 NPs affects the overall porosity and the adsorption-desorption isotherms obtained through the Brunauer Emmet and Teller theory indicate a decrease of surface area and pore volume of 45% and 64% respectively. Furthermore, after the treatment, the formation of a homogeneous dense phase into the bone matrix is observed as indicated also by the increase of the Vickers microhardness (more than 40%). Additionally, by means of a paleogenetic analysis we showed that authentic genetic data could be retrieved from bones even after the consolidating treatments.

Figure 1 shows some SEM micrographs collected before (A) and after the application of two different consolidation treatments. Micrograph B has been collected after the application of a solution of diammonium phosphate aqueous solution (DAP, treatment 1) while micrograph C has been collected after the application of DAP and a dispersion of Ca(OH)2 nanoparticles (treatment 2). Both the consolidation treatments lead to the progressiverecovery of a much more compact structure and to the formation of a homogeneous texture (Figure 1B and C) with an apparent decreaseof the dimensions of the open pores. This effect is more pronounced especially for bone sample subject to treatment 2.

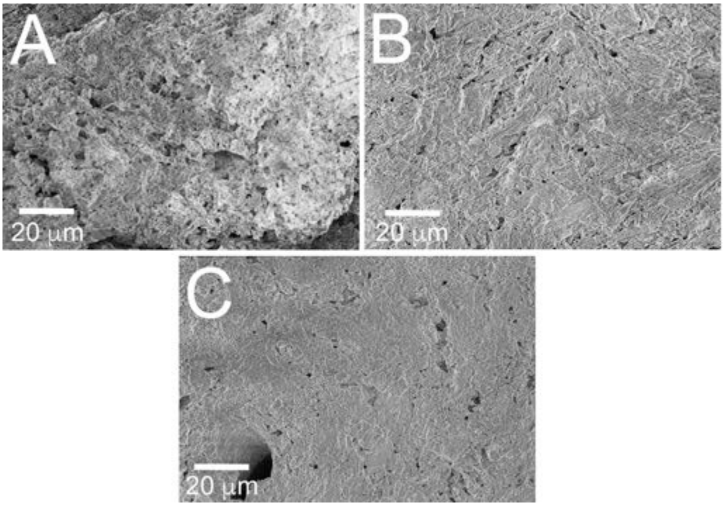

Fig. 1: SEM micrographs of Iron Age bone fragments. Image A has been collected from a sample before the consolidation treatment; micrograph B was collected after the application of the consolidation treatment 1; micrograph C was collected after the consolidation treatment 2.

Moreover, one of the most important innovation introduced in this work is that, for the first time, the efficacy of the consolidation treatment has been evaluated not only by considering the effect of the consolidants on the physico-chemical point of view, but also analyzing the impact of the consolidating materials applied onto the bone matrix on the molecular characterization of genetic material. Indeed, paleogenetic analysis on treated and untreated fragments from the same bone specimens demonstrate that the consolidating materials proposed in this study do not substantially affect the ability to recover endogenous DNA molecules. No change in damage patterns of the genetic material -due to the antiquity of the sample- seems to be induced by the consolidant protocols tested.

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1A – LCA of urban systems: a framework for the sustainability assessment of cities

S. Maranghi, M.L. Parisi, A. Facchini (IMT School for Advanced Studies Lucca), A. Scala (ISC CNR), R. Basosi

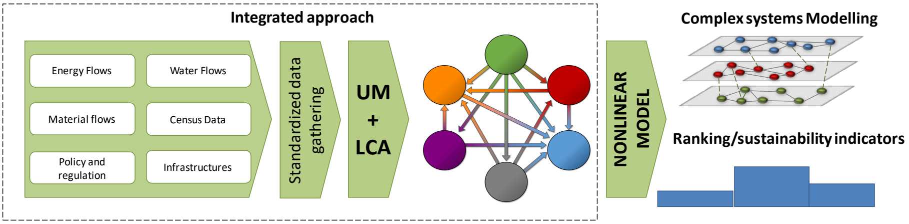
Aims

In recent decades, the close correlation between urban development and the concept of sustainability has become increasingly evident and important. This is demonstrated by European Union policies concerning EU cities and the United Nations 2030 Agenda for Sustainable Development, including sustainable development goal (SDG) 11: sustainable cities and communities. In the context of increasing urbanization, it is essential to find innovative methods to manage urban living systems and to establish a standard method for assessing the environmental performance of cities and their infrastructures. A unified and complete methodology for assessing policies for urban sustainability that takes into consideration urban complexity is currently lacking. In this paper, we develop a multi-dimensional measure framework applied to cities, aimed at unveiling, in a second phase, the interconnections among a set of urban dimensions identified by means of an approach based on urban thermodynamics and complex systems, aimed at integrating the urban metabolism (UM) and life cycle assessment (LCA). We also suggest key indicators for investigating and comparing the sustainability of cities, based on information concerning energy, material, and information flows for six urban sub-dimensions. Together, these sub-dimensions and their components describe the urban environment, providing the level of data granularity needed for the UM and LCA approaches.

Results

Expansion of urban environments, while doubtless bringing advantages and merits, is linked also to global challenges of sustainability, particularly in regions where the process of urbanization is still unfolding. Cities and urban communities can play a crucial role in the global work of improving sustainability. So we propose an approach based on urban thermodynamics to measure the sustainability of cities as complex systems by integrating urban metabolism (UM) and life cycle assessment (LCA). By means of a multiscale view of the city, we propose a synergy between UM and LCA with the aim to cope with urban sustainability both from the macroscale point of view (i.e. Urban Metabolism) and both from the microscale point of view (i.e. LCA). Our combined approach involves implementation of UM and LCA at an urban scale that is suitable for both approaches.

Our proposed multi-layer model also allows for a better comparative characterisation of urban sustainability based on synthetic indicators. Having a more detailed representation of urban flows and their interdependences, finding synthetic indicators and ranking is eased by the fact that we can use the typical metrics of multilayer complex networks.



This approach extends the multi-layered survey proposed for UM and includes in UM and LCA information flows, which are rarely considered in such studies. Together with information flows, we included data on quality of life, as a measure of how effective metabolic flows are in the development of the city. This includes a qualitative aspect into the framework of material flow analysis, e.g., it can be useful to assess how the same quantity of energy is used differently. In addition to this, we also pointed out how our multi level approach may represent a significative advantage for the application of this kind of analysis yielding a multiplex network approach to urban systems.

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1A – Lead-free perovskite solar cells coupled to plasmonic nanoarrays

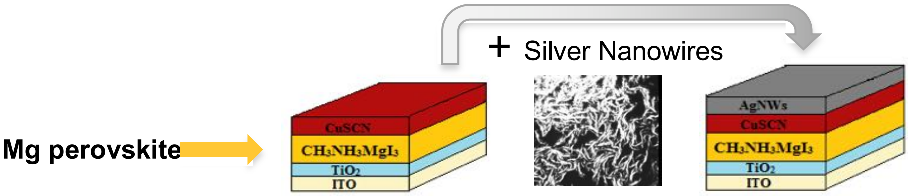
G. Caminati, B. Muzzi, G. Lucchesi

Aims

In the active search for low-cost source of energy, perovskite solar cells represent one of the most active areas. Several recent contributions focus on the study of lead-free solar cells with acceptable conversion efficiency. We propose a novel, non-toxic magnesium perovskite solar cell (CH3NH3MgI3) that, thanks to the plasmonic enhancement due to silver nanowires ordered coating, exhibits promising efficiency and long-term stability.

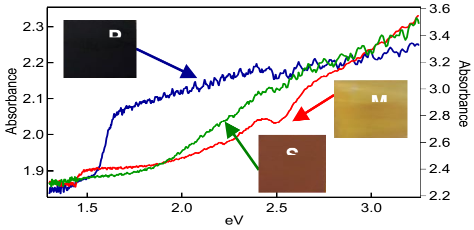
Results

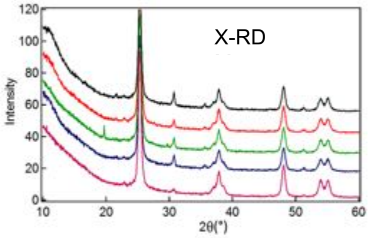
Magnesium perovskite photoactive layer was prepared by means of sequential spin-coating and/or drop-casting techniques on ITO covered glass substrate. We explored the effect of different experimental conditions (temperature, humidity and oxygen content) on perovskite structure and performance. Perovskite structure and layer morphology were obtained by X-ray diffraction and Confocal Laser Scanning Microscopy. The photophysical properties of the samples were studied by means of absorption and fluorescence spectroscopy whereas reflectance spectroscopy provided information on the energy gap.



The properties of Mg perovskite layer were compared to lab-built lead- and tin- based perovskites using the same techniques.

Solar cells of the three perovskites were built using drop-casted CuSCN as Hole Transport Layer before cathode coating. The efficiency of the solar cells was comparatively determined measuring current and potential under irradiation as a function of time.





A significant increase of efficiency was obtained intercalating a nanolayer of Silver nanowires (AgNW) between the HTL and the cathode. Different transfer procedures, i.e. Langmuir-Blodgett and drop-casting techniques, were explored to obtain an ordered and uniform AgNW layer in order to maximize the resulting efficiency by means of surface plasmonic coupling.

The results showed that coupling Mg-base perovskite with AgNW layers provide solar cells with efficiency close to Pb-based cells but Mg perovskites resulted more stable with respect to aging and photodegradation. These promising results pave the way to eco-friendly devices not only for solar energy conversion but also in LED technology.

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1A – Magnesium phosphate cements for bone tissue engineering

R. Gelli, M. Tonelli, F. Ridi, P. Baglioni

Aims

The use of magnesium phosphate-based cements (MPCs) in the biomedical field has recently come under investigation in the scientific community, as these materials display many intriguing properties in the replacement and/or integration of calcium phosphate-based bone cements; however, the diverse preparation conditions reported in the literature make it difficult to evaluate how the modification of a specific parameter in the preparation of the paste affects the final properties of the material. Our research aimed at preparing and characterizing MPCs by mixing a tri-magnesium phosphate powder with a solution of di-ammonium hydrogen phosphate, so to form struvite as a final setting product. The influence of several parameters on the properties of the final materials was investigated.

Results

In the framework of new materials for orthopedic applications, Magnesium Phosphate-based Cements (MPCs) are currently the focus of active research in biomedicine, given their promising features. In the literature several formulations are currently reported and because of these diverse preparation conditions, it is difficult to evaluate how the modification of a specific parameter in the preparation of the paste affects the final properties of the material. This project aimed at preparing and characterizing MPCs by mixing a tri-magnesium phosphate powder with a solution of di-ammonium hydrogen phosphate, so to form struvite as a final setting product. The powder to liquid ratio and the concentration of the aqueous solution were systematically varied, and their effect on the properties of the final product was studied. [1] The handling properties of the pastes were investigated, as well as the compressive strength and the porosity of the final material. The crystallinity, the microstructure and the specific surface area were assessed with a multi-technique approach which allowed us to relate the amount of formed struvite with the properties of the material, and to identify the preparation conditions to be used to obtain a cement with desired features.

Taking the next step, the loading of MPCs with active molecules to be released in the proximity of newly-forming bone was investigated, as this strategy represents an innovative approach to enhance the in vivo performances of the biomaterial. In particular, we prepared and characterized MPCs containing citrate, an ion naturally present in bone which presents beneficial effects when released in the proximity of newly forming bone tissue. The cements were characterized in terms of handling properties, setting time, crystallinity and microstructure, so to unravel the effect of citrate concentration on the features of the material. Upon incubation in aqueous media, we demonstrated that citrate could be successfully released from the cements, while contributing to the alkalinization of the surroundings. The cytotoxicity of the materials towards human fibroblasts was also tested, revealing the importance of a fine modulation of released citrate to guarantee the biocompatibility of the material.

Currently, our research is moving towards the inclusion of halloysite nanotubes in the formulations, in the attempt to increase their mechanical properties and to introduce in the cements possible reservoirs to be filled with active molecules (such as antibiotics) that can be released slowly in time.

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1A – Mineral particles, project funded by EUSMI - European Soft Matter Infrastructure Forschungszentrum Juelich GmbH 52425 Juelich, Germany

L. Gentile, G. Palazzo

Aims

Soil organic matter (SOM) plays a major role in the global carbon (C) cycle, since soils contain over three times more C than the atmosphere or terrestrial vegetation. Hence, decomposition of even a small part of the SOM pool can have a major impact on the quantity of CO2 and other greenhouse gases in the atmosphere and thus Earth´s climate. SOM originates from the microbial decomposition of plant and animal litter material. During this process, the dead organic material is progressively degraded into, smaller pieces by the activity of extracellular enzymes and radicals.

It is largely unknown why some SOM persists for millennia (recalcitrant SOM), whereas other SOM decomposes readily (labile SOM). The traditional view assumes that recalcitrant SOM consists of plant residues and *de novo*-synthesized, large-molecular sized, so-called humic substances whose chemical structure renders them resistant to degradation. Recently this view has been challenged by data indicates that the molecular structure alone does not control SOM stability. Instead, the persistence of SOM arises from complex physicochemical interactions between SOM and the bio-geological environment.[1,2] According to a recent proposed model [2], SOM are continuously processed into smaller molecules by decomposing microorganisms. This is accompanied by an increasing degree of oxidation of the decomposition products, which increases their water solubility and, possibly, also their propensity to be incorporated into colloidal aggregates and their reactivity towards mineral particles. The formation of molecular aggregates and mineral interactions will protect the SOM from microbial degradation. In new model for stabilizing SOM, the SOM present in the aqueous phase, usually referred to as dissolved organic matter (DOM), is the key SOM fraction relevant to the formation of organic matter-mineral associations. However, the structure and dynamics of molecular aggregates in DOM and their interaction with mineral particles have not been described in detail. Recently Gentile et al. [9] reported the coexistence of two kinds of water-soluble SOM: molecular and colloidal fraction. Here the focus is on the complex processes of SOM sequestration at the molecular to nm and µm length scales, directly relevant for microorganisms.

“The ILVA Industrial Site in Taranto” published by the European Parliament describes how environmental pollutants resulting from the production process at ILVA cause negative health impacts: “particulate matter smaller than 10 micrometres that are capable of penetrating deep into the respiratory tract and causing significant health damage), polycyclic aromatic hydrocarbons (PAHs) in particular the benzo(a)pyrene, dioxins and heavy metals that can be carcinogenic.[10,11] Here a contaminated soil from Taranto, Puglia (Italy) will be investigated by using several techniques to understand the effect of heavy metals on the colloidal fraction of the DOM. Furthermore, the results will be compared with an uncontaminated soil.

The colloidal properties of DOM will be investigated by using advanced physical chemistry techniques, such as X-ray and light scattering. The colloidal properties of organic matter will primarily be studied by small angle X-ray scattering (SAXS), a powerful technique to resolve the size and shape of (monodisperse) macromolecules, pore sizes, characteristic distances of partially ordered materials, and much more. SAXS has been widely used in biochemistry and colloidal science,[4] but very few studies have appeared in the environmental science literature.[5] Here SAXS will provide information on the aggregation of colloidal DOM induced by heavy metals. Static and dynamic light scattering will be used as complementary techniques to obtain information on size and shapes of the aggregates.[6–8] Finally, high-resolution NMR will be useful to characterize the chemical composition of the molecular fraction dissolved in water, while solid-state NMR will be useful to have some ideas on the overall composition. The combination of scattering and spectroscopy will provide a new level of comprehensive understanding of the colloidal property of organic matter and the effect of contamination from heavy metals.

Results

The dissolved organic matter consists of both fractal-like colloids, of a hundred nanometers and small molecular DOM. SAXS, SLS, and DLS were used to obtain structural information on the DOM colloidal fraction. The SAXS data at q-values between 0.004 and 0.02 $Å^{-1}$, shows scattering power law, $I(q) \sim q^{(-m)}$, with $m \approx 3$, 2.3 and 1.8 for Mottola, Gioia del Colle, and Massafra, respectively. The element analysis of the investigated solutions shows Al to be 0.875, 0.248 and 0.127 mg/l, while Fe is 0.329, 0.156 and 0.088 mg/l per Mottola, Gioia del Colle e Massafra, respectively. The higher presence of minerals could lead to a more complex fractal aggregation of the organic matter leading to different m values.

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1A – Nanocomposite electrodes for the simultaneous determination of hydroxycinnamic acid structural analogs

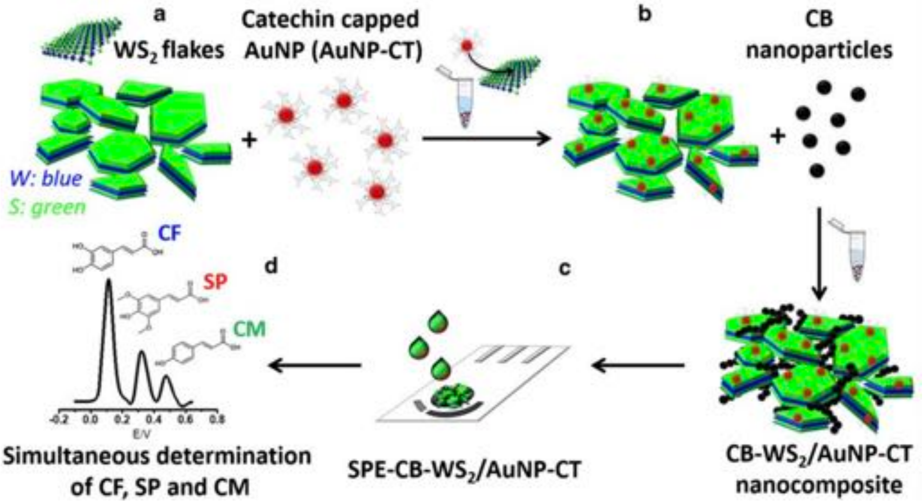
F. Della Pelle, G. Ferraro, E. Fratini, D. Compagnone* (*Faculty of Bioscience and Technology for Food Agriculture and Environment, University of Teramo, Teramo, Italy)*

Aims

The proposed sensor is the first example exploiting the simultaneous determination of these compounds in food samples. Given its excellent electrochemical performance, low cost, disposability, and ease of use, this SPE-CB-WS2/AuNP-CT nanocomposite sensor represents a powerful candidate for the realization of electrochemical devices for the determination of (bio)compounds with high passivation tendency.

Results

A high-performance electrochemical sensor based on WS_2 decorated with AuNP-CT and supported in a CB network was successfully developed and applied to the simultaneous determination of a three hydroxycinnamic acid (hCN) structural analogs (accordingly to the hydroxyl moieties' arrangement in the phenol structure) in food samples. The proposed sensor takes advantage of the AuNP-CT metallic properties, demonstrating electroactivity towards hydroxyl moieties through assembly in the WS_2 flakes that result in an enhanced conductivity with an exceptional antifouling activity due to WS_2. The final assembly of WS2/AuNP-CT into CB network exhibited a further conductivity enhancement without loss of antifouling performance.



The nanomaterial based synergistic effect of the sensor results in enhanced selectivity, sensitivity, and reproducibility in the simultaneous determination of class-selective hCN structural analogs in food samples. Given its excellent electrochemical performance, together with its low cost, disposability, and ease of use, this SPE-CB-WS_2/AuNP-CT nanocomposite-based sensor represents a powerful candidate for the development of electrochemical devices for the determination of (bio)compounds with high passivation tendency.

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1A – Prospective life cycle assessment of third-generation photovoltaics: a long-term scenario approach

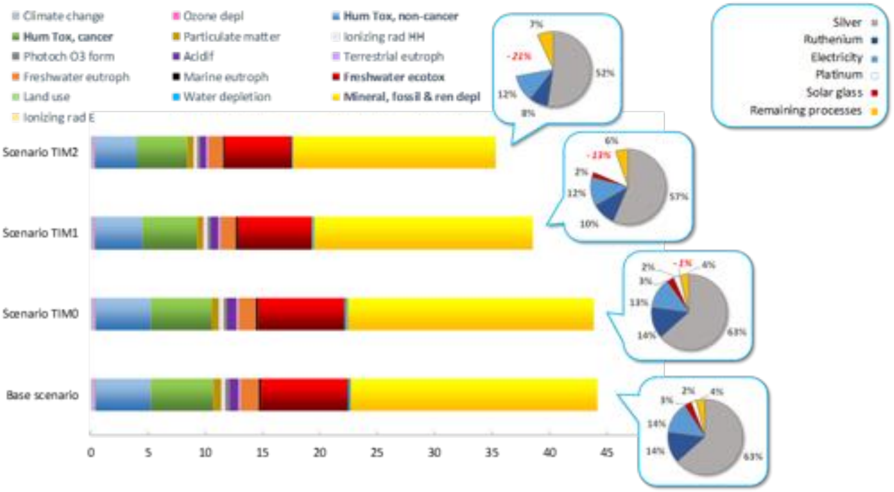
M.L. Parisi, S. Maranghi, L. Vesce (CHOSE, Università di Torvergata, Roma, Italy), A. Sinicropi, A. Di Carlo (CHOSE, Università di Torvergata, Roma, Italy), R. Basosi

Aims

The development of sustainable technologies for energy generation should undergo sustainability assessment. A well-recognized, valuable tool to accomplish this task is the life cycle assessment. The aim of the project is the definition of a long-term approach, using prospective life cycle assessment, based on predictive scenarios featuring technological development and energy mix evolution to investigate the opportunities and constraints related to the mass-production potential of third-generation PV technologies.

Results

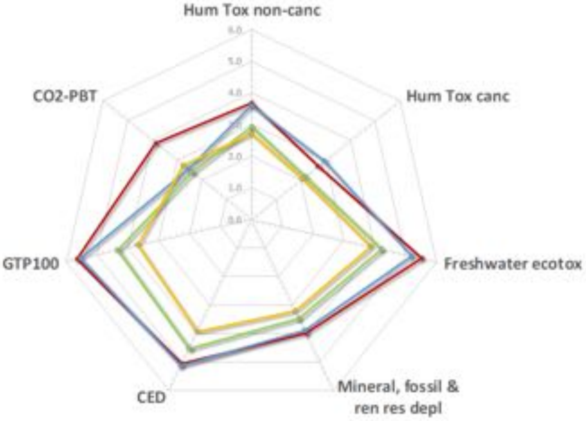
The Dye Sensitized Solar Cell technology is taken as a case study due to the access to detailed and robust primary data of dye sensitized solar module (DSSM) produced by the Italian Dyepower consortium at the pre-industrial scale. The use phase is modeled based on building integrated photovoltaics applications. Results obtained from the hypothetical use phase scenario were pivotal to highlight the hotspots of the process and to emphasize the alternative materials and engineering solutions that could allow for further decrease in the environmental footprint of the DSSMs.



The eco-profile of the pre-industrial manufacturing process of DSSM shows that the consumption of direct energy during the fabrication procedure (ca 35% of the global

CED indicator) is a crucial point for the industrial optimization and development. However, the consumption of some raw materials, such as silver, ruthenium and glass (ca 90% of the global impact on ILCD 2011 impact categories) employed in the module configuration is necessary for generating significant improvement of the environmental profile of DSSM.

The long-term prospective eco-profile of DSSMs as a future renewable European electricity-generating technology shows the potentiality of the BIPV application. The results emphasize the relevance of the technological improvement, even in a future European electricity mix characterized by a remarkable share of renewable sources. However, beyond a threshold, for some impact and photovoltaic performance indicators, a further improvement would be possible by exclusively replacing some materials among the components of the DSSM



From a general point of view, the analysis shows that research and development for efficiency, stability and durability should be coupled with technological improvement to reach the best performances in terms of environmental sustainability and circular economy.

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1A – Smart Nanostructured Functional Materials: for Biomedical and Environmental Applications

M. Monduzzi, M. Piludu, A. Salis, et al.

Aims

This project aimed to exploit bottom-up nanotechnology strategies based on the fundamental knowledge of chemical, physical and colloidal sciences to produce highly versatile platforms based on hybrid materials with specific functional activity in biomedical, environmental and catalytic applications. Using various types of synthesis, functionalization and characterization, different types of functional materials have been obtained. In particular, solid matrices based on ordered mesoporous silica nanoparticles (MSNP) have been studied. Natural biomaterials, such as polysaccharides, proteins including some enzymes, synthetic functional groups such as amino acids and peptides have been used for the functionalization of particles. Several chemical-physical characterization studies have been carried out, both on functionalizing agents and on solid matrices (before and after the various functionalization phases) using BET, TGA, SAXRD, TEM, FT-IR, DLS and Zeta potential measurements. Furthermore, the effect of electrolytes and simulated body fluids for functional materials characterized by polar or charged interphases was examined to investigate the stability and interactions induced by changes in surface charge.

Results

Some studies have been carried out using functionalized mesoporous silica-based nanoparticles (MSNP) for different types of applications, in particular in the biomedical field, and imidazolized Zeolites for environmental applications. The biomedical application of nanoparticles is mainly associated with their surface properties and stability and interactions in biological media. Surface functionalization plays a key role in determining biodegradation, cytotoxicity and biodistribution through specific interactions mediated by biomacromolecules. A typical example is given by different proteins that lead to the formation of nanoparticles coated with a protein *corona*. MSNPs can be used as carriers for prolonged drug release. These MSNPs were then used to study the interaction with BSA and to highlight the role of different biopolymers. BSA conjugated with gold particles was used to highlight the adsorption of the protein to the surface of the MSNP by electron transmission microscopy (TEM). Figure 1 schematically illustrates the use of MSNPs, and also two images of fluorescence and TEM that visualize biocompatibility and internalization assays in cell lines.

Environmental applications have involved the preparation of a diagnostic tool for heavy metals, and the preparation of biocatalysts. In particular, the MSNPs were used to prepare modified glassy carbon electrodes coated with the Nafion ion-exchange polymer for the electrochemical detection of Cd (II). The biocatalysts were prepared by encapsulating enzymes on frameworks consisting of zeolites functionalized with imidazole.

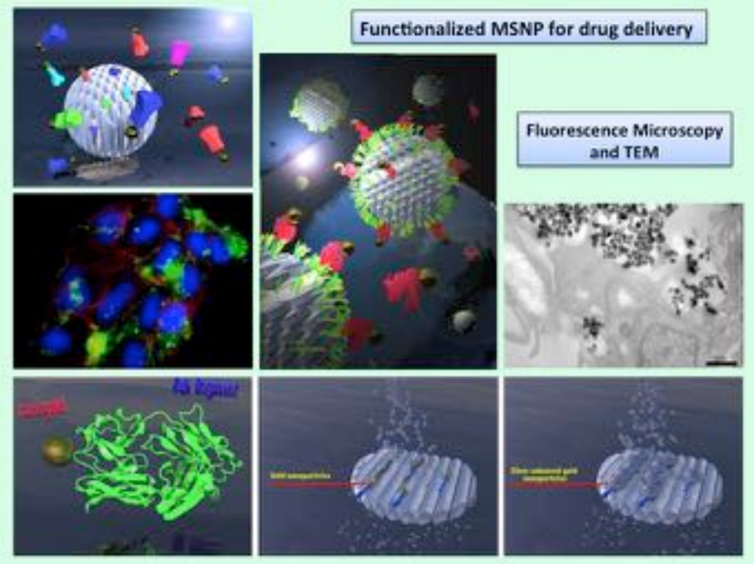

Figure 1: Schematic representations of MSNP together with fluorescence microscopy and TEM images.

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1A – Understanding interactions between polymer coated surfaces and model biopolymers- ITN-MSCA “BIOCLEAN” Project Number: 722871

H. Mateos, N. Cioffi, G. Palazzo

Aims

Most real-world ubiquitous and costly microbiological problems are rooted in biofilms including clinical infections, corrosion, loss of process efficiency such as heat transfer, dental plaque, food contamination, cleaning household surfaces, water processes, fabrics and laundry. Since the development of antimicrobial resistance (AMR) is faster than the limited penetration and neutralization on the biofilm’s outer surface the biofilm are less susceptible to chemically diverse biocides and disinfectants. Furthermore, the shortage of water is going to be a worldwide problem and consumers become consciences of water usage for personal cleansing, reducing water consumption for cleaning their homes. For these reasons it is advisable to develop new methods that deliver hygienic clean surfaces without the use of anti-microbial agents and reducing the water consumption.

Results

We have preliminarily characterized a pool of surface modifying polymers in terms of molecular weight, hydrodynamic size, titratable groups, zeta-potential and isoelectric point, surface activity and elemental composition. This was done using static light scattering (SLS), dynamic light scattering (DLS), titrations, laser Doppler electrophoresis (LDE), tensiometry and X-ray photoelectron spectroscopy (XPS). An analogous study was conducted on a pool of solid surfaces representative of those found in a home (particularly in a kitchen or in a bathroom) by means of XPS, contact angle measurements and scanning electron microscopy (SEM).

Subsequently, the experimental strategy to probe the adsorption of surface modifying polymers and it impact on the interaction of proteic soil was implemented in the case of glass as a surface and BSA as model soil. The choice of glass as surface allows the use of surface plasmon resonance (SPR) to probe the whole process.

Using SPR it was possible to calculate the surface coverage of the polymers on glass at increasing concentrations. Absorption constants were calculated by fitting these curves to a Langmuir isotherm and plotted in figure for each of the polymers.

A model bioprotein, BSA, was chosen in order to monitor the interactions with glass surfaces coated with 3 polymers. The results from SPR, as shown in figure, indicate an affinity of BSA for Polymer2, forming a layer that remains there even after flushing with water. However, BSA did not significantly interact with neither polymer 1 nor polymer3.

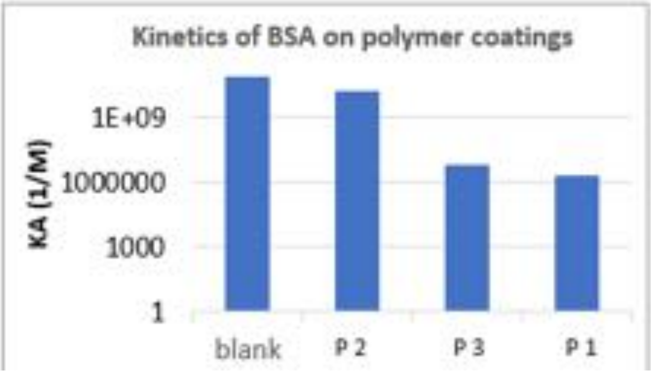

Fig. 1: Affinity constants of BSA for bare glass and coated with Polymer 1, Polymer 2 and Polymer 3, where the y-axis is shown in log scale.

This project is currently in progress.

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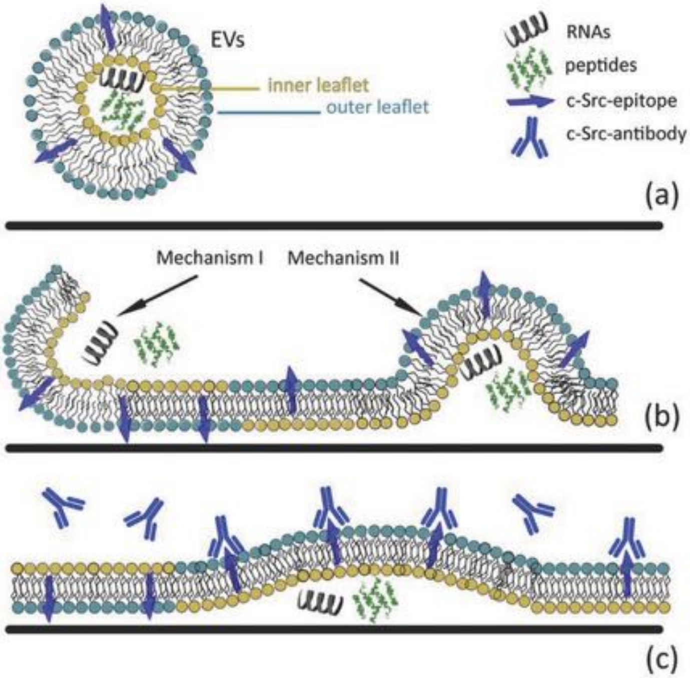
1B – Biogenic Supported Lipid Bilayers from Nanosized Extracellular Vesicles

C. Montis, F. Valle, D. Berti, P. Bergese

Aims

Supported lipid bilayers (SLBs) reproduce biological membranes providing surface biosystems of great interest for fundamental studies and for new biomedical applications. The realization of synthetic surfaces mimicking structure and function of biological membranes is an open challenge. Therefore, in this work we report the first example of supported lipid bilayers obtained from extracellular vesicles (EVSLBs).



Results

Silica-supported EVSLBs are formed from nanosized EVs—separated from culture media of prostate cancer model TRAMP-C2 murine cells—following a characteristic crowding-rupture-fusion pathway. It consists of the deposition on silica substrates of diluted dispersion of EVs in NaCl solution, added with CaCl2 buffer.

The determination of the EVSLBs' properties was performed by the combination of different surface sensitive techniques, such as Quartz Crystal Microbalance with Dissipation monitoring (QCM-D), Confocal Laser Scanning Microscopy (CLSM), Fluorescence Correlation Spectroscopy (FCS) and liquid phase Atomic Force Microscopy (AFM).

EVSLBs display peculiar properties at different length scales, such as 2.5 nm roughness, lipid-raft-like domains, and cushioned patches (with the cushion filled with the native

EV biomolecular cargo), which preserve the native EV membrane orientation with the proto-oncogene tyrosine-protein kinase Src (c-Src) accessible to antibody recognition. The experiments reveal simple EV fusion to obtain SLBs, maintaining the key features of the original TRAMP-C2 EV membranes, that constitutes the first example of 2d EV engineering.

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1B – Bioplastics and their degradation in composting conditions

E. Carretti, T. Lotti
In collaboration with Prof. C. Lubello, Prof. R. Gori
and Ing. F. Ruggero

Aims

The results of a composting lab-scale test carried out on plastic films, are presented. The first test material (Mater-Bi®) is composed by starch, additives and polybutylene adipate terephthalate (PBAT). The test lasted for 45 days and was developed in three replicates under different temperature and moisture conditions, with the aim to assess the influence on plastic degradation of less favourable composting conditions as short thermophilic phase, absence of moistening, and a combination of the two factors. The chemical nature and the morphology of the material and of its single components have been investigated before, during and at the end of the composting process, by means of different analytical techniques. Thermo Gravimetric Analysis (TGA) allowed to obtain activation energy and weight loss; Fourier Transform InfraRed spectroscopy (FTIR) and Scanning Electron Microscopy (SEM) were used to study changes in the polymeric and morphological structure, and visual analysis provided information on the size of the plastic particles. The results show that the biodegradation of PBAT is strongly influenced by the environmental conditions (temperature and moisture); on the contrary, in all the three replicates, both starch and additives are completely biodegraded within the first days of the process.

Results

Some composting test have been carried out on plastic samples composed by AMter-Bi® following three different protocol reported in Table 1.

Table 1. Process conditions (temperature, moisture and duration of the phases) of the experimental composting tests.

	Thermophilic phase			Maturation phase		
	T (°C)	Moisture (%)	Time (day)	T (°C)	Moisture (%)	Time (day)
A	58±2	55-60	5	35±5	45-50	40
B	58±2	40-50	5	35±5	20-30	40
C	58±2	55-60	20	35±5	45-50	25

Starch and additives follow a trend that is almost constant for the three process conditions A, B and C: they present an average weight loss of 40.5 ± 3% and of 85%, respectively. On the contrary, for PBAT the degradation depends upon the composting conditions with a weight loss ranging 17.2% (sample B) up to, 90.4% in sample C (thermophilic phase of 20 d, Figure 1).

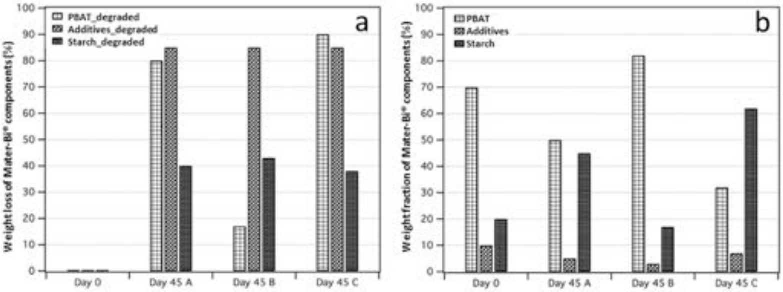

Figure 1. The graphs show a) the weight loss WL (%) and b) the weight fraction WF (%) of each Mater-Bi® component at day 45 for samples A, B and C in comparison with day 0.

The image of not degraded Mater-Bi® (day 0) is reported in Figure 2 and indicate the presence of a heterogeneous microstructure; the main evidences of the material is the presence of some circular spots which dimensions range in the order of few hundreds of nm probably composed by starch. Upon degradation, strong changes in the microstructure of Mater-Bi® occur. With the progress of the composting process, images reported in Figure 2 indicate the progressive disappearance of the circular spots with the formation of small holes (in the order of hundreds of nanometres) in correspondence of the grains that were present before composting. Being that from TGA we observed that the composting process progressively induces a strong degradation of the starch constituting the original Mater-Bi®, it is reasonable to suppose that these circular spots are made mainly by starch.

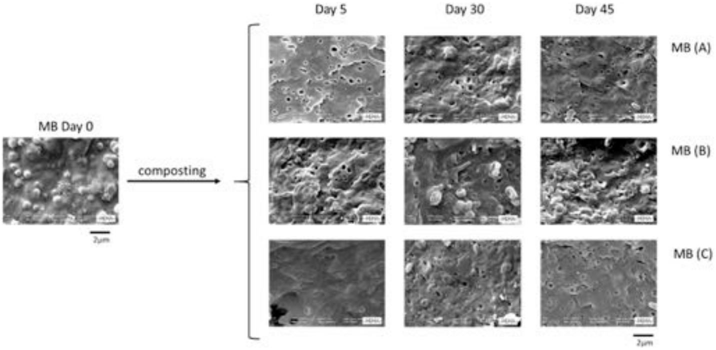

Figure 2. SEM micrographs of degraded samples A, B and C during (day 5 and 30) and at the end (day 45) of the composting process, x20000.

To carry out an exhaustive analysis of the biodegradation process, this study highlights the necessity to use a synergic approach based on the use of different instrumental techniques, giving complementary information. This approach allows a complete kinetic analysis of the composting process and shows the influence of the environmental conditions on the biodegradation of starch, additives and PBAT, allowing to extend the knowledge on the behaviour of bioplastics in a composting process

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1B – Chemical characterization of liposomes containing nutraceutical compounds: Tyrosol, hydroxytyrosol and oleuropein

C. Bonechi, A. Donati, G. Tamasi, A. Pardini, H. Rostom, G. Leone, S. Lamponi, M. Consumi, A. Magnani, C. Rossi (Department of Biotechnologies, Chemistry and Pharmacy, University of Siena)

Aims

Tyrosol, hydroxytyrosol and oleuropein are among the major phenolic compounds in fruits, leaves and oils from *Olea europaea* L. These natural antioxidants molecules revealed several beneficial effects on human health, but a low bioavailability and accessibility to targeted site. Liposomes are drug/nutraceutical delivery carriers, used for driving bioactive molecules to desired target tissues, decreasing potential side effects and protecting the encapsulated molecule from enzymatic metabolic processes.

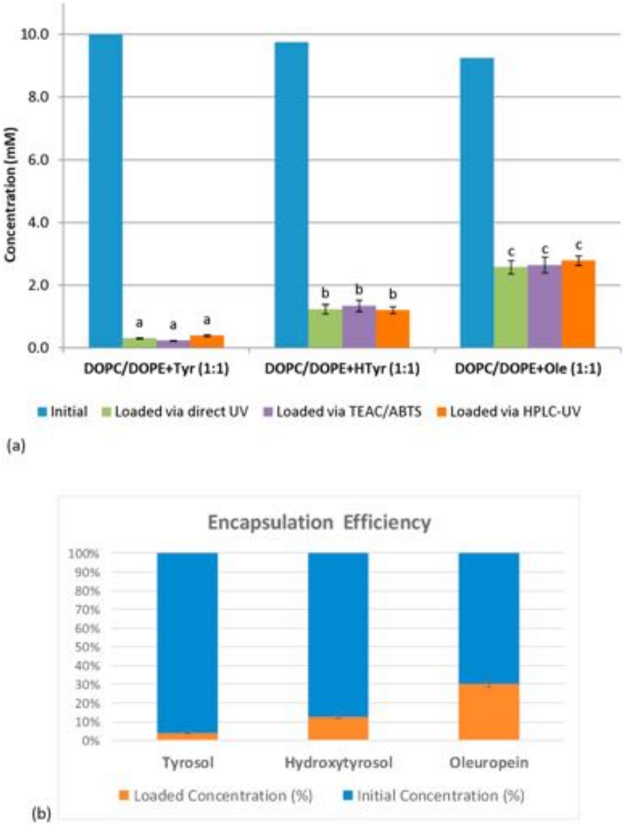
In this study, zwitterionic liposomes containing tyrosol, hydroxytyrosol and oleuropein were synthesized and characterized for their size and surface charge. Particular attention was devoted to the determination of encapsulation efficiency (EE%), quantifying the loaded Tyr, HTyr and Ole amount, by using three different techniques: direct UV spectrophotometry, High Performance Liquid Chromatography and Trolox Equivalent Antioxidant Capacity assay. The results revealed higher EE% for oleuropein. Cyto-toxicity and cyto-compatibility of liposomes were also tested on human chondrocyte cells.

Results

In the present work zwitterionic liposomes preparation containing three different nutraceutical compounds found in the fruit, leaf and oil of *Olea europaea* L. (tyrosol, Tyr; hydroxytyrosol, HTyr, and oleuropein, Ole) have been synthesized and characterized.

Determination of the average size of liposomes showed a slight change, statistically not significant, in the mean size of diameter of liposomes loaded with tyrosol and hydroxytyrosol. These data evaluated together to EE% suggests that both molecules where successfully integrated with in the liposomes while a decrease in the mean size of liposomes loaded with oleuropein has been noted which could suggest that the incorporation of oleuropein in liposomes occurred trough the bilayer membrane, changing the typical bilayer conformation of the liposomes. The overall charge of liposomes, which showed to be more negative for oleuropein suggest the better physical stability for this preparation, indicating a less probability of aggregation of liposomes, versus time, containing oleuropein than liposomes loaded with hydroxytyrosol and tyrosol.

The comparison of the values of the encapsulation efficiency (EE%) using Ultraviolet spectroscopy, TEAC assay and HPLC-UV analysis, confirm the better incorporation of oleuropein with respect of hydroxytyrosol and tyrosol within the liposomes.



(a) Initial and loaded concentrations (expressed as mM) in liposomes for Tyr, HTyr and Ole as determined via UV direct photometric quantification, TEAC/ABTS assay and HPLC-UV analysis (different letters indicate significant differences, $p < 0.05$, Tukey's test). (b) Graphical representation of the encapsulation efficiency (EE%) for the liposomes loaded with Tyr, HTyr and Ole, as determined via HPLC-UV analysis.

The difference in ATR-FTIR spectra between empty and loaded liposome preparations, suggest that the three nutraceutical compounds expose the hydroxylic groups on the surface of the liposomes, hence confirming their preferential incorporation within the lipid bilayer. Cyto-toxicity assay of the different liposomal preparation by human chondrocytes shows that liposomes are not cyto-toxic at any concentration.

Therefore, the zwitterionic liposomes loaded with natural compounds are important *drug-delivery system* to increase the bioavailability of antioxidants in the osteoarthritic pathologies and to reduce the collateral effect of classical drugs.

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1B – Chemical messengers for digital molecular communication

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Aims

Efficient, transmission and decoding of information is at the basis of any technological advancement. Although the dominant communication protocols, employing electromagnetic waves, are capable to transmit high information loads extremely quickly and over very long ranges, there are still fields where alternative communication approaches are desirable or even necessary. For example, the miniaturization of nano-devices is hampered by the need of antennas of sufficiently large size to detect electromagnetic waves. More importantly, the storage and transport of information along human bodies, which may allow the development of novel and personalized therapies based on the real-time monitoring and treatment of patients, requests the use of radiation-free approaches to avoid both any risk of hazard generated by electromagnetic waves sufficiently energetic to penetrate tissues and organs and any possible interference between different devices working simultaneously. Thus, how devices could communicate in cases like these? As with many other scientific and technological developments the reply arises from the observation of natural processes. Evolution has developed many effective communication systems exploiting molecules for message swapping in living organism. Biological molecular communication occurs both on the micro and nanometric scale for the exchange of inter and intracellular information, through a long-range communication system such as the exchange of pheromones between animal species. However, efficient chemical communication is only possible in nature because highly specific messengers and receptors have been developed in thousands of years of evolutionary optimization. Each messenger/receptor couple is able to transfer the information, that is the presence of absence of the messenger itself, and the many information required for the proper functioning of a living body are stored and transferred by thousands of chemical messengers developed by nature.
The aim of the project is the developing of a communication procedure where information is encoded in no-specific molecular messengers in binary code.

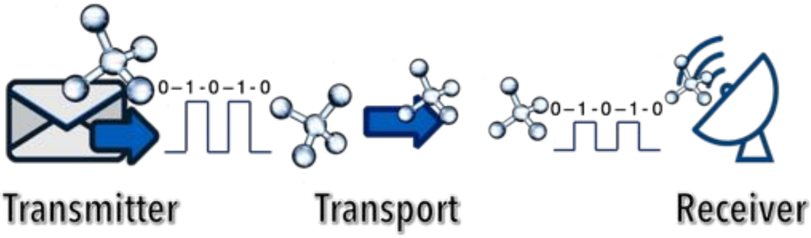

Figure 1– Synoptic Representation of the Molecular Communication Process

Conceptually, the idea is quite simple: a transmitter releases small amounts of chemical messenger which is propagated in an aqueous or gaseous medium up to a receiver which is responsible for detecting and decoding the information encoded in these particles (see Figure 1). Although the concept of digital molecular communication has been hypothesized around 10 years ago, the transfer from theory to practice has not yet been developed. A small niche of telecommunications researchers has modelled the process from a theoretical point of view. Very few prototype basic systems have been developed.

Results

We are developing a fully working prototypal molecular communication platform inspired by the nature and scientifically based on the already theorized protocols to develop the suitable molecular messengers to achieve effective information transfer. Transmitter releases a concentration impulse of fluorescent nanoparticles, acting as molecular messenger, that it subsequently propagates within the transport medium until it reaches the receiver, where the signal is translated it into the initial message.
Results have been published on international journal on physical chemistry filed.

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1B – Development of liposomal formulations as drug delivery systems

G. Leone, M. Consumi, C. Franzi, G. Tamasi, S. Lamponi, A. Donati, A. Magnani, C. Rossi, C. Bonechi (Department of Biotechnologies, Chemistry and Pharmacy, University of Siena)

Aims

Liposomal formulations were obtained mixing 1,2-dioleoyl-sn-glycero-3-phosphocholine (DOPC) and 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (DOPE) with synthetic lovastatin or lovastatin extracted from Red Yeast Rice (RYR) to prepare a vehicle able to overcome both the disadvantage of lovastatin, i.e. its poor oral bioavailability and side effects. Liposomal formulation obtained combining DOPC, DOPE and hydro-alcoholic extract of RYR showed optimal physico-chemical, mechanical and thermal characteristics and the strongest inhibition activity versus 3-hydroxy-3-Methyl glutaryl coenzyme A (HMG-CoA) reductase.

The aim of this paper is the evaluation of effectiveness of liposomes on synthetic and RYR lovastatin inhibitory activity against HMG-CoA-reductase.

Results

Liposomes were an efficient vehicle for lovastatin. Lovastatin from RYR is more efficient than synthetic lovastatin. The best extraction solvent was the hydro-alcoholic one which, starting from 1000 mg of RYR, guaranteed the encapsulation of about 6 mg which had a similar effect than the 20 mg/day dose of synthetic lovastatin, actually the most used daily dose, since myalgia incidence is proportional to the dose (ranging from 0.1% at 20 mg/day to 1.5% at 80 mg/day).

Physico-chemical characterization of liposomal formulations (A: DOPC-DOPE and RYR alcoholic extract; B: DOPC-DOPE and RYR hydro-alcoholic extract; C: DOPC-DOPE and standard lovastatin in EtOH; D: empty liposomes) by particle size, zeta potential and lovastatin encapsulation efficiency

Composition	mg[a]	mg[b]	E.E.	D (nm)	PI	ζ (mV)
A:DOPC-DOPE + R (EtOH)	20.6	3.2±0.1	9%	155±17	0.40	−37±7
B:DOPC-DOPE + R (EtOH:H_2O)	35.4	6.4±0.2	31%	450±23	0.35	−32±7
C:DOPC-DOPE + Lov	28	3.9±0.1	14%	263±15	0.47	−29±5
D: DOPC-DOPE	–	–	–	85±11	0.30	−18±5

a mg of extracted lovastatin.

b mg of encapsulated lovastatin.

Consequently, the amount of lovastatin from RYR uploaded in liposomal formulation (sample B) is sufficient to exert the same effect of the common dose of lovastatin (20 mg/day). However, it is possible to slightly increase the amount of lovastatin uploaded by the liposomes reaching 10 mg which is the recommended daily dose of lovastatin from RYR to gain the claimed effect, increasing the RYR amount to 1800 mg or even higher, i.e. 2,400 mg, which are common tested doses of RYR.

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1B – Effect of flow conditions and geometrical parameters on the electrochemical detection with band microelectrodes

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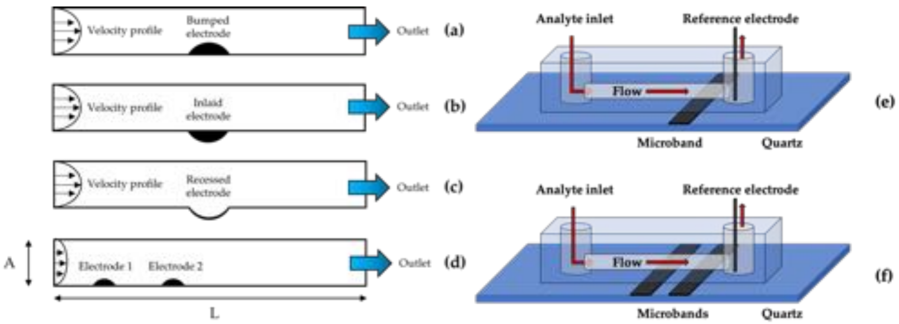
Aims

The realization of microelectrodic devices coated with biocompatible and conductive materials, cover a critical interest in medicine, optoelectronics and electrocatalysis. Showing both conductivity and low-immunoresponse characteristics, the realization of melanin-based microsensors was considered. As the effect of transport conditions and geometrical parameters on the electrochemical performance of microbands electrodes constitute a fundamental step in devices realization, computer simulations based on the finite element analysis were performed to obtain a flexible model that would serve as aid for the design and realization of microelectrodic devices.

Results

The mass-charge transport of electroactive species on channel microelectrodes was modeled using the finite element method implemented in a commercial package (COMSOL® Multiphysics). A dimensionless form of the governing equations was used to evaluate the effect of channel height, electrodic interdistance, electrodes geometry, and flow conditions on key electrochemical parameters, such as the electroactive species collection percentage and electrodic currents.



The better electrochemical performances of bumped microelectrodic geometries (a) in respect of inlaid (b) and recessed (c) configurations were evaluated from the dimensionless formulation of the convective-diffusive problem. The results were then extended to the study the "trail effect" generated by the presence of neighboring microelectrodes (d), and to evaluate the geometrical settings for its minimization.

Due to the dimensionless nature of the formalism used throughout the model, the adaptability of the obtained results to different specific cases of study by the use of proper scaling factors was demonstrated.

The present work was thus proposed as a valuable tool for the design of microelectrodic devices (e, f), and constitutes a first step for the modeling and realization of melanin-based microsensors, were the low-immunoresponse and UV-radiation absorption capabilities of this heterogeneous biomaterial could be exploited.

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1B – Effect of nanoemulsion stabilizers on solubility and in-vitro digestion of curcumin

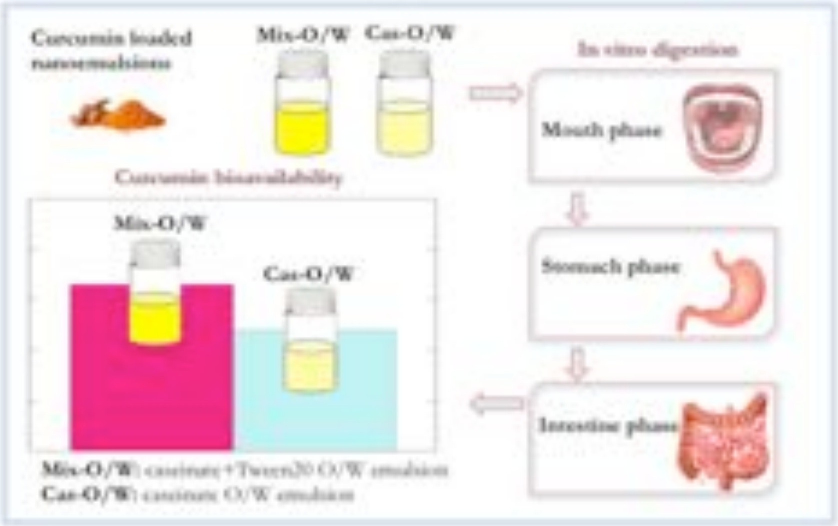
F. Cuomo, G. Cinelli, A. Ceglie, F. Lopez

Aims

The use of curcumin, a hydrophobic natural compound, is associated with anti-inflammatory, anti-carcinogenic and antimicrobial properties. Since it is a poor-water soluble molecule, its use in several food products and beverages is limited, as well as its oral bioavailability. Encapsulation of curcumin in nanoemulsions is a strategy to overcome these limitations and the use of low molecular weight surfactants in combination with a natural protein, sodium caseinate, has recently been applied to improve the stability of nanoemulsions in the acidic environment. Protein/surfactant (Mix-O/W) stabilized nanoemulsions are proposed as a curcumin carrier to enhance its bioavailability. The effectiveness of the delivery system was evaluated through an in-vitro digestion process.

Results

pH sensitivity of sodium caseinate (isoelectric point pH 4.6) was studied and improved by using a blend of Tween 20 and sodium caseinate as nanoemulsion emulsifier. The results obtained through dynamic light scattering demonstrated that the diameters of the dispersed phase in Mix O/W nanoemulsions were smaller than those stabilized by caseinate only (Cas-O/W), indicating that the mixed system was more stable. The two types of O/W nanoemulsions, Cas-O/W and Mix-O/W nanoemulsions, were loaded with curcumin and tested through a simulated gastrointestinal digestion process to evaluate their delivering effects of curcumin.



It was first demonstrated that the amount of curcumin solubilized through Mix-O/W nanoemulsion was higher than that in Cas-O/W nanoemulsion. Cas-O/W nanoemulsions, indeed, at their best, solubilized about 55 µg/mL of curcumin while Mix-O/W nanoemulsions reached a curcumin concentration around 180 µg/mL. Furthermore, for both the systems an increase of curcumin loading capacity was recorded with the rise of incubation temperature.

Finally, after the in-vitro simulated digestion process, the potential curcumin bioavailability was evaluated and the data suggested that Mix-O/W nanoemulsions provided more than twice the amount of curcumin compared to Cas-O/W nanoemulsions. On balance, the outcomes of this investigation demonstrated that the mixed emulsifier system offered a higher amount of lipophilic compound bioavailable delivered with a low fat intake compared to nanoemulsions stabilized by sodium caseinate.

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1B – Effect of temperature on the phase behavior of hydroxypropyl cellulose in presence of sodium dodecyl sulfate and glycerol

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Aims

The aim of this research is to describe the complexation process which occurs between hydroxypropyl cellulose (HPC) and sodium decyl sulfate (SDS) in terms of temperature gradient experiments due to HPC thermo-sensitivity. In addition, the aim is to evaluate how the presence of glycerol affects the lower critical solution temperature (LCST) and the structure of the aggregate of HPC/SDS below and above this temperature.

Results

The cellulose HPC derivative is a surface-active non-ionic thermo-responsive polymer being soluble in both water and organic solvents. It is used as emulsifier, stabilizer, thickener and film former in foods, cosmetics and paints. The thermo-responsivity depends by the lower critical solution temperature (LCST) of the polymer in aqueous solutions which depends on the molecular weight of the polymer and on the ionic strength of the solution (i.e. presence of electrolyte).[1] This kind of polymers form molecularly mixed complexes with anionic surfactants, due to a process known as complexation, similar to surfactant micellization in solution, occurring above a critical association concentration (cac), which is lower than the corresponding critical micellization concentration. [2] While this process between HPC and SDS has been widely studied, there is a hypothesis on the morphology of the complex at room temperature and still there is a lack of information on the complex and on polymer aggregate morphology when the temperature is raised over the LCST.[3]

Fluorescence, DLS and SANS measurements were performed on samples with a polymer concentration of 1% w/w. 8-Anilinonaphthalene-1-sulfonic acid (ANS) was used as a fluorescent probe. The spectra analysis shows a signal blue shift, indicating that ANS is in a more hydrophobic environment, proving the aggregates formation. The value of the wavelength corresponding to the maximum emission peak for each measurement has been reported as a function of temperature (Fig. 1A). The SDS presence causes the shift of the LCST at higher temperature compared to the one without the surfactant, while the presence of glycerol causes a LCST decrease, probably thanks to its hygroscopicity which disadvantages the interaction between the polymer and the water. DLS indicated that once passed the LCST, the presence of glycerol even if it causes a lowering of the LCST it leads to the formation of smaller aggregates compared to the sample where the solvent is only water (Fig. 1B). A stronger reduction of the aggregates dimension was observed when the surfactant is present in solution.

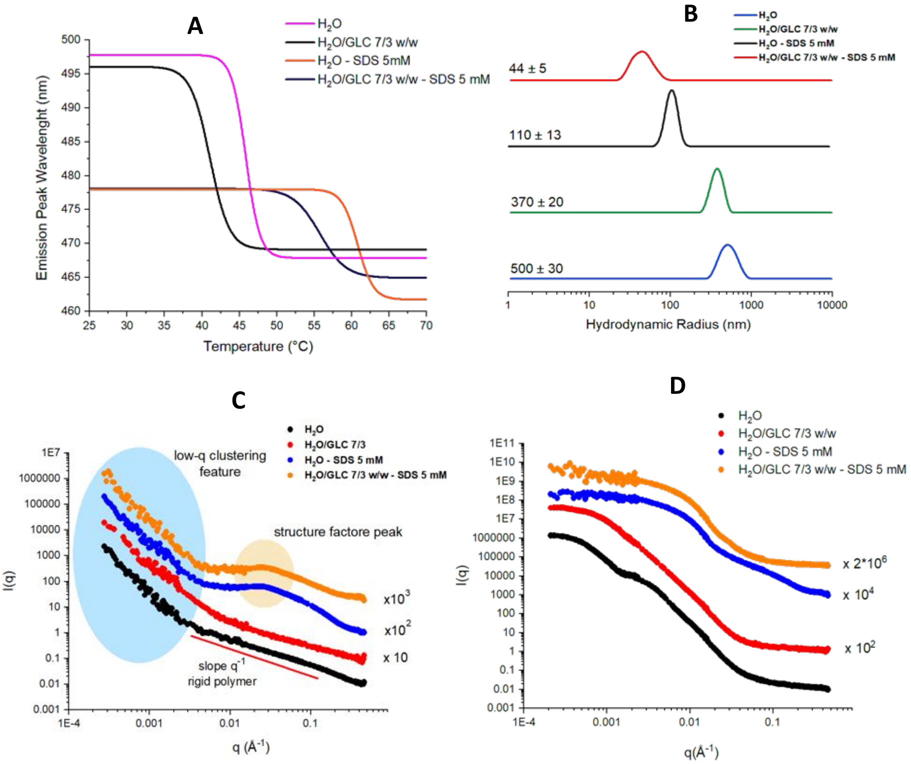

Fig. 1: Fluorescence measurements (**A**) and Hydrodynamic Radius distribution of the aggregates from DLS at 65°C (**B**). SANS measurement at 25 °C (**C**) and at 65 °C (**D**).

SANS confirmed the aggregates size, also furnishing insights on the particles structure and morphology. Below the LCST at 25°C (Fig. 1C) the increase of intensity at low-q is a feature of the formation of polymer cluster [4]. The curves best fitting indicated that the ‘’clustering intensity’’ is higher in presence of glycerol feature of a worse polymer-solvent interaction. The curves of SDS-containing samples show a structure factor peak signaling the formation of micelle, also hypothesizing the formation of a ‘’pearl necklace’’ structure. Above the LCST at 65°C (Fig. 1D), the aggregates formed by the HPC and by HPC/SDS systems have an ellipsoidal morphology.

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1B – evFOUNDRY - The Extracellular Vesicle Foundry (Horizon 2020 FET-Open project, No 801367)

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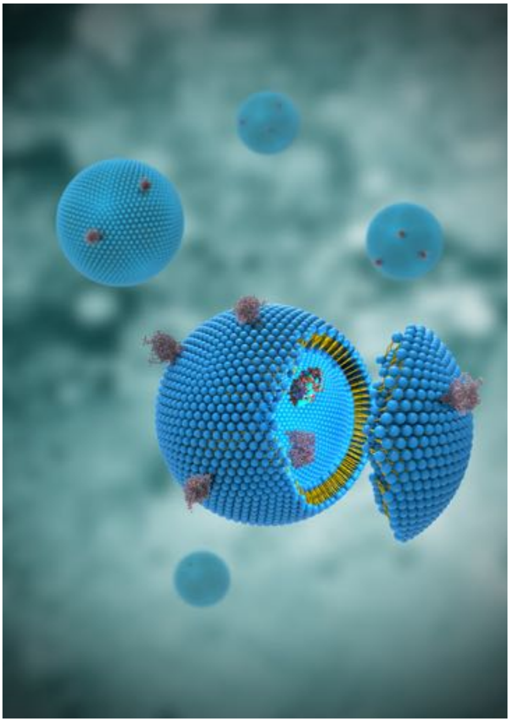
Aims

Extracellular vesicles (EVs) are natural cell-derived membrane-bound nanoparticles containing proteins and nucleic acids, which are newly recognized as the universal agents of intercellular and inter-organismal communication.

EVs are reshaping our perspective on life sciences, environment and public health. They are under intensive investigation as early disease multi-biomarkers, while EV-based personalized therapeutic agents and vaccines have produced enticing results in early-phase clinical trials.

FET-Open project evFOUNDRY targets the unmet knowledge and technology able to streamline production of therapeutic EVs from sustainable sources, drawing the baseline for future EV bioprocessing, which is necessary for effective EV medical translation and opens to new biogenic nanotechnology.



Results and References

http://www.evfoundry.eu/

1B – Exploiting interfacial chemical reactions to drive the formation of 2D materials at the air/water interface

G. Li Destri, N. Tuccitto, T. Amato, G.M.L. Messina, G. Marletta

Aims

Liquid surfaces and interfaces have been extensively used to drive the assembly of molecules and nanoscopic objects into two-dimensional (2D) structures, by using the intrinsic asymmetry of surfaces and interfaces as template to obtain continuous monolayers upon spreading or adsorption of amphiphilic species. Additionally, liquid interfaces and surfaces have also been exploited as an ideal asymmetrical reaction environment by using reagents that are mutually insoluble in one of the two fluid phases so that the reaction is intrinsically confined at the interface, leading to the formation of coordination polymer monolayers and nanosheets. In spite of these successes, following in situ and real time monolayer or nanosheet formation is not always possible, as it generally requires the occurrence of characteristic signals such as diffraction peaks. In this framework, we report a novel experimental approach using a water insoluble di-iminic ligand (DI), which is progressively hydrolyzed upon spreading at the water subphase. This approach allowed us to easily monitor the in-situ formation of the coordination polymer monolayer using the evolution of the surface pressure with time with a simple Wilhelmy balance.

Results

Figure 1a reports the time evolution of surface pressure of a DI monolayer spread at the air/water interface. The gradual decrease of surface pressure is due to the ongoing of the hydrolysis reaction, which leads to the formation of a water-soluble product (isobutylamine) and of a non-surface active di-aldeidic one (DA). As a result, hydrolysis is shifted toward the reagents if DI is spread on an isobutylamine solution (Fig. 1a, red curve), while DA monolayer does not form (Fig. 1a, blue curve)

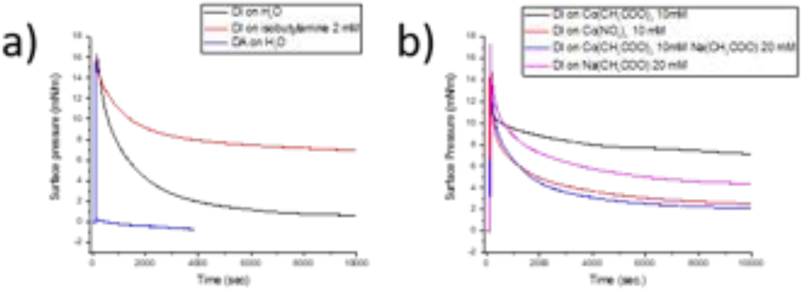


Fig. 1. Evolution of the surface pressure of DI and DA monolayers (a), effect of coordinating ions and pH on the interfacial hydrolysis of DI (b).

These results point out that surface pressure evolution with time can be exploited to monitor the hydrolysis of the ligand. As a result, if the ligand is spread on solutions containing the proper coordinating ion, the hydrolysis is arrested because of the coordination polymer monolayer formation (Fig. 1b). However, it is to mention that the mere presence of suitable coordinating ions is not sufficient to arrest the hydrolysis and to lead to the formation of the coordination polymer monolayer. In fact, the coordination reaction occurs exclusively at basic pH, as revealed by curves of Fig. 1b.

The formation of the coordination polymer monolayer was also confirmed ex situ by AFM imaging of monolayers deposited on solid substrates via the Langmuir-Schaefer method. The results are reported in Fig. 2 showing that, while in the presence of a proper coordinating ion an homogeneous monolayer is formed (Fig. 2a), if the ligand is spread on pure water it forms droplets (Fig. 2b) which, because of the hydrolysis, disappear with time (Fig. 2c)

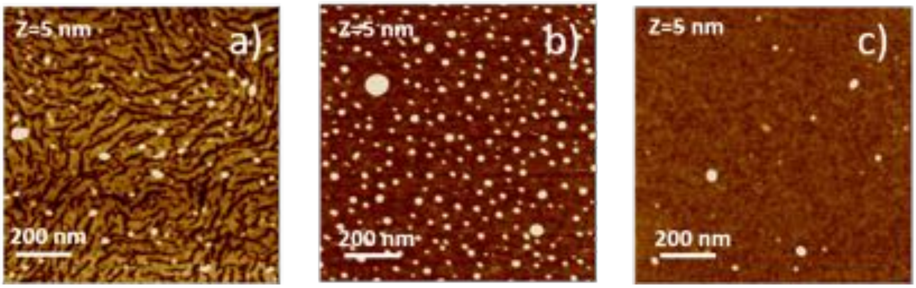


Fig. 2. AFM height images of DI ligand monolayer spread on a coordinating ion solution (a), spread on water and immediately deposited on solid substrate (b), spread on water and deposited on solid substrate after 1 hour (c).

These results confirm that 2D coordination polymer monolayer can be easily followed by exploiting competitive interfacial reactions such as hydrolysis and coordination. Additionally, they show that the spreading behavior of the ligand is not as straightforward as one would expect, as it is dramatically influenced by the subphase composition. The reason of this behavior can have either thermodynamic or kinetic origin, as it could be caused by a significant reduction of the interface free energy upon coordination or by the reduction of the spreading energetic barrier in the presence of proper ions. Further studies are ongoing to shed light onto this phenomenon.

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1B – Extracellular Polymeric Substances (EPS) extracted from anammox bacteria: structural, mechanical and applicative properties

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In collaboration with Prof. C. Lubello

Aims

The recovery of biopolymers from the waste sludge produced in wastewater treatments and their application in other industrial sectors, would substantially increase the environmental and economical sustainability of the process, promoting the development of a circular economy. In this study, extracellular polymeric substances (EPS) extracted from anammox granular waste sludge, were investigated and characterized. Rheological and differential scanning calorimetry measurements on EPS aqueous dispersions indicate the formation of an extended 3-D network above a threshold concentration, with a clear dependence of the mechanical and water retention properties on EPS content. The structural characterization, performed with transmission electron microscopy and small angle X-ray scattering, reveals the presence of functional amyloids as putative structural units, observed for the first time in an EPS-based hydrogel. As a proof of concept of the applicative potential, we explored the water and grease resistance provided to paper by an EPS coating. These results shed light on the structural details of EPS-based hydrogels and pave the way for the possible use of EPS-based materials as a cheap, ecofriendly alternative to commonly adopted paper coatings, in line with a circular economy patter for wastewater treatment.

Results

extracellular polymeric substances extracted from anammox granular waste sludge are able to form a hydrogel with solid-like mechanical properties, without any additional chemical cross-linker. Rheological and DSC analysis showed that for EPS concentrations above 17% w/v an extended 3D network is formed conferring to the material high mechanical and water retention properties (Figure 1). The structural characterization of the material suggests that fibrillar functional amyloids (which presence is shown in the TEM micrograph reported in Figure 2) represent the structural units of the 3D network formed in concentrated EPS dispersions.

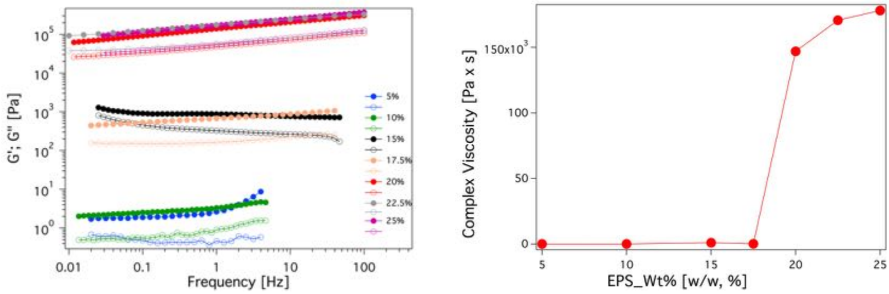

Fig. 1: Left: Trend of the elastic modulus G’ (full symbols) and of the viscous modulus G” (open symbols) as a function of the oscillation frequency of the applied shear stress for the investigated EPS based systems (amplitude strain, γ: 0.5%). Right: Trend of the complex viscosity, *η**, as a function of the EPS network concentration.

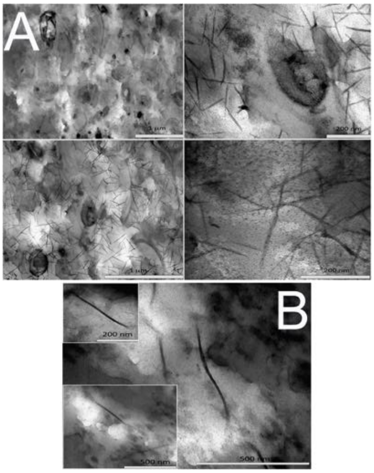

Fig. 2: TEM electron micrographs of (A) natural granules and of (B) EPS hydrogel 25 wt% (the thick of the thin sections is 100 nm).

Interestingly, diluted EPS dispersions can be successfully used to produce homogenous films with extremely low roughness. As a proof of concept, the application of EPS as a coating agent on paper greatly improves the water and grease resistance of the treated substrate. The reported properties of EPS-based materials could open new scenarios for the exploration of its potential applications as a resource in the context of circular economy.

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1B – Fourier-Transform Rheology and AFM Micromechanics of Soft Materials

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Aims

The mechanical properties of materials at rest are typically characterized by measuring frequency-dependent viscoelastic moduli, either macroscopically using rheometry, or at the micro/nanoscale by means of oscillatory AFM micromechanics. Both techniques present drawbacks associated with the technical complications of precisely controlling the amplitude and frequency of the oscillation. An alternative is represented by performing technically simpler measurements in the time-domain, to which an accurate Fourier Transform procedure can be applied to extract frequency-dependent moduli. We applied this approach to conventional rheological creep tests and AFM indentation and relaz.

Results

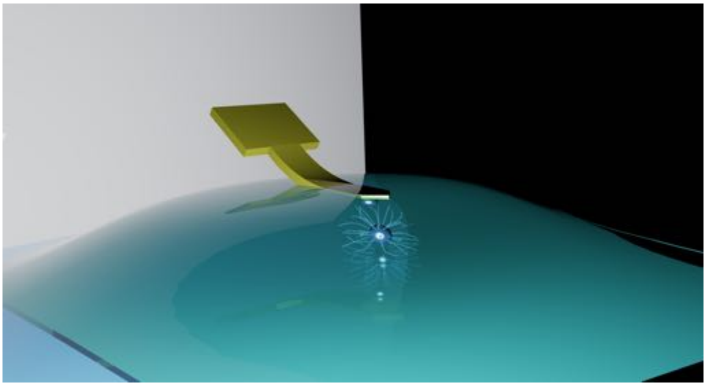

Fig.: Sketch of an AFM indentation experiment to measure the viscoelasticity of a single colloidal particle.

We applied the FT approach to creep tests measured in the rheometer to extract the viscoelastic moduli of dense colloidal suspensions. We found that, due to the fast sampling response of the rheometer in creep tests, a higher frequency domain can be achieved compared to conventional oscillatory measurements, even though tool inertia might be a limiting factor.

In AFM we used indentation and relaxation experiments (see a sketch in the figure) to determine the viscoelastic properties of single ds-DNA coated colloids in different saline buffers. We found that particles are stiff in the absence of salt, due to the stretched configuration of the DNA chains on the colloid surface, while they become suddenly soft with the addition of salt, due to the DNA progressive neutralization and collapse. Thus, the salt-dependent counterion distribution determines the particle degree of softness. A closer look at the frequency-dependent viscoelastic properties suggests that the energy dissipation at low frequencies (i.e., long times) is dominated by the collective force relaxation in the corona, whereas at high frequencies (i.e., short times) chain dynamics might be more important. Finally, we report that particles with a thicker DNA corona are softer, which can be associated with a lower DNA density in the outer side of the corona and/or a weaker contribution of the rigid core of the colloid.

The proposed approach can be generally applied to the determination of macroscopic or local viscoelastic moduli of soft materials.

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1B – Functional nanocomposites based on clay nanotubes

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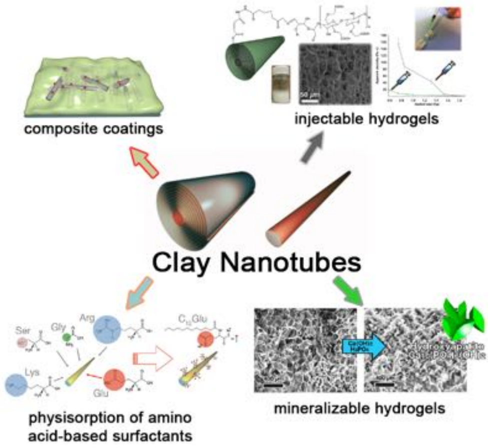
Aims

This project aims at the design, preparation and characterization of functional composites based on nanotubular clays, namely, imogolite nanotubes (INT) and halloysite nanotubes (HNT).

Results

Hybrid materials were obtained through different strategies, leveraging the different inner and outer surface chemistries of these nanotubes and their different aspect ratios, aiming at the preparation of biocompatible formulations of interest in the field of bone tissue engineering. Biodegradable composites were prepared through the introduction of HNTs in a PHBV matrix, so to impart novel mechanical and cation-exchanging properties, especially to transport Sr(II) ions at the treatment site.1 HNTs were also used to tune the rheological properties of carboxymethylcellulose (CMC), aiming at the formulation of an injectable composite for the minimally invasive treatments of local bone diseases.2 INTs were shown to enhance the mechanical stability of gelatin-based hydrogels and, more importantly, to promote their mineralization ability towards the formation of Hydroxyapatite.3 Thanks to the alumina surface, which makes INT very interesting as adjuvants in the formulation of pharmaceuticals, we explored the possibility to selectively adsorb amino acids and amino acid-based surfactants on these nanotubes and to use it as drug-delivery vehicles.4



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1B – Hierarchically self-assembled Frank-Kasper phase of CeO2-NPs superlattice induced by hydrophobic coating

N. Gallucci, G. Vitiello, I. Russo Krauss, L. Paduano

Aims

The aim of this research project is the physico-chemical investigation on the hierarchical organization of functionalized CeO_2 nanoparticles due to the presence of a hydrophobic coating by a combined approach of different techniques.

Results

Cerium oxide (CeO2) is used as an ultraviolet absorber [1], catalyst [2], polishing agent [3] and gas sensors [4]. In recent years, cerium oxide nanoparticles (CeO2-NPs) have attracted a great interest in the biomedical field, due to their pro-oxidant and anti-oxidant properties [5]. Particularly, CeO2-NPs have found to show both anti-oxidant and pro-oxidant behavior on different cells, mostly depending on: i. the presence of defects (i.e. oxygen vacancies) in the lattice structure, ii. the cerium oxidation states (Ce3+ or Ce4+) on the NPs surface and iii. the environmental conditions (such as local pH in cell systems). The functionality of CeO2-NPs can be related to their size and morphology, strongly depending by the synthesis methods, as well as to their hierarchical organization in the presence of templating agents. The physicochemical properties of the NPs (magnetic, fluorescent, optoeletric or redox activity) can be modulated either during the synthesis phase, choosing the appropriate synthetic approach and the synthesis conditions (e.g., precursor, pH, temperature, reaction time), or through the structuring of a hierarchic organization of singles entities in ordered phases (cubic, hexagonal), a process modulated by the interaction of the NPs amphiphilic coating. The single NPs and their more complex structures can become multifunctional entities able to perform, selectively, different specificities and/or implement their intrinsic physico-chemical properties finding, therefore, applications in different fields, from catalysis to electrochemistry, from photochemistry to biosensing and nanomedicine.

We have synthesized CeO2-NPs by thermal decomposition of Ce(NO3)3·6H2O in presence of oleylamine (OL), as capping agent, thus obtaining small nanoparticles (~ 5 nm) with spherical morphology. In order to disperse the nanoparticles in water, their surface has been functionalized using oleic acid (OA) or sodium oleate (SO). The preliminary data indicated that functionalized NPs showed a colloidal stability for a long time. Dynamic light scattering (DLS) data showed a hydrodynamic radius (Rh) of 300 nm for OA-OL-CeO2-NPs, while the Rh of SO-OL-CeO2-NPs was about 100 nm. Interestingly, Cryo-TEM images of OA-OL-CeO2-NPs indicated that the NPs organize forming Frank-Kasper phases, suggesting a key role of the oleic acid (OA) in inducing a hierarchically organization of the NPs. On the other hand, no similar evidences were obtained for SO-OL-CeO2-NPs. The difference in the organization driven by OA and SO is also evident from preliminary SANS experiments (Fig. 1).

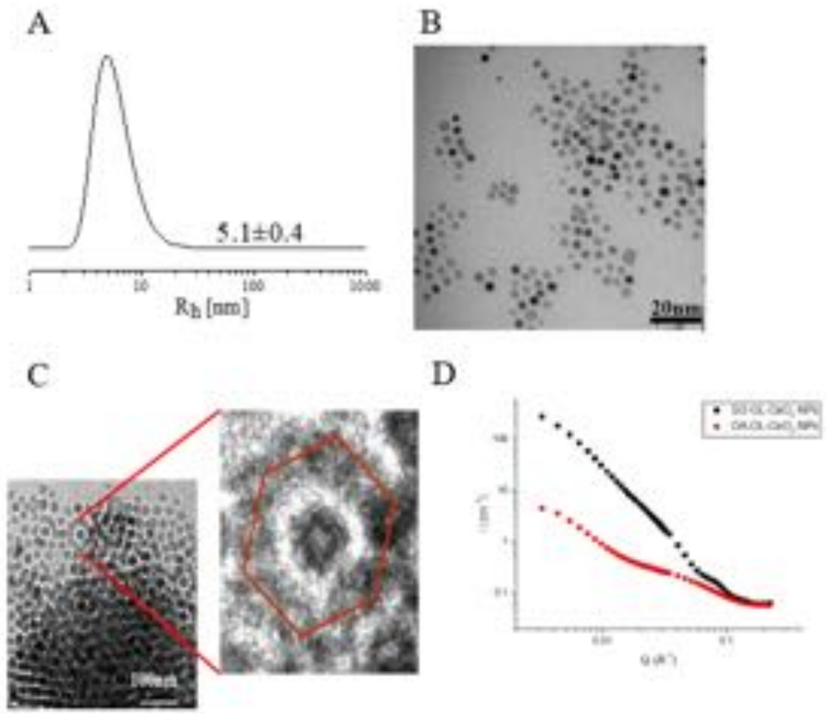

Fig. 1: Hydrodynamic radius distribution of OL-CeO2-NPs in chloroform (A); TEM image of OL-CeO2-NPs (B); Cryo-TEM image of OA-OL-CeO2-NPs in water (C); SANS data of SO-OL-CeO2-NPs (black squares) and OA-OL-CeO2-NPs (red circles) in D2O (D).

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1B – Hyaluronan-based graft copolymers bearing aggregation-induced emission fluorogens

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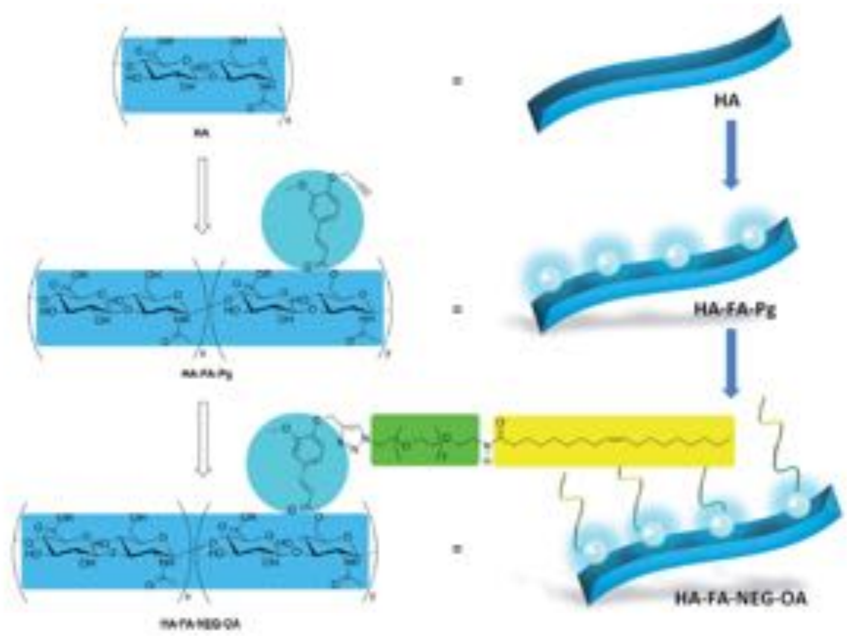
Aims

In order to develop a technology platform based on two natural compounds from biorenewable resources, a short series of hyaluronan (HA) copolymers grafted with propargylated ferulic acid (HA–FA–Pg) were designed and synthesized to show different grafting degree values and their optical properties were characterized in comparison with reference compounds containing the same ferulate fluorophore.
Interestingly, these studies revealed that the ferulate fluorophore was quite sensitive to the restriction of intramolecular motion and its introduction into the rigid HA backbone, as in HA–FA–Pg graft copolymers, led to higher photoluminescence quantum yield values than those obtained with the isolated fluorophore.
Thus, the propargyl groups of HA–FA–Pg derivatives were exploited in the coupling with oleic acid through a biocompatible nona(ethylene glycol) spacer as an example of the possible applications of this technology platform. The resulting HA–FA–NEG–OA materials showed self-assembling capabilities in aqueous environment. Furthermore, HA–FA–NEG–OA derivatives have been shown to interact with phospholipid bilayers both in liposomes and living cells, retaining their fluorogenic properties and showing a high degree of cytocompatibility and for this reason they were proposed as potential biocompatible self-assembled aggregates forming new materials for biomedical applications.

Results

We have developed a technology platform based on two natural compounds from biorenewable resources, namely low molecular weight HA playing the role of the macromolecular carrier, and FA playing the role of the aggregation-induced emission (AIE) fluorophore bearing clickable propargyl groups. Thus, a short series of hyaluronan-based graft copolymers (HA–FA–Pg) were designed and synthesized to show different grafting degree values and their optical properties were characterized in comparison with reference compounds containing the same ferulate fluorophore. Interestingly, these studies showed that the push–pull structure of the cinnamic scaffold of ferulate fluorophore was quite sensitive to the restriction of intramolecular motions (RIM) phenomenon, thus showing fluorogenic properties. In fact, model compound HA–FA–Pg-1F showed a typical aggregation-induced emission behavior, and the introduction of ferulate fluorogen in the rigid HA backbone as in HA–FA–Pg graft copolymers led to PLQY values in the solutions higher than of the corresponding value obtained with the solution of model compound HA–FA–Pg-1F in dichloromethane.



In the attempt to demonstrate the usefulness of the technology platform, the propargyl groups of HA–FA–Pg derivatives were exploited in the coupling with a third natural component from biorenewable resources (i.e. oleic acid) through a biocompatible spacer composed of nine monomeric units of ethylene glycol. The resulting HA–FA–NEG–OA derivatives showed selfassembling capabilities in aqueous environment and for this reason were characterized as potential biocompatible selfassembled aggregate forming material for biomedical applications.

In particular, HA–FA–NEG–OA derivatives were demonstrated to interact with phospholipid bilayers both in liposomes and living cells retaining the fluorogenic properties and showing a high degree of cytocompatibility.

On the basis of its high modularity, we envisioned for this technology platform a broad applicability. In fact, a broad range of polymeric carriers can be used beside to different fatty acid residues and oligo(ethylene glycol) spacers, with ferulate playing the central role of natural small molecule fluorogenic clickable linker.

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1B – Hybrid humic acids/metal oxides nanomaterials: from design to technological applications

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Aims

Design and characterization of multifunctional hybrid humic acid/TiO_2 nanomaterials, synthetized by a wet-chemical approach in order to valorize biowaste.

Results

Humic acids (HAs), which are heterogeneous, redox-active organic macromolecules that, thanks to their carbogenic diversity and tunable redox behavior, provide an important source for novel materials. Indeed, HAs present different functional groups (i.e. quinones, phenols and carboxylic acids) in their chemical structures, which are responsible of different properties, such as easy metal ions chelation, antibacterial, antioxidant as well as anti-inflammatory activity, regenerable red-ox behavior.

Despite their offered great potentialities, several challenges still need to be faced, mainly related to poor selectivity as well as short life-time, due to leakage and/or degradation phenomena as well as poor stability in aqueous environment. A valid strategy to overcome these disadvantages can be based on a conjugation of the HA moieties onto a foreign matrix, made of either organic and/or inorganic phase.

A new synthetic approach to hybrid nanomaterials was recently proposed, wherein inorganic oxides were employed as catalysts and structure directing agents in biopolymers building up [1-3]. The inorganic nanostructured component, i.e. TiO_2, proved able to tune biopolymers supramolecular structure, thus ultimately improving their properties [1-4]. A ceramic templated approach was exploited to produce hybrid HA-based nanostructures, showing uniform size distribution and a good chemical and colloidal stability in aqueous solution as demonstrated by DLS and SANS analyses.

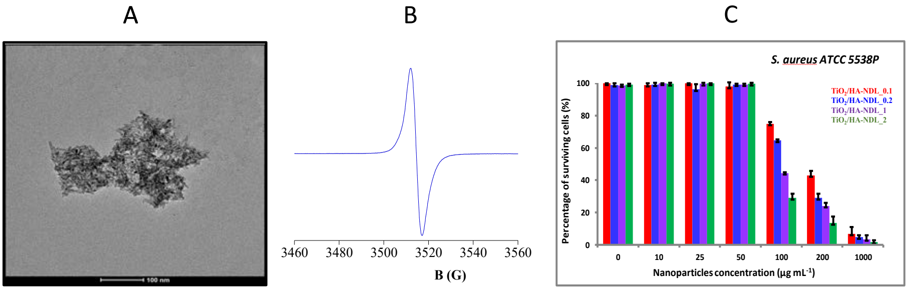

Fig. 1: TEM image (**A**) of HA/TiO_2 in aqueous suspension; EPR spectrum of carbon-centered radical species typical of HAs (**B**); antimicrobial activity of HA/TiO_2 NPs (**C**).

To shed light on the relationships between structural and functional properties of the nanohybrids, a wide physico-chemical characterization was realized by a combined approach of different techniques, among which Dynamic Light Scattering (DLS), Small-

Angle Neutron Scattering (SANS), TEM and Electron Paramagnetic Resonance (EPR) analyses (Fig. 1), in order to relate the morphological, surface and redox properties (generation of reactive oxygen species, ROS) of these nanohybrids with their functionality. These novel nanohybrids showed an interesting multifunctionality, as antimicrobial agents against Gram-negative pathogens of different strains and, at the same time, as sequestering agents towards three different antibiotics, usually found in aqueous solution as possible active agents for water remediation.

Obtained results disclosed the high potential of this approach to HA valorization, converting organic wastes into cutting-edge functional materials for many innovative applications such as biological as well water remediation.

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1B – Hybrid PVA-xanthan gum hydrogels as nucleus pulposus substitutes

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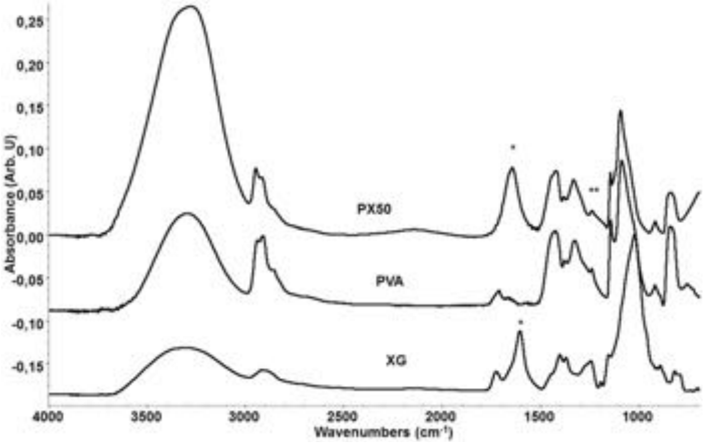
A. Donati, C. Rossi, A. Magnani (Department of Biotechnologies,
Chemistry and Pharmacy, University of Siena)

Aims

Hybrid hydrogels were synthesized mixing poly(vinyl alcohol) (PVA) and xanthan gum (XG) in different molar ratios and using trisodium trimetaphosphate, as crosslinking agent, to obtain potential nucleus pulposus substitutes. Human Nucleus Pulposus (NP) is a hydrogel-like tissue with peculiar properties, which determine its role in supporting and dissipating spinal loads. Hydrogel obtained mixing PVA and XG in molar ratio 4:1 (PX25) showed mechanical, swelling, and thermal properties, i.e., heat capacity, which make it a good candidate as a potential NP substitute. Preliminary cytotoxicity tests pointed out that the developed materials did not show any signs of cytotoxicity towards NIH3T3 cells.

Results

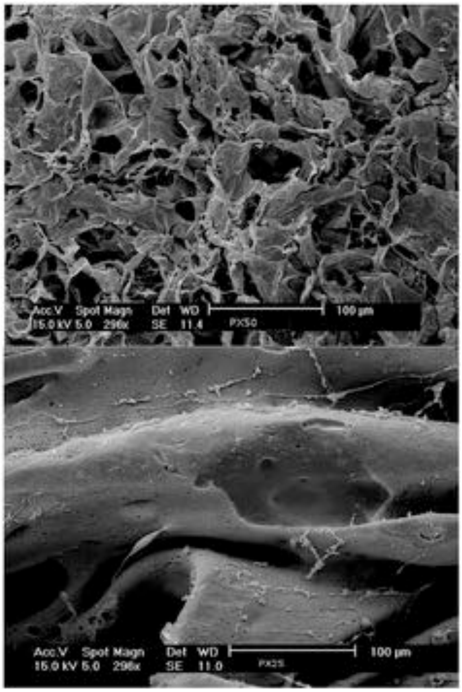
To study the physic-chemical properties the hydrogels were analysed by infrared spectroscopy.



Infrared spectra of the hybrid hydrogels were superimposable and showed the typical bands of both the polymers and bands related to the presence of crosslinking arms. In (a), the infrared spectrum of PX50, used as example, was depicted and compared with the IR spectra of native polymers. The band centred at 1600 cm-1, related to the asymmetric stretching of carboxylate group, confirmed the presence of xanthan gum and the band centred at 1237 cm-1, which is related to P[sbond]O[sbond]C, confirmed the crosslinking reaction. However, the obtained IR spectra showed very large bands, thus TGA was used to confirm interactions among the components.

The morphology of swollen hybrid hydrogels was analyzed by SEM and the obtained micrographs were reported in (b). The total amount of interstitial fluid dispersed in a polymeric matrix depends on the material network which affect the hydration of polymeric components thus generating the correct swelling pressure to ensure the physiological behavior of NP.

Hybrid hydrogel PX25 showed a homogeneous structure characterized by the presence of very small pores with a diameter ranging from 500nm to 1.5 mm whereas PX50 showed a porous texture with micrometric pores homogeneously distributed inside the sample bulk. Micrographs confirmed the trend observed in term of mesostructure withPX25 showing smaller pores than PX50.



Hybrid hydrogels were obtained mixing PVA and Xanthan Gum in different molar ratios. The crosslinking procedure permitted to obtain a PVA matrix containing Xanthan gum as confirmed by infrared spectroscopy, thermogravimetric analysis and RET. Among the obtained hydrogels, PX25 showed rheological, mechanical and swelling properties superimposable with those of human nucleus pulposus.

Moreover, the developed hydrogel had a heat capacity, at 37 °C, which can stimulate chondrocytes proliferation and, as a consequence, proteoglycan production, which is the key in homeostasis of the tissue.

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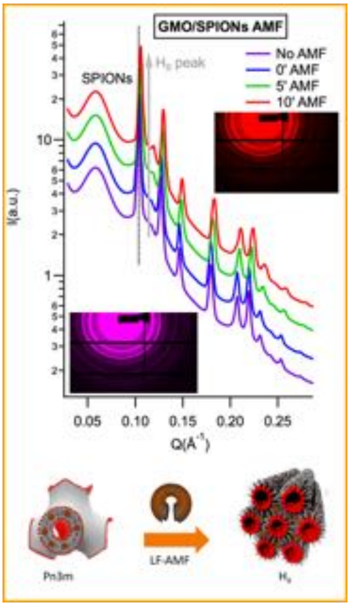
1B – Hybrid systems from magnetic nanoparticles and lipid mesophases

L. Caselli, C. Montis, D. Berti

Aims

Synthesis and characterization of hybrid lipid and magnetic nanoparticles systems as smart drug delivery carriers. Effect of alternating magnetic field on mesophase behavior.

Results



The inclusion of Fe3O4 nanoparticles in lipid structure, allows the combination of the lipid biocompatibility with the responsiveness to magnetic stimuli of such nanoparticle, making suitable candidates for a controlled drug delivery and release.

The organization of SPIONs within the lipid scaffold can lead to locally enhance SPIONs concentration and improve magnetic response, overcoming the current limitations of hyperthermic treatments. Structural thermotropic and magnetotropic behavior of glyceryl monooleate (GMO)/water mesophases, loaded with hydrophobic SPIONs was investigated with Small-Angle X-ray Scattering (SAXS). Low amounts of SPIONs deeply alter the phase behavior and thermotropic properties of the mesophases, promoting a cubic to hexagonal phase transition, which is similarly induced upon application of an Alternating Magnetic Field (AMF). Moreover, in the hexagonal phase we proved that SPIONs spontaneously self-assemble within the lipid scaffold into a linear supraparticle. The phase behavior was analyzed with Helfrich's theory, which shows that SPIONs affect the mesophase both from a viscoelastic and from a structural standpoint. Finally, the dispersion of these cubic phases into stable magnetic colloidal particles, which retain their liquid crystalline internal structure, is addressed as a promising route towards magneto-responsive drug-delivery systems (DDS).

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1B – Influence of composition and size asymmetry on the vitrified states of binary colloidal mixtures

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Aims

Amorphous solids states are ubiquitous in nature and technology, from food to medicine and engineering materials. Often, these systems present a high degree of structural complexity and are formed by several components. Binary mixtures of hard sphere-like colloids represent the simplest, tunable model system that can be used to study the properties of multi-component amorphous solids. By combining confocal microscopy and differential dynamic microscopy, we explore how variations in the mixture composition and particle size ratio affect the microstructure and dynamics of the particles, and consequently the mechanical properties of the system. This understanding provides a way to a bottom-up design of the response of the system in order to fulfill the needs of processing conditions.

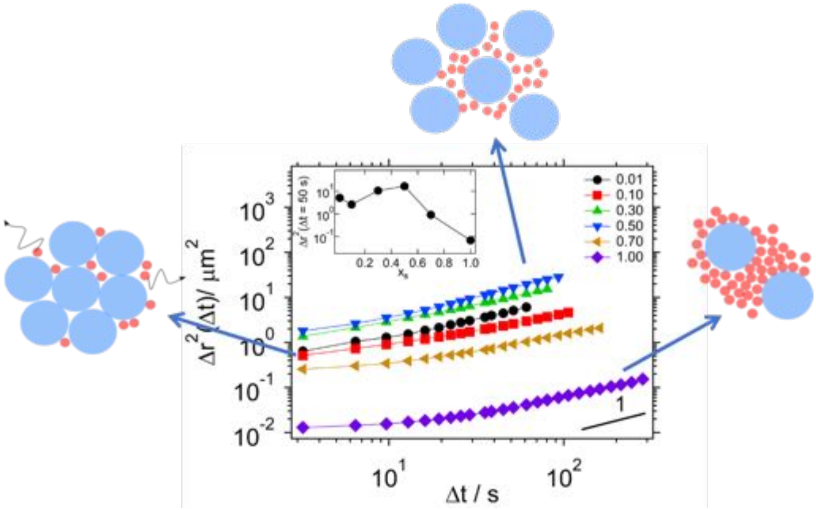

Fig.: For a size asymmetry of 1:4, the dynamics of the small particles reveal different states depending on composition: sub-diffusion due to confinement (left), solid melting (center) and re-solidification (right).

Results

Determination of the structure and dynamics of colloids, obtained from particle tracking and differential dynamic microscopy (DDM) applied to confocal microscopy experiments, reveals the strong influence of the size ratio and mixture composition on the non-equilibrium, vitrified states of dense suspensions. For similar sizes of the colloids, both species are vitrified to form an amorphous solid and composition variations act as polydispersity in shifting the critical volume fraction where the formation of the solid.

Increasing size asymmetry instead different states are observed depending on composition: When a small fraction of small particles fills the voids of a dense suspension of large particles, a single glass state is formed, in which only the large particles are dynamically arrested while the small particles are still able to diffuse within them. At intermediate compositions instead a double glass is formed, in which both species are dynamically arrested, or, for size ratios exceeding 1:3, the solid is melted into a high packing fraction fluid. For large fractions of small particles, the large particles act as defects in the homogeneous and dense solid formed by the small particles.

In the single glass state, the dynamics of the small particles are significantly coupled to the dynamics of the large particles and evidence anomalous diffusion which is related to the characteristic time of the opening of channels in the dense matrix of the large spheres. These findings have important consequences in general for transport phenomena in crowded environments, like the cell interior, cell membranes, porous matrices. The melting of the glass at intermediate compositions on the other hand shows a route for the transport of high particle content dispersions in a fluid state.

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1B – Interaction with human serum proteins of phosphocholine-functionalized nanoparticles

I. Russo Krauss, G. Vitiello, L. Paduano

Aims

The aim of this research is the investigation of the interaction of small SPIONs covered by an amphiphilic double layer of oleic acid/oleylamine and 1-octadecanoyl-sn-glycero-3-phosphocholine with two abundant human plasma proteins, human serum albumin (HSA) and human transferrin (HTF). We highlighted the SPION effects on protein structure and stability, by means of spectroscopic techniques, as well as the possible formation of a protein corona on the NP surface or of NP-protein aggregates, by means of a combination of scattering and spectroscopic technique, in order to assess biocompatibility of phosphocholine-functionalized SPIONs.

Results

Nanoparticles (NPs) are increasingly exploited as diagnostic and therapeutic devices in medicine. Among them, superparamagnetic nanoparticles (SPIONs) represent very promising tools for magnetic resonance imaging, local heaters for hyperthermia and nanoplatforms for multimodal imaging and theranostic. However, the use of NPs, including SPIONs, in medicine present several issues, first the encounter with the biological world and proteins in particular. Indeed, nanoparticles can suffer from protein adsorption, which can affect NP functionality and biocompatibility [1].

We found that SPIONs covered by a double layer of oleic acid/oleylamine and 18LPC [2] are able to interact with both the abundant human plasma proteins HSA and HTF, but the kind and strength of interaction is crucially dependent on the nature of the protein.

In the case of HTF the interaction is rather weak and no stable complex forms. Notably CD and fluorescence analysis indicate that SPIONs do not affect HTF secondary and tertiary structure [3], differently to what found differently coated SPIONs with similar dimensions, which cause irreversible changes of the protein conformation that may be at the basis of NP toxicity [4].

In the case of HSA a tight NP-protein complex forms, characterized by a binding constant of ~10^8 M^{-1} as determined by fluorescence quenching experiments and a well-defined geometry of interaction. HSA seem able to form both a hard and a soft corona on the SPION surface. DLS analysis show that upon extensive washing of protein excess, only SPION/HSA complexes with $R_H \approx 10$ nm are present.

The small dimension of our SPIONs can be called into play for their biocompatibility, at least with respect to interactions with proteins: indeed in the presence of a strong binding between a quite large protein such as HSA and the NP surface, no significant conformational change is detected for the protein. NR analysis was performed to analyse the interaction between HSA-covered SPIONs and lipid bilayers used as membrane models: protein-covered NPs are able to interact with and adhere to the surface of the lipid bilayers without removing lipids nor affecting the membrane structure, further pointing towards a high biocompatibility of the overall system.

Finally the HSA layer tightly bound to the SPIONs could be exploited for further functionalization of NPs, by taking advantage of the carrier properties of this protein, which have often been used to deliver drugs and diagnostic probes [3].

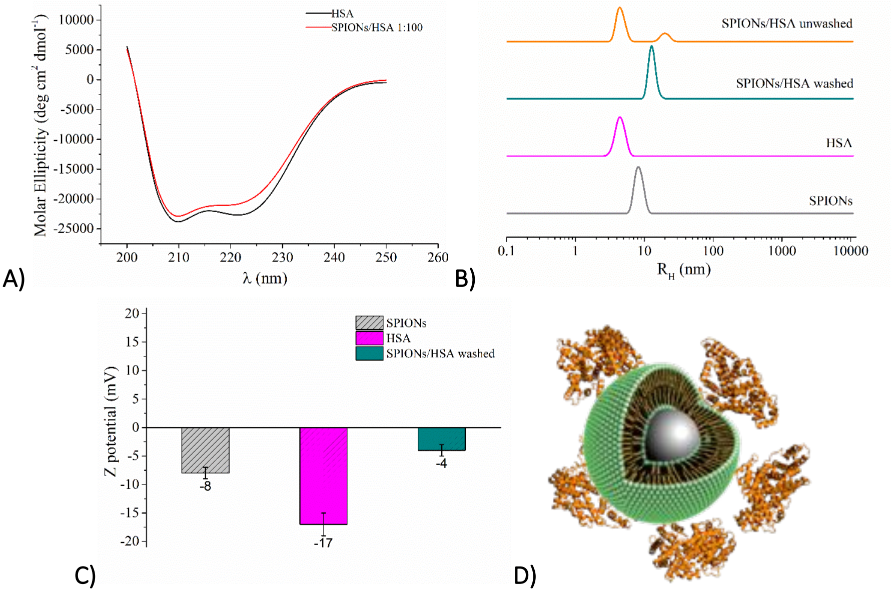

Fig. 1: A) Comparison of CD spectra of HSA in the absence and in the presence of SPIONs, B) DLS profiles of SPIONs/HSA with respect to isolated NP and protein, C) comparison of zeta potential values for SPIONs/HSA after removal of protein excess with respect to those of isolated NPs and protein, D) a sketch of the SPION/HSA complex

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1B – In-vitro digestion of Curcumin loaded in one layer polyelectrolyte capsules

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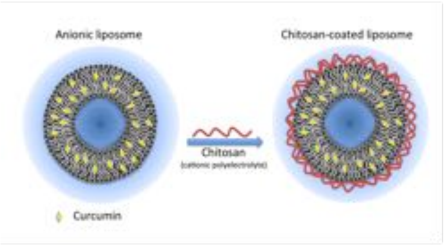
(Departamento de Quimica, Coimbra University, Portugal),
B. Lindman (Physical Chemistry, Lund University, Sweden),
F. Lopez

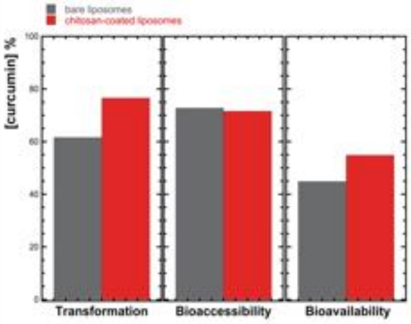
Aims

The wide-spread use of curcumin (from the rhizome of the *Curcuma longa*) is associated with its anti-inflammatory, anticarcinogenic and antimicrobial properties. The principal limitation for the application of curcumin in food and pharmaceuticals is its low solubility in water and its poor bioavailability. Several strategies have been set up in order to overcome the insolubility in water. Among them, colloid systems, such as micelles, liposomes or compartmentalized environments offer great potential of application. Here, curcumin was encapsulated in liposomes and chitosan was used to cover and protect the liposome. An in-vitro digestion model has been applied to study the effect of the use chitosan coating on the bioavailability of curcumin.

Results

Curcumin encapsulated into chitosan-coated liposomes is better absorbed than curcumin loaded into bare anionic liposomes. By means of DLS and ζ-potential it was first demonstrated that chitosan was able to stabilize curcumin-loaded liposomes. Anionic liposomes and cationic assemblies, were used for in-vitro digestion tests. The digestion model used simulates the food/beverages ingestion from mouth to the small intestinal phase. In every digestion compartment, the collective z-potential was measured also in the presence of the curcumin-loaded nanocontainers. It was demonstrated that chitosan-coated liposomes in the mouth phase interact with mucin because mucin is negatively charges at the mouth pH. The layer of mucin that probably covers the chitosan-coated liposomes provides a further protection to curcumin during the other digestion phases. This protection makes more bioactive curcumin available for the absorption in the raw digesta and in the bile salt micellar phase.





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1B – Ionic exchange resins and hydrogels for capturing metal ions in selected sweet dessert wines

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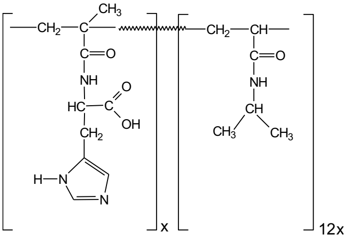
Aims

Samples of sweet and dessert wines, Vin Santo (VSR) from Malvasia grapes, and Granello (GR) from Sauvignon grapes were collected and analyzed for the content of selected macro- and micro-nutrients (Na, K, Mg, Ca, Mn, Fe, Cu and Zn) and of Pb. GR wines had low levels for Fe, Cu and Zn, when compared to VSR and particularly Zn was two orders of magnitude lower. Methods to decrease the content of Zn and Cu in VSR, as well as those for reducing at the same time, the concentrations of Ca, Mg and K in both VSR and GR, to avoid the formation of opalescence and depots of metal tartrates, were studied. Synthetic hydrogels containing L-histidine residue as well as commercial ion exchange resin Lanxess Lewatit L-207 and L-208 (legally allowed in the agro-food industry) were tested.

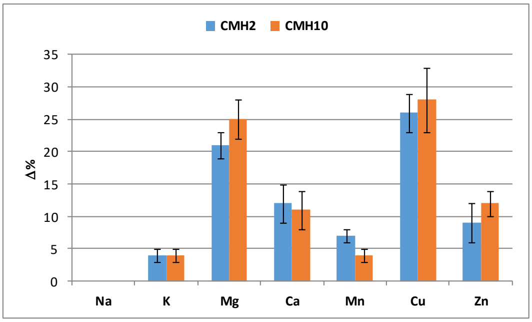
Results

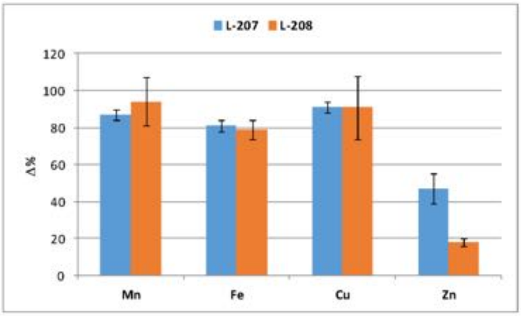
Selected macro- and micro-nutrients were analyzed on GR and VSR wine samples, from the sampling time up to stabilization, that occurred within ca 2 months. Synthetic hydrogels poly(N-methacryloyl-L-histidine-co-N-isopropylacrilamide), NIPAAM/MHIST molar ratio 12, cross-linked with 2 and 10 mol% of N,N'-ethylene-bis-acrylamide (CMH2 and CMH10) were tested. The overall relative lowering effects on Cu and Zn contents, for GR wine were by 25% and 10%, respectively. These materials have never been tested for wine treatments, neither for research or industrial purposes, and it has to be noted that these materials are expensive in terms of working time and cost of synthesis, purification, swelling, and regeneration.

Commercial ion exchange resin Lanxess Lewatit L-207 and L-208 were then assayed. The L-207 resin revealed a great lowering effect on the concentrations of Mn, Cu and Zn, being 75%, 91% and 97%, respectively in VSR wines and 77%, 76% and 92%, respectively, in GR wines. The content of Zn was reduced from 49.3±1.2 mg/L in the original wine down to 1.1±0.1 mg/L within 48 h of contact. The effects on the character of the dessert wines by the resin L-207 was also taken under control, measuring pH and color index.



CMH2 and CMH10





Particular attention was also devoted to the ecological aspects related to the treatments of dessert wines with L-207 resin, requesting activation and regeneration processes. The waste materials are in fact aqueous acidic solutions, but their acidity and amount are small when compared to the amount of treated wine. Hypothesizing the treatment of 1 hL of wine, the usage of about 5 L of HCl (2M) activating solution, 10 L of water used for the washing, and 2 L of discarded acidified wine, can be predicted. These acidic solutions need to be neutralized by treating them with NaOH (ca 0.4 kg), before being discarded as waste (ca 15 L of salt solution). Furthermore, the turnover of the resin has to be considered, mostly because of erosion and reduced activity. On assuming an erosion by ca 2% each treatment cycle (1 hL), times 10 cycles (10 hL of treated wine), it means that less than 500 g of resin are predicted to be disposed to waste. This corresponds to 2000 bottles (0.5 L each) of the final product, ready for the market. The exhausted resin could be sent back to the resin producer for overall reconditioning.

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1B – Linear Viscoelasticity and Yielding of one and two component colloidal glasses: link to microstructure and dynamics

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[5]Department of Chemical Engineering and Biotechnology, University of Cambridge, UK.

Aims

The determination of the link between mechanical response and microstructure of amorphous solids is of primary importance for their microscopic design and for the optimization of their processing conditions. Using model amorphous solids obtained from one and two-component colloidal dispersions we investigate such link, in particular how the linear viscoelastic properties are determined by the quiescent microscopic dynamics of the system and the structural rearrangements that govern the transition to flow at sufficiently large deformations. We combine for this purpose rheometry and in-situ confocal microscopy.

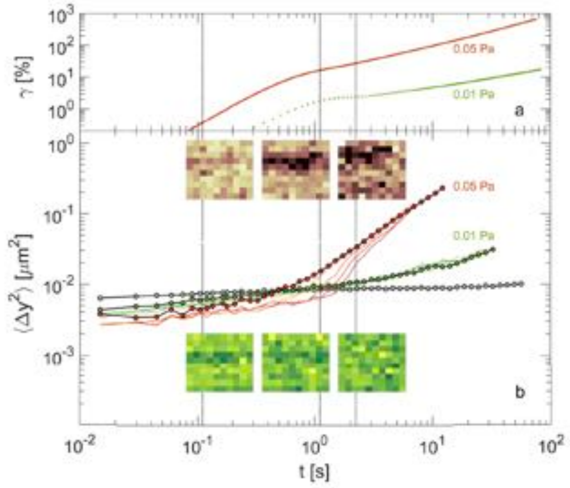

Fig.: Strain (top) and Mean squared displacement (bottom) measured simultaneously in rheo-confocal experiments for different applied stresses (as indicated). Images indicate the presence of regions with higher dynamical behavior (darker) in the field of view.

Results

In terms of linear viscoelasticity, we were able to semi-quantitatively link the frequency-dependent viscoelastic moduli to the microscopic dynamics of the colloid, by comparing experiments, simulations and Mode-Coupling Theory. In binary mixtures, either the large or the small particles mainly determine the moduli, depending on composition.

Under application of sufficiently large stresses or strains, the transition to flow is characterized by the rearrangement of the nearest neighbors, as observed from the rheo-confocal measurements and structural analysis. During this rearrangement we observe super-diffusive dynamics (see Figure) which turn into diffusion when the local neighborhood has been rearranged. We found that application of a constant strain rate is more efficient in rearranging the local structure, while under application of constant stress the yielding process is more heterogeneous and characterized by hotspots of locally enhanced dynamics (See pictures in the figure). However, both procedures lead to the same steady state of flow of the system.

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1B – Lipid-stabilized oil-water interfaces studied by Microfocusing Small Angle X-ray Scattering

I. Clemente, E. Di Cola, K. Torbensen, F. Rossi, A. Abou-Hassan, S. Ristori (University of Florence, Italy; Université Grenoble-Alpes, France; UPMC, France; University of Salerno, Italy)

Aims

Microconfined dispersed systems such as simple water in oil (w/o) emulsions possess interesting interfacial properties and a wide range of applications. Microfluidics is an advanced technique that allows precise control and enhanced flexibility in the fabrication of microemulsions. In this work, a microfluidic device was used to prepare w/o emulsions, stabilized by the phospholipid 1,2-dimyristoyl-sn-glycero-3-phosphocholine (DMPC) and other intercalating dopants. The stability and internal arrangement of such-built systems were investigated by Microfocusing SAXS, that performs raster scans of the sample with high spatial and temporal resolution.

Results

W/o emulsions were loaded on a capillary and then irradiated to obtain 2D- and 1D-SAXS intensity plots. The former in Fig.1 clearly showed the presence of an extended (~100 µm) diffuse scattering pattern at the liquid/liquid interface, stabilized by swollen and uncorrelated DMPC bilayers.

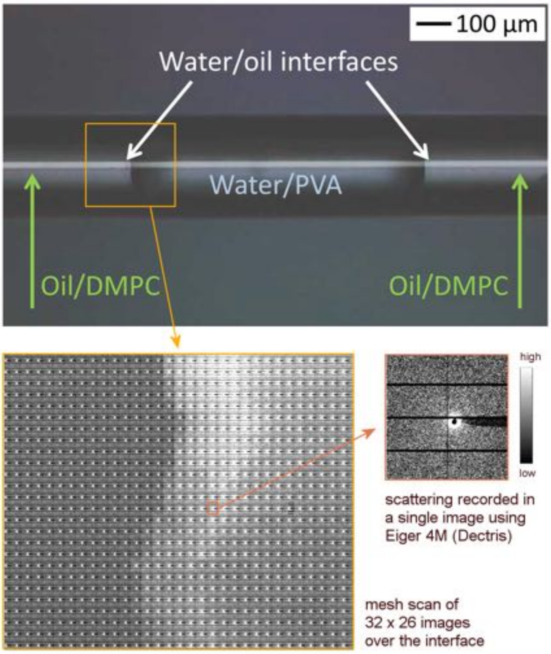

Figure1

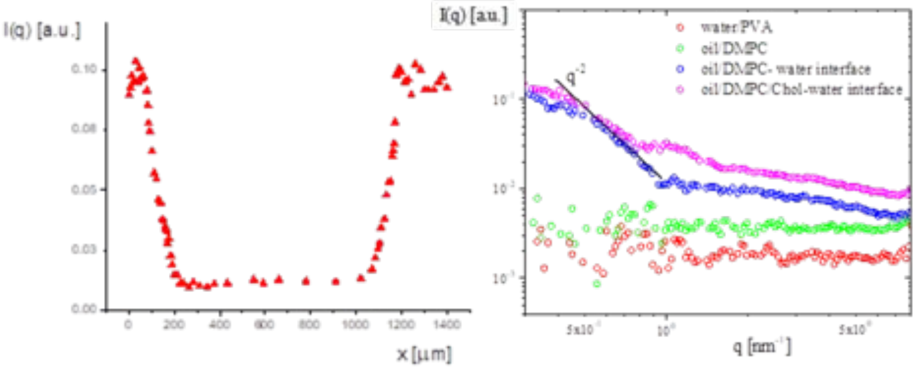

Figure 2

Axial scans (fig.2 left) along the droplets confirmed the presence of excess diffuse intensity corresponding to the stabilized interfaces, whereas the lower signal middle phase accounted for the internal aqueous phase (PVA). We investigated the variations in aggregation and bilayer stiffness through the addition in small percentage of other dopant molecules. 1d SAXS plots (fig.2 right) showed the profiles of both only DMPC and DMPC Cholesterol-doped samples, with respect to aqueous and oil bulk phases. In either emulsion samples a typical q-2 decay of locally flat objects could be seen, and for the Cholesterol-doped one inter-bilayer correlation was evident. Indeed, Cholesterol is known to impose a degree of rigidification in lipid bilayers. The only-DMPC sample did not show correlation, suggesting the presence of single and swollen self-assembled bilayers, which extended through the interface and stabilized it. Furthermore, no evidence of micelle aggregation could be seen in the bulk phases. We believe that this work could bring a contribution to the field of fabrication of microconfined lipid-stabilized water/oil interfaces by means of microfluidics and to the knowledge about their stability and communication abilities.

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1B – Liquid crystalline nanoparticles applications in nanomedicine

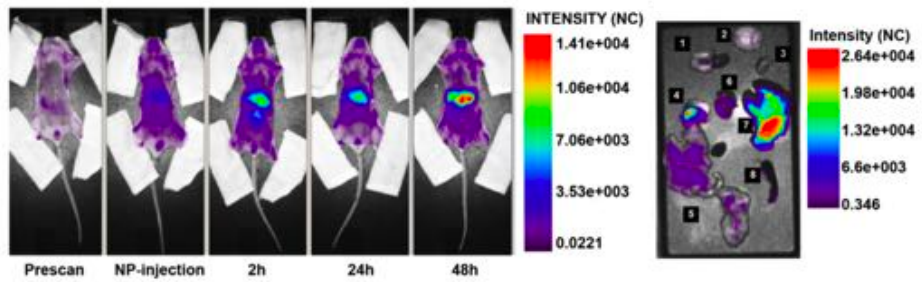
S. Murgia, C. Caltagirone, V. Lippolis, M. Monduzzi, et al.

Aims

Soft nanoparticles characterized by lamellar, bicontinuous cubic, and hexagonal inner structure (namely liposomes, cubosomes, and hexosomes) were systematically investigated in vitro and in vivo to explore their potential as pharmaceutical formulations.

Results

Hexosomes doped with docetaxel (a potent anticancer drug) and stabilized with a mixture of commercial and folate- and rhodamine-conjugated PF108 were formulated as theranostic tools in oncology. This nanoparticle showed good colloidal stability and drug release properties. Moreover, cytotoxic assays showed a 20-fold higher toxic effect of the drug-doped hexosomes against HeLa cells with respect to hexosomes not loaded with the drug. We also provided the first proof of principle for in vivo fluorescence optical imaging application in a healthy mouse animal model. Cubosomes loaded with a C_{14} modified 5.5 Cyanine (to allow a better encapsulation within the lipid bilayer), administered at a non cytotoxic concentration, allows both exogenous contrast for NIR fluorescence imaging with high efficiency and detailed chemospecific information.



Polymer free cubosomes loaded with photosensitizing dyes were formulated for the photodynamic therapy of skin malignant melanoma. Bioimaging studies demonstrated these nanoparticles were effectively internalized by Me45 and MeWo cell lines, while photodynamic activity experiments proved their significant cytotoxicity effect after photoirradiation.

Finally, to address the serious concerns posed by the use of adrenaline used in cardiopulmonary resuscitation, this drug was encapsulated into PEGylated, anionic liposomes by a pH-driven loading technique. This formulation showed excellent stability and release properties (as confirmed by two different in vitro release-testing methods), while cytotoxicity tests against human endothelial cells proved its biocompatibility.

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1B – Macro- Micro- and Nano-porous Gelatin Hydrogels

M. Bonini, R. Gelli, G. Mugnaini

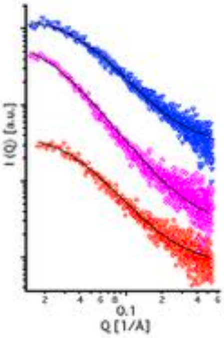
Aims

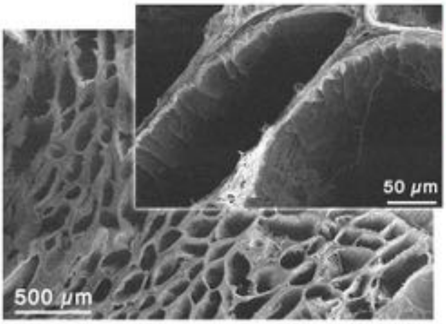
The aim of this project is the development of novel protocols based on emulsions, templates and/or cryoporation to prepare gelatin structures with controlled porosities ranging in the macro, micro or nano-scale. These systems are then investigated for their potential application in fields such as food, delivery of actives, and supported cell growth.

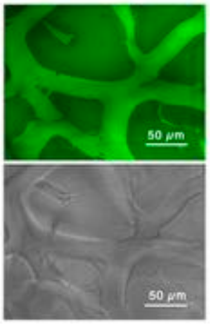
Results

Gelatin hydrogels have recently found many applications in different industrial applications, such as the controlled release of pharmaceuticals, tissue engineering and food formulations. Biocompatibility, biodegradation, thermal responsivity, water uptake and porosity are probably the most relevant properties in those applications.

In this project we developed different protocols for the preparation of gelatin hydrogels crosslinked either with glycerol diglycidyl ether or glutaraldehyde. The hydrogel structure was modified through cryoporation (i.e., controlled formation of ice crystal within the hydrogel, followed by sublimation of ice) or by the use of oil-in-water-in-oil emulsion strategies, resulting in the formation of porosities ranging from tens of nanometres up to hundreds of microns. The structure of these systems is investigated at different length scales by means of Small Angle Scattering of X-Rays (SAXS), Field-Emission Scanning Electron Microscopy (FE-SEM), Optical microscopy and Laser Scanning Confocal Microscopy (LSCM), showing that pore sizes and pore wall thicknesses could. The diffusion properties are evaluated by kinetic release experiments, as well as by Fluorescence Correlation Spectroscopy and Fluorescence Recovery after photo-bleaching. These results open the way towards for the smart design of gelatin-based hydrogels with predictable diffusive properties.







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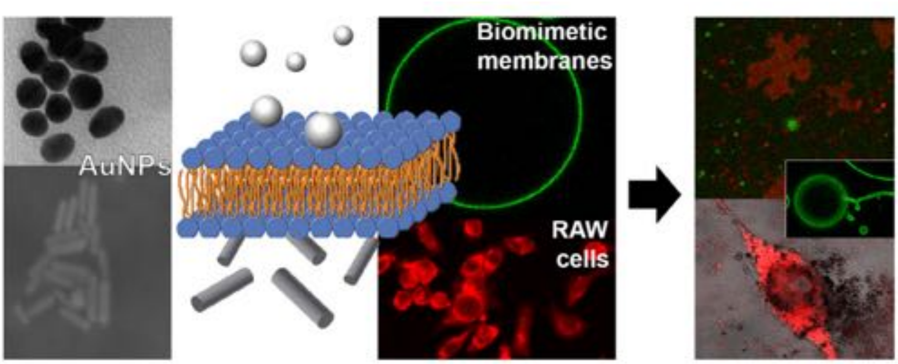
1B – Model lipid bilayers to mimic non-specific interactions of nanoparticles with plasma membranes

C. Montis, P. Bergese, L. Caselli, D. Berti

Aims

We investigate non-specific interactions of inorganic nanoparticles (AuNPs) with synthetic and biogenic membranes, proving a correlation between the findings on synthetic and real cell membranes, which is still lacking.



Results

A comprehensive data set was generated by systematically varying the structural and physicochemical properties of AuNPs (size, shape, charge, surface functionalization) and of the synthetic membranes (composition, fluidity, bending properties and surface charge), which allowed to unveil the matching conditions for the interaction of the AuNPs with macrophage plasma membranes in vitro. This effort directly proved for the first time that synthetic bilayers can be set to mimic and predict with high fidelity key aspects of nanoparticle interaction with macrophage eukaryotic plasma membranes. It then allowed to model the experimental observations according to classical interface thermodynamics and in turn determine the paramount role played by non-specific contributions, primarily electrostatic, Van der Waals and bending energy, in driving nanoparticle-plasma membrane interactions

Non-specific interactions controlled Au NPs approach with both model membranes and the macrophage membranes, proving the utility of biomimetic membranes as simple models to investigate and predict the NPs behavior with cell membranes. In a future perspective, a complete understanding of natural membrane will need the increase of structural and functional complexity of model membranes.

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1B – Nanostructuring-driven protein-surface interactions

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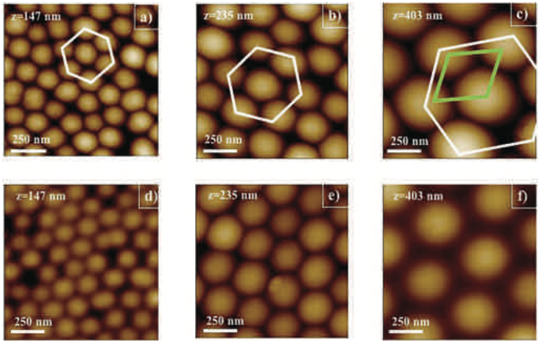
Aims

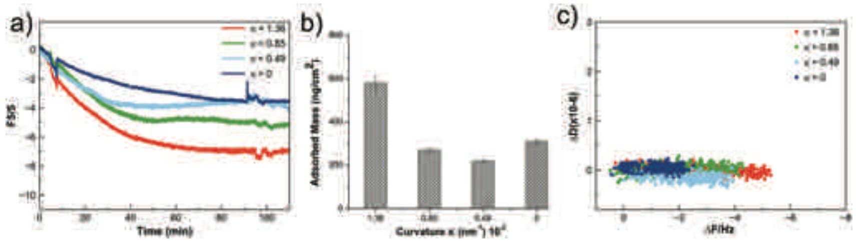
Nanostructured surfaces have a dramatic effect on the amount of protein adsorbed and the conformational state and, in turn, on their performances in tissue engineering applications. Here we describe an innovative method to prepare silica-based nanostructured surfaces with a reproducible, well-defined local curvature, consisting of ordered hexagonally packed arrays of curved hemispheres, from nanoparticles of different diameters (respectively 147 nm, 235 nm and 403 nm). Experimental and theoretical study of laminin, taken as a model protein, to study the nanocurvature effects on the protein configuration at nano- structured surfaces have been done. It is shown that nanocurvature may drive the orientation of rigid proteins by means of a "geometrical resonance" effect, involving matching of dimensions, charge distribution and spatial arrangement of adsorbed molecules and adsorbent nanostructures. Overall, the results pave the way to unravel the nanostructured surface effects on the intra- and inter-molecular organization processes of proteins.

Results

Regular hexagonal close-packed 2D structures have been obtained by using NPs of three different diameters 147 nm, 235 nm and 403 nm, with nominal thickness and center-to-center distance of the nanoparticle arrays determined by the diameter of the employed NPs in a close-packed arrangement.

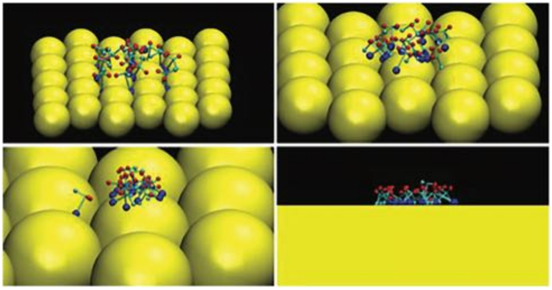


Laminin adsorption was studied by means of QCM-D technique for each nanostructured surface. The quantitative adsorption data were used to obtain information on the protein organization for different curvatures. The data indicate that the surfaces with the highest curvature yield a threefold adsorption of laminin with respect to the lower curvature surfaces and twofold with respect to flat surfaces. At the same time, the enhancement of the laminin adsorption occurs only above a nanocurvature threshold.



The higher adsorption suggests that laminin molecules are adsorbed with a different orientation onto low curvature and flat surfaces, i.e., with a different molecular packing.

The role of surface nanocurvature on the laminin adsorption has been analyzed by using mesoscale models for the protein and the surfaces and their interactions have been simulated by applying the Montecarlo algorithm.



The experimental and theoretical results shed light on the close connection between the nanostructure of surfaces and protein adsorption. The curvature effect is depending on the asymmetric nature of the adsorbing molecules and the enhancement or decrease of the protein adsorption involves drastic orientation effects, which can be modulated by a "geometrical resonance" between the dimension and spatial arrangement of the adsorbing molecules (i.e., their tertiary and quaternary structures) and the nanocurved structures. In general, these arguments seem to have a wider validity, as suggested by their analogy with models developed for globular macromolecules end-attached to nanocurved surfaces, as well as for the dependence of protein conformational changes on their relative dimension with respect to the surface roughness. Overall, the results reported here must be read in the framework of nanostructuring on bio- macromolecule adsorption and their intra- and inter-molecular organization processes.

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1B – New experimental approaches for the development of lubricant additives

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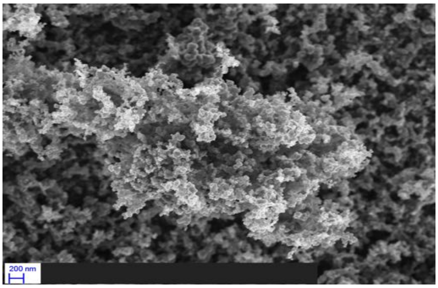
Aims

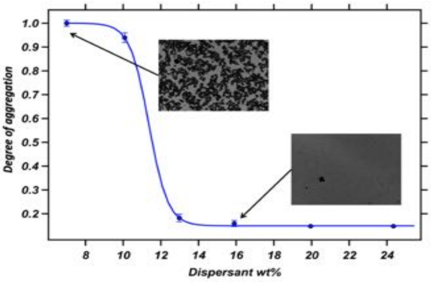
Development of new experimental and methodological approaches for the design of innovative additives in the field of engine lubricants.

Results

In the last decades, the industrial research has grown to develop more efficient engines and reduce their maintenance costs. One of the main factors affecting engine performances is the formation of carbonaceous particles during the normal operation of the engine, which is responsible for the change in the lubricant oil viscosity, eventually leading to engine failure. To reduce the formation and growth of carbonaceous particles, commercial lubricants contain many chemical additives. Among them, oil-soluble dispersants are used to inhibit the growth and aggregation of carbonaceous deposits.

It is therefore necessary to develop an innovative, cheap and easy to implement lab-scale methodology to evaluate the dispersive effectiveness of a lubricant oil formulation containing different additives. Our approach is based on the direct rank of the dispersion power of the lubricant formulation. In particular, optical microscopy was employed to evaluate the interaction between a series of additives with different chemical structure and molecular weight and carbonaceous substrates. Our results indicate that the dispersant ability is strictly connected to the dimension of the polar portion of the additive.





This study represents an advancement in the knowledge of lubricant chemistry and in the comprehension of the main parameters affecting the dispersant performances of different kinds of amphiphilic molecules. The correlation between the colloidal behavior of the amphiphiles and their dispersant efficacy can be used to guide the synthesis of novel oil soluble dispersants with enhanced activity against the carbonaceous particulate deposition in lubricant media.

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1B – Peelable polyvinyl alcohol highly viscoelastic dispersions loaded with nanostructured fluids: a new class of cleaning tools for works of art

E. Carretti, G. Poggi, E. Fratini, L. Dei and P. Baglioni

Aims

Complex systems made of High Viscosity Polymeric Dispersions (HVPD) based on polyvinyl acetate (PVA), borax and water and loaded with microemulsions were developed.

These nanostructured systems can provide a new resource for the cleaning of painted surfaces.

→ The oil-in-water microemulsion (composed by H_2O, sodium dodecyl sulphate, SDS, 1-pentanol, 1-PeOH) is effective in the removal of unwanted hydrophobic polymers from the porous substrates of mural paintings.

→ 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 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, 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 and the mechanical action and repeated washings usually necessary for the complete removal of traditional gels can be avoided. 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 confined o/w microemulsion has been characterized by Small Angle X Rays Scattering (SAXS) and rheology in order to obtain informations about both the structure (i. e. the radius of the nanodroplets and their polydispersity) and the mechanical behavior, with particular attention on the effects induced by the presence of the PVA based 3D network. In particular, the experimental data indicate the persistence of the nanostructure of the o/w microemulsion (this is a fundamental requirement to warrantee the cleaning efficacy of the system) and that the relaxation of the PVA network occurs through a sticky reptation mechanism.

Contact angle, TOF-SIMS, 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.

Moreover, recently, we have found that inside the HVPDs, apart organic solvents and o/w microemulsions, it is possible to insert also 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.

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1B – Poly(vinyl alcohol) Microgel Prepared through Liquid-Liquid Phase Separation

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Aims

The use of technologies based on soft polymer particles represents an effective way to deliver target molecules with a specific function. Poly(vinyl alcohol), PVA, is among the most common species used for preparing polymer particles. This is, thanks to its low-toxicity, noncarcinogenicity, good biocompatibility, and desirable physical properties of the resulting particles such as a rubbery or elastic nature and a high degree of swelling in aqueous solutions.[1] To design a well-performing delivery system, it is fundamental to rationalize both the aggregation and the structural properties of such particles. For this, we present the kinetic and structural characterization over time of PVA microgels obtained through a salting-out process in the presence of NaCl.[2] The preparation of PVA aggregates without the use of chemical cross-linkers does not modify the structure of the polymer, preserving its original properties of biocompatibility and biodegradability. The addition of a species that reduces the solubility of the polymer (known as cosmotropic species) triggers the polymer aggregation, inducing a local phase separation. As a result of such aggregation, a colloidal dispersion is formed. PVA can show an aggregation behavior in NaCl solutions similar to that already found for EVOH,[3] which differs chemically from PVA due to the presence of ethylene sequences along the polymer chain. Understanding the relationship between the aggregation regime and the corresponding morphological, microstructural, and internal dynamic features is mandatory for any potential application of polymer microgels in technological fields.

Results

PVA microaggregates are widely used in various field, including biomedicine, catalysis and environmental science.[4] PVA particles prepared through salting-out are formed following an easy protocol, which does not require the use of chemical cross-linkers and that guarantees, at the same time, a compact structure where hydrogen bonding represents the main interaction among polymer chains. To rationalize the aggregation process of PVA in the presence of NaCl as a salting-out agent was necessary the use of various experimental techniques, including DLS, SLS, SANS, TEM. As a result, it was found that NaCl induces a liquid phase separation in solution with the formation of spherical PVA microaggregates, which increase their size and compactness over time. The radius of gyration of the aggregates over time follows a power-law with their molecular weight with an exponent quite close to 0.33, typical of spherical homogeneous particles, a result confirmed by TEM images. The PVA aggregation, upon increasing salt concentration, occurs under a reaction-limited aggregation (RLA)[5] mechanism, which leads to an increasing polymer density that reflects in a more compact aggregate.

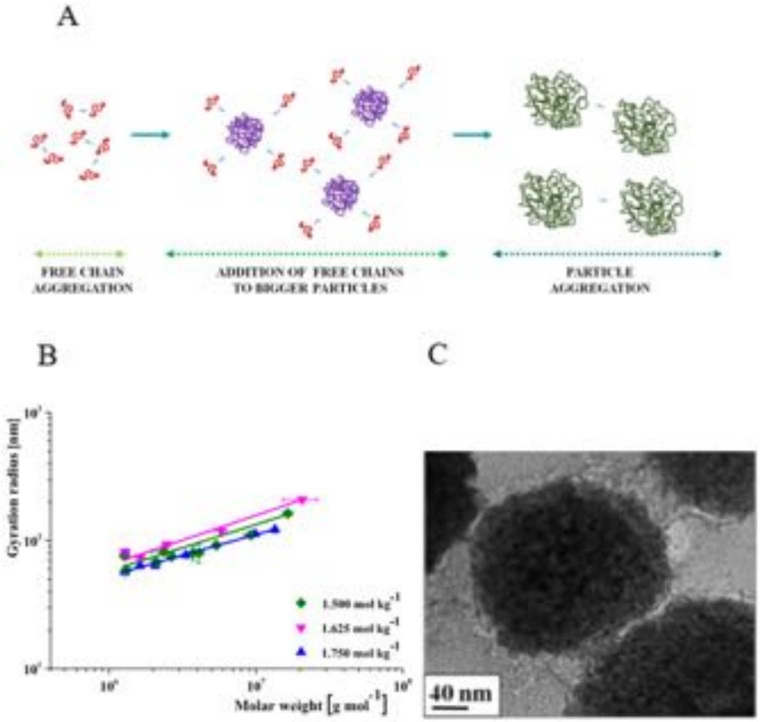

Fig. X: Sketch representation of the hypothetical PVA aggregation mechanism. Violet particles are the result of the free chain aggregation; over time, these also self-aggregate (green particles), forming large particles and eventually precipitate (A); Dependence of gyration radius on aggregate molar weight at three different NaCl concentrations (B); TEM image (C).

The microparticle preparation based on the salting-out process constitutes a novelty and is a cheap and easy protocol that allows tuning both particle size and density by varying the salt concentration.

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1B – Protective effect of quercetin and rutin encapsulated liposomes on induced oxidative stress

C. Bonechi, A. Donati, G. Tamasi, G. Leone, M. Consumi, C. Rossi, S. Lamponi, A. Magnani (Department of Biotechnologies, Chemistry and Pharmacy, University of Siena)

Aims

Natural antioxidants show many pharmacological properties, but poor solubility and inability to cross cell membrane. Liposomes are biocompatible and phospholipid vesicles able to carry hydrophilic, hydrophobic, and amphiphilic molecules. This work focus on the synthesis of anionic, cationic and zwitterionic liposomes, loaded with quercetin or rutin, and on the evaluation of their cytotoxicity and protective effects against oxidative stress.

Chemical characterization was obtained by dynamic light scattering and ζ-potential experiments. In vitro cell behavior was evaluated by Neutral Red Uptake test.

All liposomes, empty and loaded with antioxidants, are stable. The cytotoxicity of both quercetin and rutin encapsulated in zwitterionic and anionic liposomes is higher than that of their solutions. Quercetin (Q) and rutin (R) loaded in cationic liposomes are able to inhibit the toxic effect of empty liposomes. The encapsulation of rutin at 5.0 $\times 10^{-5}$ and 5.0 $\times 10^{-4}$ M, in zwitterionic and anionic liposomes, protects fibroblasts by H_2O_2 treatment, while the loading with quercetin does not have effect on improving cell viability.

All data suggest that the tested liposomes are stable and able to include quercetin and rutin. The liposomes encapsulation of antioxidants makes easier their internalization by cells. Moreover, zwitterionic and anionic liposomes loaded with rutin protect cells by oxidative stress. Liposomes stability together with their good in vitro cytocompatibility, both empty and loaded with antioxidant molecules, makes these systems suitable candidates as drug delivery systems. Moreover, the encapsulation of rutin, is able to protect cells by oxidative stress.

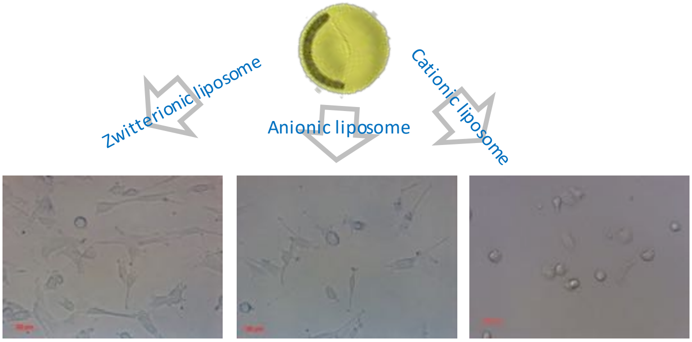
Results

All experimental chemical data suggest that the liposomes studied in this work (zwitterionic, anionic and cationic) are stable and are able to include the two antioxidants: quercetin and rutin. In fact, the size and ζ-potential values showed modifications according to chemical properties of Q and R. Liposomes are stable and not present aggregation processes versus conservation time, at least up to 3 months. The Q and R loaded liposomes show a fairly low encapsulation efficiency which does not negative influence the biological data. This result highlights that liposomes are excellent drug delivery systems for quercetin and rutin,which are protected from chemical and physical degradation processes.

Encapsulation efficiency of quercetin (Q) or rutin (R) in liposomal formulations (mean ± S.D.)

Liposome Composition	Encapsulation Efficiency (EE) %
DOPC/DOPE + Q	18.9 ± 5.3
DOPE/DOPA + Q	14.2 ± 1.9
DOPE/DOTAP + Q	15.6 ± 1.5
DOPC/DOPE + R	12.9 ± 5.2
DOPE/DOPA + R	12.3 ± 6.1
DOPE/DOTAP +R	12.9 ± 4.7

Moreover, the zwitterionic liposomes show chemical and biological properties better than the anionic and cationic vesicles. The anionic liposomes can be excellent drug delivery systems for specific compound for specific lipid concentration.



Biological results confirm that the use of liposomes as carriers, may help cell internalization of the studied flavonoids, which better interfere with cell at lower concentrations, with respect when they are free in solution. Moreover, in agreement with the evidence of neuroprotective effects of rutin against H_2O_2 induced oxidative stress in cerebral glioma cell line, rutin both in solution and liposomes loaded, interferes with the hydrogen peroxide induced toxicity, showing a good ability as cells protector. So, the loading of liposome with antioxidant molecules can be considered a good method to improve cell internalization of molecules characterized by low solubility in water media.

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1B – Quality control of fresh-cut apples after coating application

F. Cuomo, M. Cofelice, F. Lopez

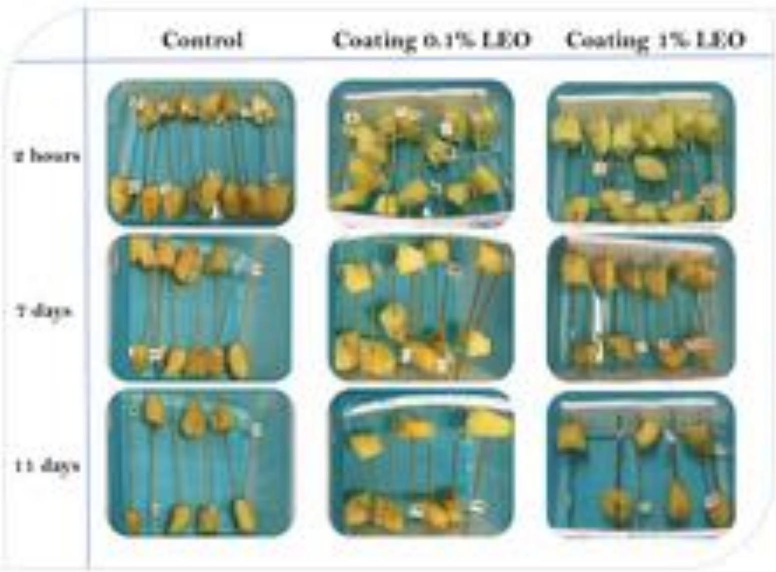
Aims

The modification in consumers' life style and the increasing attention to healthy and nutritional food products enlarged the request of ready-to-eat products, like fresh-cut fruit. This kind of commodities is highly perishable and difficult to preserve since minimal processing removes fruits natural protection. An appropriate strategy for ensuring food products protection could be the deposition of a kind of new peel produced by an edible coating on the surface of the fresh-cut fruits.

An edible coating or film is defined as a primary packaging made of edible components. A thin layer of edible material can be directly deposited on food or formed into a film to be used as a food wrap without changing the original ingredients or the processing method.

Results

To investigate on how some physicochemical quality parameters are influenced by the application of edible coatings, two nanoformulations are used for coating fresh-cut apples. The oil in water nanodispersions were made of sodium alginate suspension (1% w/w) and lemongrass essential oil (LEO) at two different concentrations (0.1% and 1% w/w) stabilized by the non-ionic surfactant, Tween 80. The rheological behavior of the nanodispersions was determined with rotational and oscillatory tests and the edible coating was applied on apple slices by dipping method.



The effectiveness of nanodispersions as edible coating was investigated on coated fruits stored at 4°C for 14 days while uncoated slices were used as control.

Physicochemical parameters like pH, titratable acidity, weight loss and total phenolic content were analyzed during storage. Both the nanoformulations had suitable rheological characteristics for being applied on fruit by dipping method, but their oil content influenced differently the fruit quality during storage. Considering all the parameters analyzed, like the slowing down of the surface browning and the positive effects on pH and TA, the nanoformulation with the low essential oil content seemed more promising and appropriate than the 1% LEO nanoformulation for being applied on ready-to-eat fresh products. As a whole the outcomes of this study offers suitable nanoformulations to be used as edible coating. Such nanodispersions are able to protect fruits stored at 4°C for several days. Deterioration events like respiration, moisture loss and enzymatic activity are mitigated after the applications of these edible films.

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1B – Rheological Characterization of Hydrogels from Alginate-Based Nanodispersions

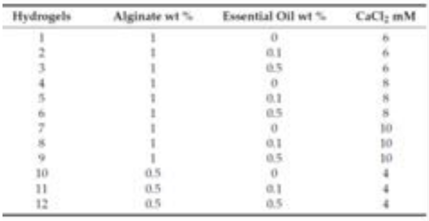
F. Cuomo, M. Cofelice, F. Lopez

Aims

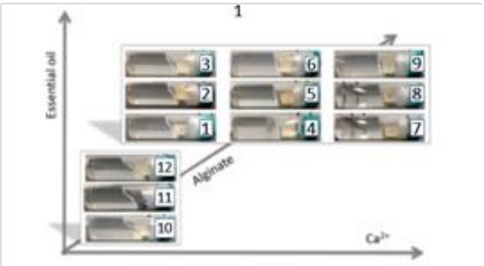
Alginate hydrogels have a high potential of application ranging from clinical practice, biomedical use and food science. Lately, an increasing interest has been focused toward complex hydrogels mainly produced by gelation of emulsion/nanoemulsion in order to design more stable materials able to encapsulate and deliver hydrophobic compounds in a hydrophilic network. Among the lipophilic phases used to formulate nanoemulsions hydrogels, a particular interest is directed to the use of essential oils. Essential oils, besides being able to solubilize lipophilic substances, have antimicrobial and antioxidant properties.

Results

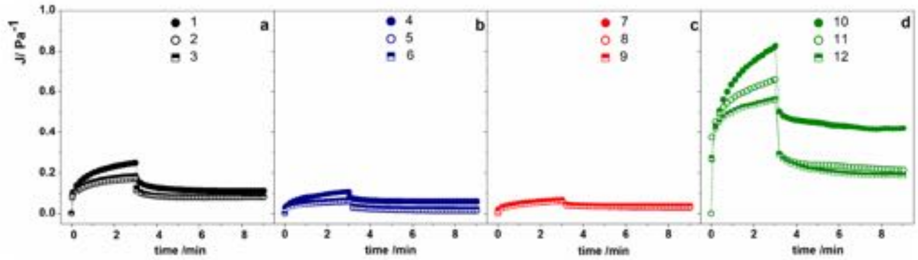
The rheological properties of hydrogel based nanodispersions made of alginate and lemongrass essential oil were analyzed. Different alginate, essential oil and calcium concentrations were considered.



Hydrogels	Alginate wt %	Essential Oil wt %	$CaCl_2$ mM
1	1	0	6
2	1	0.1	6
3	1	0.5	6
4	1	0	8
5	1	0.1	8
6	1	0.5	8
7	1	0	10
8	1	0.1	10
9	1	0.5	10
10	0.5	0	4
11	0.5	0.1	4
12	0.5	0.5	4



The flow curves of the hydrogels revealed a shear thinning behavior with the presence of a Newtonian plateau at low shear rates in hydrogel formed at low and medium calcium concentration in absence of oil and that persisted in presence of oil phase only at low alginate concentrations. Strain sweep tests allowed determining the LVE region of the hydrogels and the evaluation of the gel strength. Frequency sweep tests confirmed that the characteristics of the hydrogels were mainly influenced by the alginate and calcium concentration. The thixotropic tests revealed that after the breakage of the hydrogel structure, the complete structure restoration is a slow process and finally, through the creep recovery experiments the hydrogels were found fitting with the Burger model. Among the hydrogel systems studied, the only one that appeared in some way influenced by the presence of oil was the one with low alginate concentration that in creep recovery experiments deformed differently with the oil concentration increase.



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1B – Self-assembly of polymer ultrathin films under nanoscale geometrical distortion

G. Li Destri, R. Ruffino, N. Tuccitto, G.M.L. Messina, G. Marletta

Aims

Polymer ultrathin films have been extensively used as model system to investigate the self-assembly properties of soft matter under nano-confinement. Thanks to these studies, a number of novel technologically relevant soft nanostructures has been discovered and interfacial interactions between macromolecules and the supporting solid substrate have emerged as key factor in driving the self-assembly process. The aim of this study is to extend the knowledge on the substrate effect by simultaneously taking into account the effect of interfacial interactions and substrate geometrical features at the nanoscale on the polymer self-assembly. In particular, if nanostructured substrates characterized by periodic variations of the surface height or curvature are employed as support for the self-assembly of ultrathin polymer films, geometrical distortions of the resultant nanostructures are expected leading, provided a suitable energetic gain, to the formation of novel soft nanostructures.

Results

Substrates characterized by controlled periodic nano-curvature were prepared via soft colloidal lithography of 235 nm SiO_2 particles (Fig. 1a). Employing silica particles enables the subsequent modulation of the substrate surface free energy via octadecyltrichlorosilane (OTS) functionalization (Fig. 1b) followed by RF plasma oxidation (Fig. 1c).

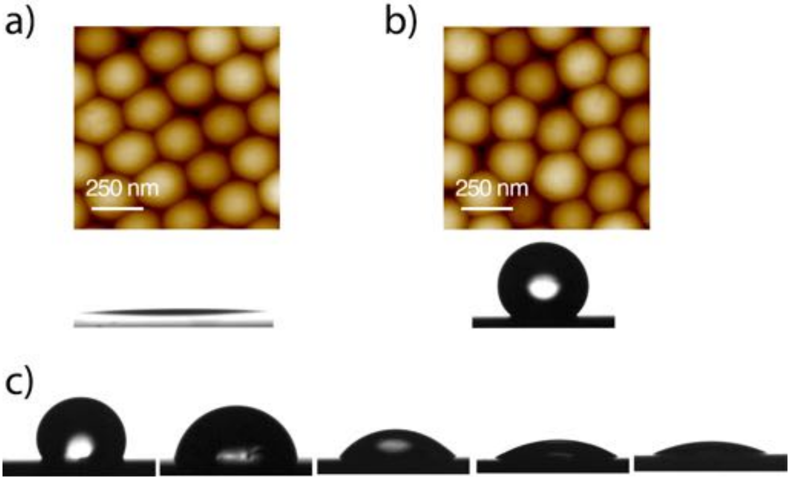

Fig. 1. 1x1 μm^2 AFM height image of 235 nm SiO_2 particle monolayer treated with piranha mixture (a) and functionalized with OTS (b). Below each image the corresponding water contact angle is reported. In (c) the water contact angles of OTS-functionalized 235 nm SiO2 particle monolayers exposed to RF Ar/O_2 plasma for progressively longer times are reported: due to the oxidation of the OTS monolayer, contact angles are progressively lower

Poly-3-hexylthiophene (P3HT) was chosen as model polymer to investigate the crystallization behavior onto substrates having constant nano-curvature and different surface free energy. Results show that, with increasing surface free energy, P3HT crystals gradually covers the particles, e.g. the nano-curved portion of the substrate, leading, as a result, to the growth of distorted crystals (Fig. 2)

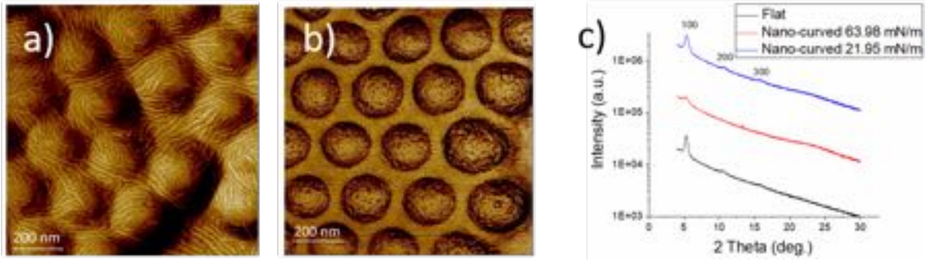

Fig. 2. 1x1 µm^2 AFM phase image of P3HT crystallized onto high surface free energy (63.98 mN/m) nano-curved substrate (a) and low surface free energy (21.95 mN/m) nano-curved substrate (b). Crystals grow on the nano-curved portions of the substrate in the case of high surface free energy ones but they don't in the case of low surface free energy ones. As a result, as revealed by GIXRD (c), crystals on high surface free energy nano-curved substrate are distorted while on low surface free energy ones the crystallinity is comparable to the case of flat substrates.

We suggest that the process is governed by two contributing driving forces: the surface free energy minimization and the maximization of the crystallization enthalpy. At low surface free energy, as there is not any significant surface energy gain from the coverage of the substrate by P3HT, the polymer does not crystallize on the curved portions of the substrates, as this would imply a distorted crystalline structure and, as a consequence, a reduced crystallization enthalpy gain. On the contrary, at high surface free energy, the lower enthalpic gain arising from the crystallization of distorted lamellae is compensated by the marked surface free energy reduction when P3HT covers the substrate. Therefore, P3HT crystallizes on any part of the substrate.

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1B – Surfactant Branching as an effective strategy for the design of high concentration/low viscosity surfactant mixtures

G. D'Errico, A. Fabozzi, L. Paduano

Aims

Physico-chemical investigation of a mixed surfactant system obtained by combining N,N-dimethyl-2-propylheptan-1-amine oxide (C_{10}DAO-branched) with a linear alkyl ethoxysulfate one (AES).

Results

The rational design of branched-tail surfactants is a suitable strategy to obtain low-viscosity surfactant-rich isotropic aqueous mixtures with negligible effects on biodegradability. This opens a way to the design of concentrated (''water-free") surfactant formulations, highly attractive for their ecological and economic benefits. The aggregation behavior of N,N-dimethyl-2-propylheptan-1-amine oxide (C_{10}DAO-branched) in aqueous mixtures was investigated across the entire composition range by polarized optical microscopy, small angle X-ray and neutron scattering, electron paramagnetic resonance, and pulse gradient stimulated echo nuclear magnetic resonance. The humidity scanning quartz crystal microbalance with dissipation monitoring technique was validated as a tool for the fast screening of surfactants phase behavior. Furthermore, the shear viscosities and viscoelastic moduli of the systems were determined by rheological measurements. Moreover, we also studied the mixtures in which the branched amine oxide is replaced by C_{10}DAO-linear.

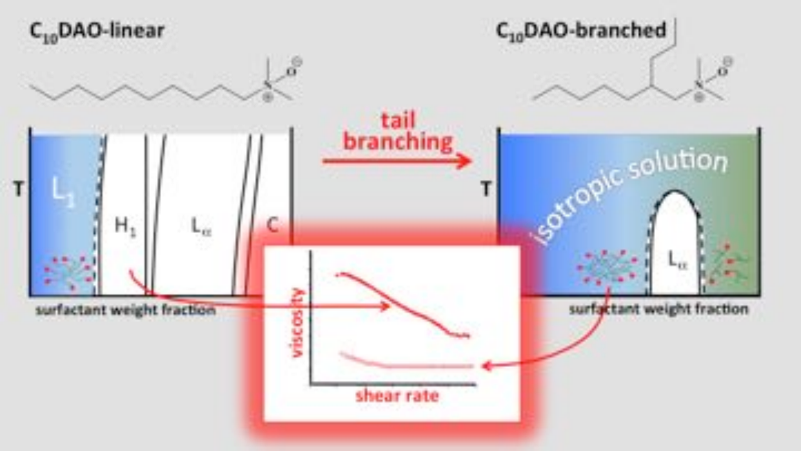

Fig. 1: Phase diagrams of C10DAOlinear and C10DAObranched in water, along with the shear viscosity at the same conce tratio (40% w/w) at 25 °C.

With respect to the linear isomer, C_{10}DAO-branched presented a much lower tendency to form lyotropic liquid crystalline phases. Except for a narrow composition and temperature range in which a lamellar structure is observed, C_{10}DAO-branched aqueous mixtures are isotropic liquids whose microstructure changes, with increasing concentration, from micellar solutions to unstructured dispersions of hydrated surfactant molecules. Low-viscosity was found for all these mixtures, including the most concentrated ones. Thus, the introduction of a single short side-chain in the tail is demonstrated to be an effective approach to increase the active concentration in surfactant formulations.

In the same direction, C_{10}DAO-branched/AES aqueous mixtures preferentially form isotropic micellar solution and lamellar structures. Low viscosity was found for all these mixtures, including the most concentrated ones. In contrast, in C_{10}DAO-linear/AES mixtures an extended hexagonal phase is detected, which presents a high viscosity. These results demonstrate tail branching and mixed aggregation to synergistically contribute to the design of high-concentration low-viscosity surfactant mixtures.

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1B – Synthesis and characterization of pullan-based hydrogels for tissue engineering scaffolds by 3D printing and Electro-Spinning

G. Mugnaini, M. Bonini, C. Resta, T. Al Kayal (Institute of Clinical Physiology, National Research Council, Massa, Italy)

Aims

This project deals with the fabrication of synthetic scaffolds made of pullulan derivates with three-dimensional printing and Electro-Spinning. Pullulan is an exopolysaccharide widely used to tissue regeneration. Here we study its chemical modification and its crosslinking to modulate mechanical properties. 3D printing and Electro-Spinning allows to fabricate scaffolds using these products as inks. Incorporation of different fillers (such as $Ca3(PO4)2$ nanoparticles, hydroxyapatite nanocrystals and clays) is evaluated to improve mechanical and rheological properties.

Results

Pullulan is a linear non-ionic polysaccharide produced in nature by fungus Aureobasidium pullulans. It is a water-soluble exopolysaccharide formed by maltotriose units connected by α (1 → 6) glyosidic bonds, while three glucose molecules linked by α (1 → 4) glyosidic bonds compose one maltotriose unit. It’s one of the FDA approved biopolymer since it is biodegradable, bio and blood-compatible, non-toxic, non-immunogenic, non-mutagen and non-carcinogenic1.

Thanks to these properties, pullulan and its derivates are promising candidates for tissue engineering and in particular for the construction of synthetic scaffolds. The term scaffold defines a three-dimensional and highly porous structure characterized by an interconnected porous network for cell growth and flow transport of nutrients, made with biodegradable and biocompatible materials, whose aim is to be a support for the regeneration of tissue.

Pullulan-based scaffolds have already been studied in literature to enhance regeneration of bone tissue since their main advantage is the facility of surface modification, respect other biopolymers.

In this project we are developing novel pullulan methacrylated derivatives to be used as inks for 3D Printing and or Electro-Spinning. 3D printing is becoming a popular technic to create 3D structures because of its ability to directly control shape and interconnected porosity of the printed structure. 3DP is based on an additive process where successive layers of material are laid down from a digital model in different shapes. A great variety of natural or synthetic polymers were developed with or without additional materials like fibers or particles as inks for 3DP. Similarly, Electro-Spinning has shown great potential in the fabrication of cellular supports.

Following the preparation of derivatives, these materials are tested as 3DP and ES inks and final constructs are tested both for their physico-chemical properties and the interaction with cells.

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1B – Synthesis and Physico-Chemical Characterization of biodegradable amino acid-functionalized PVA

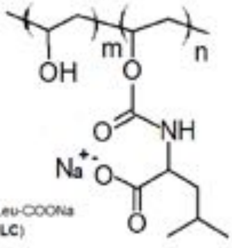
M. Bonini, C. Resta

Aims

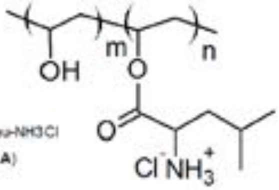
The aim of this research project is the synthesis and characterization of biodegradable polymers based on polyvinyl alcohol (PVA) a functionalized with amino acids. PVA was chosen as the polymer backbone because of its biocompatibility and biodegradability, while the amino acid functionalization is used to modify the pH and electrostatic behavior of the modified polymer.

Results

In the literature there are reports describing the syntheses of PVA derivatives modified covalently with amino acids, such as arginine or proline. However, these macromolecules expose uniquely the amino group and no syntheses are reported to obtain the same polymers exposing the carboxylic function. Among the different amino acids that could be employed to modify PVA, we chose leucine for its isobutyl side chain, which does not take to side reactions carried out and gives us a way (thanks to the proton resonance frequencies of methyl groups) to unequivocally understand from the 1H – NMR spectrum if the substitution took place and at which what percentage. The syntheses allowed us to obtain two different final polymers: a weakly basic polymer (called PLC) in which leucine exposes the carboxyl group, while the other (called PLA) exposes the amino group (weakly acid). An interesting aspect of this synthetic strategy relies on the possibility to vary the percentage of leucine functions on the polymer chain by varying the concentrations of certain reagents in specific steps of the syntheses.



PVA-Leu-COONa
(PLC)



PVA-Leu-NH3Cl
(PLA)

The behavior in water of these polymers are very interesting, especially when the polymers with different charges are mixed, resulting in the tendency to form coacervated systems. This is of outmost importance in view of the application of these polymers in pharmaceutical and biomedical fields, as well as in the formation of Layer by Layer assemblies.

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1B – Thixotropic PVA hydrogel enclosing a hydrophilic PVP core as nucleus pulposus substitute

G. Leone, M. Consumi, S. Lamponi, C. Bonechi, G. Tamasi,
A. Donati, C. Rossi, A. Magnani (Department of Biotechnologies,
Chemistry and Pharmacy, University of Siena)

Aims

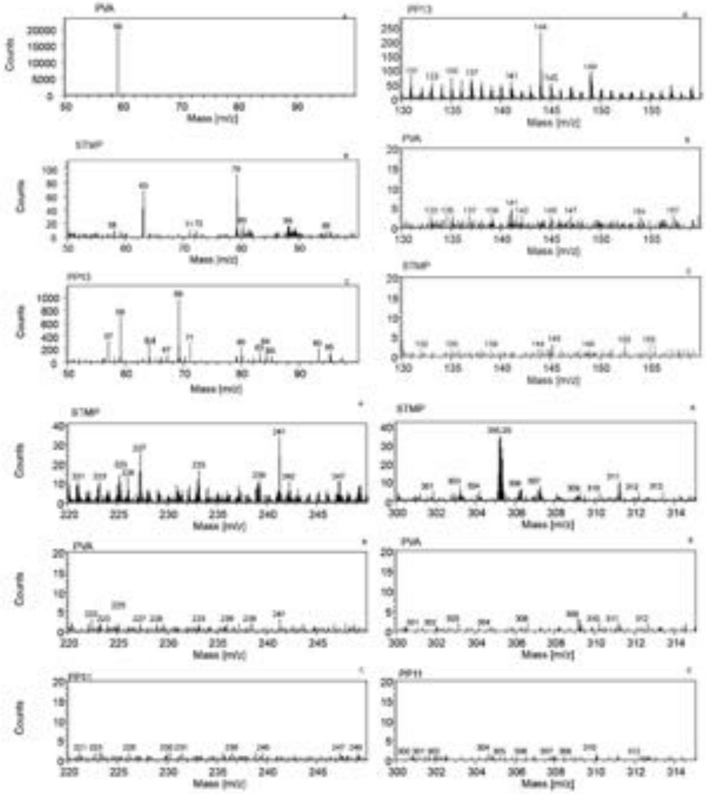
A thixotropic polyvinyl alcohol (PVA) hydrogel, containing a hydrophilic poly-vinyl pyrrolidone (PVP) core, was obtained in order to develop a preformed 3D network able to maintain injectability. PVA was mixed with PVP in two different molar ratios (1:1 and 1:3) and chemically cross-linked using trisodium trimetaphosphate (STMP), which is able to react only with PVA component. A combination of Time of Flight-Secondary Ion Mass Spectrometry (ToF-SIMS), elemental analysis and UV spectroscopy permitted to determine both the cross-linking arm length and the crosslinking degree. Hydrogels were characterized in terms of swelling pressurization, rheological and mechanical behaviour. In particular, the viscoelastic behaviour of the hydrogel was analysed in shear and compression stress under dynamic conditions and compared with the performance of healthy human nucleus pulposus. In conclusion, the study demonstrated that the scaffold obtained mixing PVA and PVP in a molar ratio 1:1 can be considered a promising material to be utilised in the replacement of nucleus pulposus.

Results

In this work, STMP was used as crosslinking agent. It is widely used as food additive being completely atoxic for humans. Cross-linking PVA with STMP has been already set up by authors. The developed procedure permits to obtain hydrogels with tuneable mechanical properties just changing the ratio between PVA and STMP. However, very stiff hydrogels were obtained when PVA and STMP are used in 1:1 ratio. A hydrophilic polymer was added to overcome their high stiffness. The presence of a hydrophilic core permits to obtain thixotropic material. A thixotropic hydrogel shows the capability to become fluid in the presence of an appropriate mechanical stimulus, whereas it recovers its structure when the stimulus was removed. This capability permits to match the advantages of an injectable hydrogel (i.e. minimally-invasive insertion) with the mechanical performance of pre-formed semi-rigid systems.

Two different molar ratios between structural polymer (PVA) and hydrophilic core (PVP) were tested in terms of swelling ratio, mechanical behaviour and heat capacity. The obtained results pointed out that adding the hydrophilic core in a molar ratio of 1:1 with the structural polymer (PP11) a potential substitute for NP could be obtained. PP11 hydrogel showed mechanical, swelling and thermal (in terms of heat capacity) behaviour similar to that of healthy human NP. Preliminary biocompatibility studies confirmed the applicability of such a hydrogel.

ToF-SIMS analysis (a) confirmed the crosslinking reaction permitting also to have information on the crosslinking arm length. Briefly, positive and negative spectra of PVA and PVP polymers, STMP and PP11 and PP13 hydrogels were recorded. Positive spectra provided few information on material chemistry. Consequently, only negative spectra were analysed considering only peaks whose intensity was at least three times the background after being normalized to their total intensity.



(a)

PVA, mixed with PVP in two different molar ratios (PP11 and PP13), was cross-linked using STMP. The presence of PVP inside the matrix affected the crosslinking arm length. ToF-SIMS analysis demonstrated that PVA chains were cross-linked by phosphate groups instead of pyrophosphate arms as found when only PVA was crosslinked using STMP. PVP amount did not significantly affect crosslinking degree, mesh size and mesoporosity. On the contrary, a higher amount of PVP significantly depleted the mechanical/rheological performance of the hydrogel. PVA and PVP in a molar ratio 1:1 (PP11) guaranteed to realize a matrix, which combined the mechanical properties of a preformed matrix with the easy injectability of a physical matrix, thanks to its thixotropic properties. Moreover, PP11 hydrogel showed a heat capacity compatible with that of human cartilage and it was compatible with cell adhesion and proliferation.

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1B – Xanthan Gum–Chitosan: Delayed, prolonged, and burst-release tablets using same components in different ratio

M. Consumi, G. Leone, S. Pepi, G. Tamasi, S. Lamponi, A. Donati, C. Bonechi, C. Rossi, A. Magnani (Department of Biotechnologies, Chemistry and Pharmacy, University of Siena)

Aims

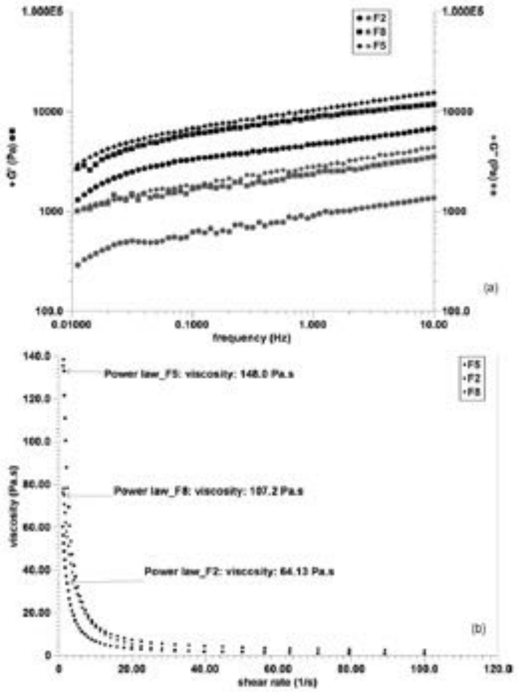
Chitosan and xanthan gum were combined in nine different percentages without using any cross-linking agent. The obtained physical matrices were able to give a burst, delayed, or prolonged release of red yeast rice (RYR) on the basis of xanthan gum percentage. In fact, thermal analysis, swelling behavior, and rheological analysis pointed out that a slight interaction among xanthan gum and RYR was present.
This was reflected in a burst release when the amount of xanthan gum was under the 30%. On the contrary, a prolonged release was observed when the xanthan gum percent was higher than 70%. A delayed release was observed using similar percentage of the polymers (i.e., F5–F7). The effect of the formulation on RYR inhibition activity toward 3-hydroxy-3-methyl-glutaryl-coenzyme A reductase and on cholesterol production was also evaluated.

Results

A versatile drug carrier can permit the realization of pharmaceutical vehicles usable for the administration of a large amount of drugs, thus being useful for several diseases.
Generally, chitosan–xanthan gum PECs have been obtained by dissolving polymers in aqueous medium, mixing them in close proportions (1:1 or similar), drying, and purifying. It is a time-consuming process especially for scale-up processes.
In this article, matrices were obtained by pressing polymers directly in dry state without using any cross-linking agent, thus reducing time and cost of the manufacturing process.
Nine formulations were obtained combining chitosan and xanthan gum in different percentages. The purpose of this study was to verify whether just changing the relative amount of the two polymers was possible to modify the release profile of RYR. For scale-up procedures, the possibility to have different vehicles without modifying the polymeric component can appear as a money-and time-saving procedure.
Besides the hydration characteristics of a polymeric system, the viscosity and the mechanical properties of the swollen layer critically influence the drug release from a hydrophilic matrix. Thus, rheological properties could predict drug release from hydrophilic matrices. The highest stiffness was found in the presence of a polymer ratio close to 1 (i.e., F5 and F6) and then it decreased. The trend of G′ and G″ of three formulations (i.e., F2, F5, and F8) was reported in (a). As shown by the graph, both moduli did not change significantly with the frequency thus emphasizing their stability.

Moreover, the absence of any cross-over region indicated the absence of gel to sol transformation. A reduction in stiffness should indicate a faster drug release.

Flow curves were used to analyze the behavior of the swollen matrices with the increase in shear rate. Flow curves of three formulations were plotted in (b). The plots showed the dependence of their viscosity on shear rate. All matrices exhibited shear thinning property, because their viscosity decreased as increasing shear rate.



(a)

The obtained results pointed out that a slight interaction among xanthan gum and RYR was present. This was reflected in a burst release when the amount of xanthan gum was under the 30%. On the contrary, a prolonged release was observed when the xanthan gum percent was higher than 70%. A delayed release was observed using similar percentage of the polymers (i.e., F5–F7).

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1C – Computational spectroscopy of redox-active radicals and proteins

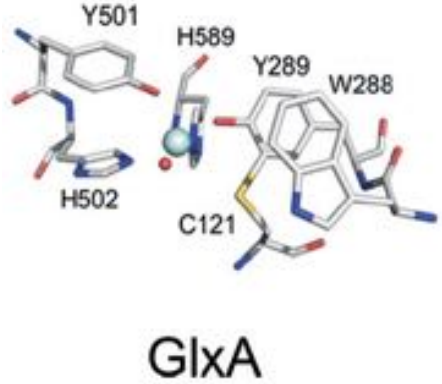
R. Basosi, A. Sinicropi

Aims

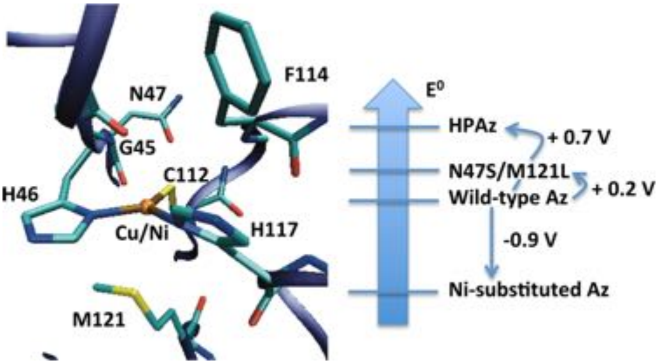
State-of-the-art quantum-mechanics methods are used to characterize the electronic and magnetic properties of redox-active amino acids involved in long-range electron transfer pathways in proteins. The results obtained are expected to shed new light on the catalytic mechanism involving radical species and thus open the way to a comprehensive understanding of radical-mediated ET reactions. Moreover, the quantum-mechanics methods are used to estimate reduction potentials (E^0) values of wild-type Azurin, two mutants (N47S/M121L and HPAz) and a Ni-substituted Azurin. The employed strategy is able to predict the lowering or increasing of E^0 of the wild-type, Nickel-substituted and mutated Azurin.

Results

The concerted redox action of a metal ion and an organic cofactor is a unique way to maximize the catalytic power of an enzyme. An example of such synergy is the fungal galactose 6-oxidase, which has inspired the creation of biomimetic copper oxidation catalysts. Galactose 6-oxidase and its bacterial homologue, GlxA, possess a metalloradical catalytic site that contains a free radical on a covalently linked Cys–Tyr and a copper atom. Such a catalytic site enables for the two-electron oxidation of alcohols to aldehydes. When the ability to form the Cys–Tyr in GlxA is disrupted, a radical can still be formed. Surprisingly, the radical species is not the Tyr residue but rather a copper second-coordination sphere Trp residue. This is demonstrated through the introduction of a new algorithm for Trp-radical EPR spectra simulation. Our findings suggest a new mechanism of free-radical transfer between aromatic residues and that the Cys–Tyr cross-link prevents radical migration away from the catalytic site.



Azurin (Az) from *Pseudomonas aeruginosa* is a redox active protein belonging to the family of cupredoxins. Cupredoxins span a wide range of reduction potentials (E^0) going from stellacyanin having the lowest potential of ca. 184 mV to rusticyanin showing the higher potential of ca. 680 mV. Several works have been devoted to the understanding of the factors influencing E^0 by changing primary coordination sphere ligands or exploring secondary coordination sphere mutations. To this goal, a series of Az mutants have been designed and showed that E^0 could be tuned over a very broad range (between 90 mV and 640 mV) without significantly perturbing the metal binding site. Among these mutants, the HPAz variant showed the highest E^0 value (970 mV) ever reported for Az while a significant lowering of E° value (-590 mV) has been reached in a Ni-substituted Az. In this paper, we computed the B3LYP energies and Gibbs free energies of oxidized and reduced models of wild-type Az, Ni-substituted Az and two mutants (N47S/M121L and HPAz) of the protein Az to estimate their E^0. The results show that the employed strategy is able to reproduce the experimental lowering or increasing of E^0 among the studied Az proteins.



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1C – Design and characterization by computational methodologies and life cycle assessment of organic sensitizers for solar cells

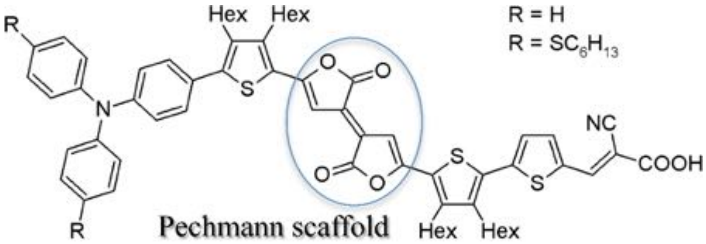
S. Mohammadpourasl, M.L. Parisi, S. Maranghi, R. Basosi, A. Sinicropi

Aims

The aim of the project is the design, computational characterization and synthesis of new organic dyes for the production of Dye Sensitized Solar Cells, along with the environmental assessment of their photovoltaic performances trough life cycle analysis.

Results

Dye sensitized solar cells (DSSCs) are based on third-generation photovoltaic (PV) technology with a great potential for Building Integrated PV market and for indoor applications due to their high performance under diffused and low-intensity illumination. The first DSSC was created by O'Regan and Gratzel in 1991. The dye plays a crucial role in DSSCs since it governs the photon harvesting process to make solar-to-electricity conversion. The most efficient organic dyes are made of a "D-π-A" structure containing an electron donor (D), a conjugated spacer (π) and an electron acceptor (A) behaving as the anchoring group. Another successful structure for dyes, "D-A-π-A" can be designed by adding an electron-withdrawing unit incorporated to conjugated π-bridge as an auxiliary acceptor. Recently, to design novel "D-A-π-A" dyes, we proposed the use of the Pechmann scaffold (see Figure below), a strong electron-withdrawing system with a brilliant red-purple colour, as an auxiliary acceptor. It allows extending the light absorption spectrum of dyes in the red/near-infrared (NIR) region and obtaining unusual blue-green coloured dyes that are currently of high interest. 13 dyes containing the Pechmann scaffold were investigated by means of Density Functional Theory (DFT) and time dependent DFT calculations performed with the Gaussian09 program package. We found that the new dyes show vertical absorption maxima ranging from 600 to 800 nm and dye electronic levels compatible with a proper use in DSSCs.



The development of these molecules as dye in DSSC should be assisted byasustainability assessment providing strategic support to minimize the environmental footprint connected with the production of PV devices. Life Cycle Analysis (LCA) is a powerful methodological tool to understand benefits and drawbacks associated with different technical options that have been proposed so far, and could be proposed in the future, for the development of the DSSC technology. To our goal, LCA has been applied to the synthetic procedure of the TTZ5 dye employed as a sensitizer in DSSC with recording good photovoltaic performance . The calculation of a full TTZ5 eco-profile allowed to compare it with the eco-profiles of other DSSC sensitizers (porphyrin-based, metallo-organic, and other fully organic dyes) previously calculated by Parisi M.L. et al, Renewable & Sustainable Energy Reviews, 2014, 39, 124-139.

LCA outcomes helped in understanding the hotspots of the TTZ5 synthesis and to advice and support in the optimization of the manufacturing procedure by implementing "greener" synthetic steps in order to decrease the environmental impacts connected with its production.

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1C – Principles of minimal wrecking and maximum separation of solid waste to innovate tanning industries and reduce their environmental impact

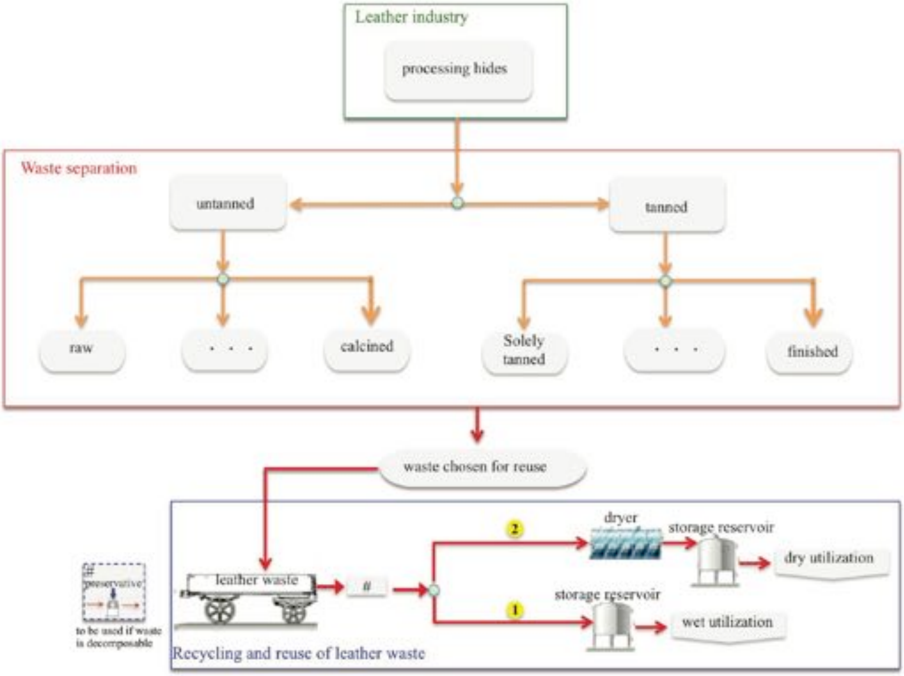
G Bufalo, F. Di Nezza, G. Cinelli, F. Lopez, F. Cuomo, L. Ambrosone

Aims

The purpose of this research strand is to find zero-waste conditions for the leather industry.

Results

The achievement of the zero-waste condition by applying principles of *maximum separation and minimal wrecking* was suggested. The idea stems from observation that leather waste is mainly composed of collagen fibres cross-linked in a three-dimensional so that their landfill or inceneration requires large amount of energy and the process turns out to be economically unfavorable. The general principle discussed above were applied to handle the solid leather waste generated in hide industries in order to manufacture paperboard for boxes and packaging commercially used, car mats, footwear, no-slip grip for chairs and laminate floor covering.



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1C – The potential of a light-sensitive protein as sensitizer for solar cells

M. Avelar, M.L. Parisi, R. Basosi, A. Sinicropi

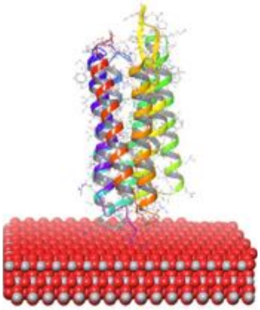
Aims

This work is part of a project recently funded by the MIUR Grant-Department of Excellence 2018-2022. The obtained results will be the basis for further studies and for the improvement of bacteriorhodopsin (bR) performances in Bio-sensitized solar cells (BSSCs).

Results

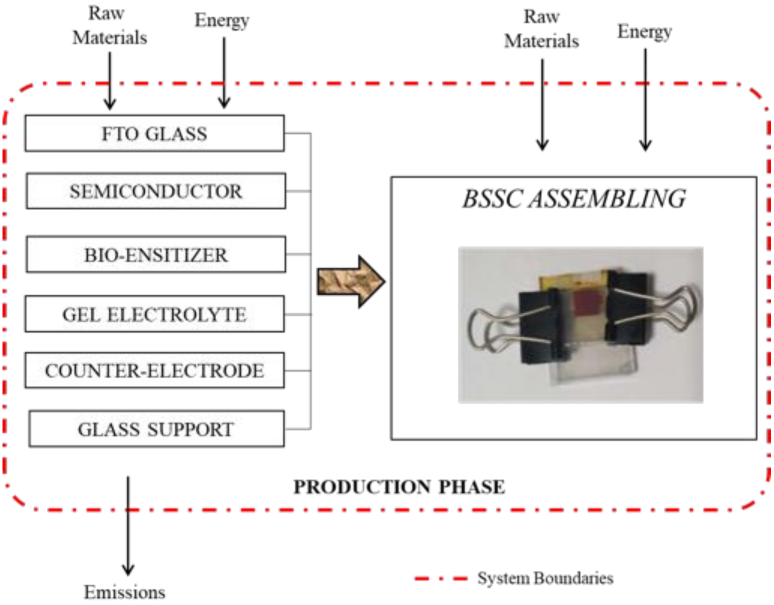
Bio-sensitized solar cells (BSSC) are third-generation photovoltaic cells based on the use of renewable energy, i.e. solar energy. Bacteriorhodopsin (bR) protein has been employed as bio-sensitizer in BSSCs. bR is a transmembrane protein that is part of the purple membrane (PM) of Halobacterium salinarum. bR is a light-sensitive protein and is a promising material for BSSC since has a thermal robustness and keeps the functional activity for long-term while absorbing the solar radiation efficiently to produce photo-induced charge generation. BSSCs were fabricated by the integration of bR into TiO2 (semi-conductor anode) with gel electrolytes and platinum as counter electrode. Although there are experimental studies employing bR in BSSCs, computational reports shedding light on the ET mechanism are still missing.

With the aim of improving BSSCs performances, insights into the electron transfer (ET) mechanisms undergoing in bR-sensitized solar cells are needed. Thus, one of the main goals of this project is to map the ET pathways in bR upon light absorption. To this aim, CP2K package will be used to run Molecular Dynamics simulations (MD) and Quantum Mechanical/Molecular Mechanical calculations (QM/MM).



From the sustainability point of view, another issue addressed in this project will be the life cycle assessment of BSSCs for the calculation of the environmental footprint of bR-sensitized solar cells. In fact, since photovoltaic technologies are known to be an emission-free technology during their operative phase, the major efforts in terms of minimization of the environmental burden associated to devices should be directed to the production of solar cell components, particularly to the sensitizer.

In this context, preliminary results show that the use of bR represents a potential alternative for the development of photovoltaic devices characterized by reduced environmental impact. Among the various scenarios analyzed, the optimization of the protein expression procedures would allow a much more pronounced environmental advantage connected to the use of biological material that does not generate burden on the environment in the end-of-life phase of the solar cell.



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2A – A remote sensing approaches to determine algal blooms in the shallow eutrophic lakes

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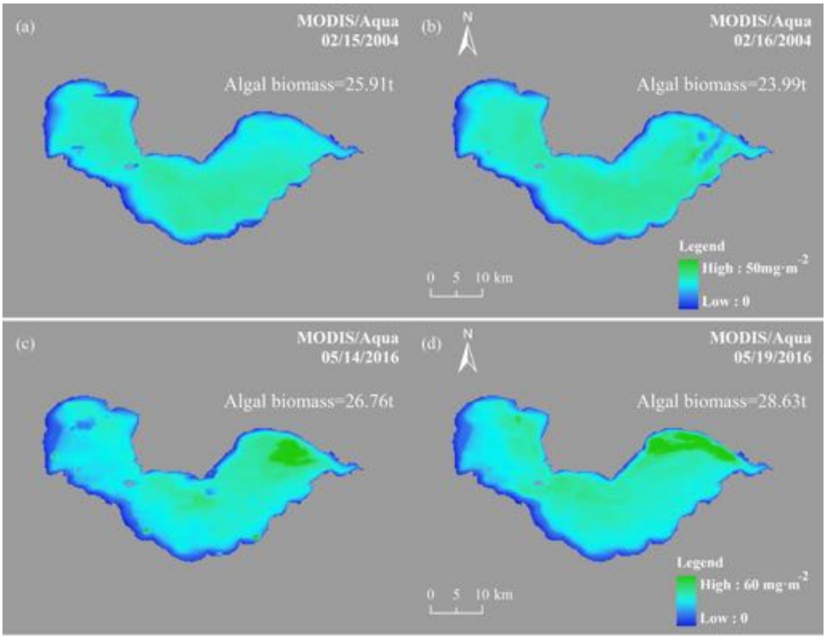
Aims

Remote sensing of algal biomass provides an indicator for eutrophication. However, most inversion algorithms of column biomass assume a homogenous distribution of phytoplankton with the water column. This study tests a new remote sensing-based algorithm to estimate column integrated algal biomass considering different possible vertical profiles. The field sampling was based on five surveys in Lake Chaohu, a large eutrophic shallow lake in China. Field measurements revealed that a significant variation in phytoplankton profiles during algal bloom conditions.

Results

The biomass retrieval algorithm developed was effective to describe the vertical variation of biomass in shallow eutrophic water. The Baseline Normalized Difference Bloom Index (BNDBI) was adopted to estimate biomass integrated from water surface to 40cm. Then the relationship between 40cm integrated biomass and whole column biomass was built based the hydrological and bathymetry data of each site. The algorithm was able to accurately estimate integrated biomass with R2=0.89, RMSE=45.94, and URMSE=28.58%. High accuracy was observed on the temporal consistency of satellite images (with the maximum MAPE=7.41%). Sensitivity analysis demonstrated that the estimated biomass integrated from the water surface to 40cm has the greatest influence on the estimated column integrated biomass. This algorithm can be used to explore the long-termed variation of biomass to improve long term analysis and management of eutrophic lakes.



Estimated algal biomass in Chaohu lake (China) in February 2004 and May 2016.

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

M. Baglioni, E. Carretti, L. Dei, D. Berti, E. Fratini, D. Chelazzi, 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 should solve the residues' issue and/or with more efficient surfctants, 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. We recently moved our focus from ionic surfactants to nonionic alcohol ethoxylates, which possess interesting (bio)degradability properties and excellent detergent power, and we explored the performances of new classes of surfactants, 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 methyl ester ethoxylates (MEE) were considered, in view of their excellent solubilization properties, with respect to more common ether ethoxylates. It was shown that MEE 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 methyl 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. Then, cleaning systems obtained by the confinement of NSFs into retentive SIPNs chemical hydrogels have been characterized from a mechanical, rheological and structural point of view. It was shown that the upload of complex NSFs does not significantly alter the rheological properties of the gels. Besides the interest from a physico-chemical standpoint, this observation has considerable importance in view of practical applications, since the inclusion of cleaning fluids should not change the optimal mechanical properties of the gels. In fact, even if their properties can be relevant for different fields related to detergency and coatings, these combined systems represent one of the most advanced solutions for the cleaning of works of art and they 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.

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2A – Application of non-TiO_2 photocatalysis for degradation of pollutants in aqueous solution

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Aims

Application of non-TiO_2 photocatalysis for degradation of pollutants in aqueous solution has received wide attention by the researchers. With this respect, the perovskite lanthanum orthoferrite $LaFeO_3$ gains considerable interest due to easy synthesis combined with large chemical stability, low-cost and non-toxicity. $LaFeO_3$ is a p-type semiconductor which possesses a relatively narrow band-gap energy around 2.5 eV. It is proposed as visible-light and UV photocatalyst for aqueous reactions, often combined with a Fenton-like reaction. As many perovskite-type oxides, $LaFeO_3$ shows a high recombination rate of photogenerated electron-hole (e^--h^+) pairs. Several strategies are developed to reduce the unfavorable electron-hole recombination process such as doping with transition metal elements, fabrication of heterojunction composite, and decoration with Ag. In this research project, we use plane $LaFeO_3$ and copper lanthanum ferrite for photocatalytic degradation of ibuprofen (IBP) and humic acids (HAs) in water solutions.

Results

This study was performed to investigate the photocatalytic performance of novel photocatalysts i.e., $LaFeO_3$ perovskite (LF) and copper lanthanum ferrite (Cu-LF). Using visible-light irradiation and in the presence of 5 mol% Cu-LF and aqueous H_2O_2 an excellent photocatalytic degradation of IBP (85 %) was observed already after 5h. Chloride water matrices could interfere with the process, as in the performed experiments decreased the amount of degraded IBP and increased the yield of the harmful degradation product 4-IBAP.

Based on the present study, photocatalytic degradation kinetics indicated the possible use of LF and Cu-LF for the degradation of humic acids as the model compound of dissolved organic matter. Furthermore, the dose effect of the respective LF and Cu-LF specimens could be related to the surface interactions in relation to the presence of the organic matter contents expressed by different molecular size fractions. Highest mineralization was achieved upon use of photocatalyst dose as 0.25 mg/mL of Cu-LF for 30 kDaHA, whereas lowest mineralization was attained for 100 kDaHA upon use of LF. Following photocatalytic degradation of humic matter, organic matrix was further characterized by EEM (Excitation-emission Matrix) fluorescence contour plots. Upon exposure to solar irradiation for 60 min, organic matrix retained humic-like and fulvic-like fluorophores excluding the formation of new fluorophoric groups that could signify destructive fragmentation products via photocatalysis. It could be emphasized that humic acids are comprised of complex and polydisperse organic compounds with undefined molecular structures; therefore, the attained results holds prime importance in comparison to the simple compounds that are used as models for activity testing. This study brings significant baseline information on the successful utilization of non-TiO_2 photocatalysts for degradation of refractory organic compounds present in natural waters as well as wastewaters upon solar light exposure.

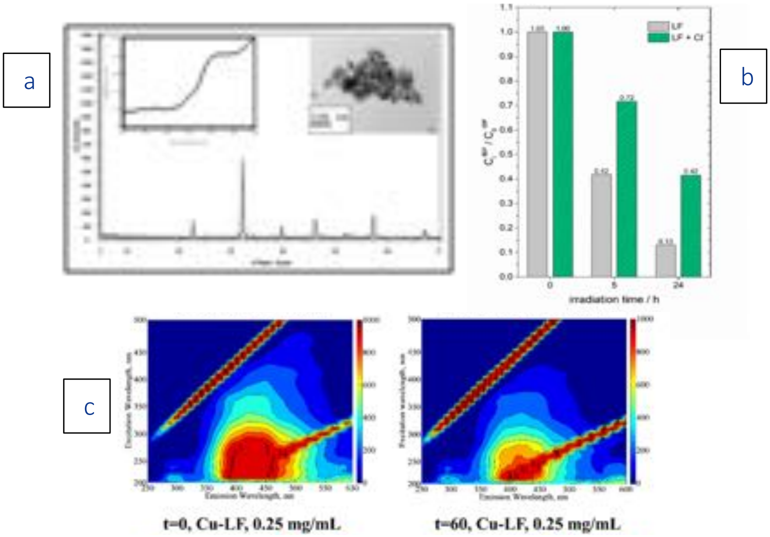

Fig. 1: a) Powder XRD pattern of $LaFeO_3$. In the inset a diffuse reflectance plot of $LaFeO_3$ powder (left) and a representative TEM image showing the nanoparticles of the material (right); b) Concentration values of IBP (C_t^{IBP}) divided by the initial IBP concentration (C_0^{IBP}) in solutions irradiated with visible-light for 5 and 24 h; c) EEM fluorescence contour plots of 30 kDaHA upon use of Cu-LF.

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2A – Film forming PVA-based cleaning systems for the removal of corrosion products from artistic bronzes and iron-based alloys

T. Guaragnone, A. Casini, D. Chelazzi, P. Baglioni, R. Giorgi

Aims

Development of plasticized PVA-based polymeric systems 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, 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 $Fe(III)Cl_3$, can also bring to new rusting processes.

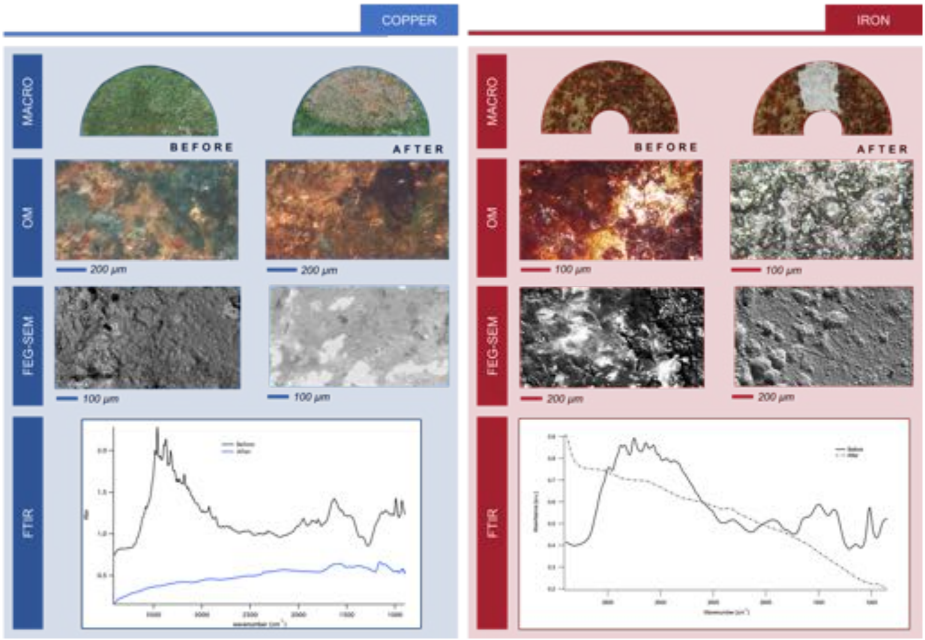
The proposed cleaning procedure consists in the application of a PVA-based polymeric solution able to form an elastic film, which can be gently peeled off from the surface upon drying. Plasticizers (different polyols) were added to the solution in order to obtain a final film with suitable mechanical 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.

For copper-based artifacts a first alkaline formulation was obtained with the addition of EDTA and then replaced with polyethylenamines which present better chelating performances and selectiveness for Cu(II). For iron-based alloys a different approach was required: the system was loaded with citric acid and corrected until pH 2 with HCl in order to demolish completely all the Fe corrosion products.

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.

The physico-chemical characterization of the system was carried out in order to investigate the kinetics of film formation, the variation in mechanical behavior of the system during drying, and the properties of the final polymeric films. The kinetics of film formation were studied by means of gravimetric and thermogravimetric methods (both scanning and isothermal) and rheology (both dynamic and rotational experiments) was used to investigate changes in mechanical behavior during evaporation of the volatile fraction of the system. The final films were characterized by means differential scanning calorimetry (DSC) and Attenuated Total Reflectance Fourier Transform Infra-red Spectroscopy (ATR-FTIR) to evaluate the crystallinity degree, which is correlated to rigidity of the polymeric film. Moreover, the viscoelastic behavior of the systems before and after the addition of EDTA and TEPA was studied by means of rheological measurements.

The cleaning processes on artificial and natural aged samples were also carried on both metal substrates and checked down to the micron scale with 2D Imaging FTIR, using a Focal Plane Array (FPA) detector, ATR-FTIR, optical microscopy and field emission gun scanning electron microscopy (FEG-SEM).



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2A – Hybrid nanomaterials for the strengthening and deacidification of paper

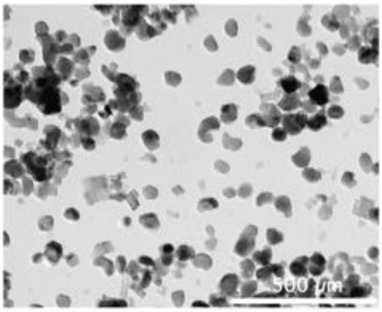
G. Poggi, Q. Xu, C. Resta, M. Baglioni, R. Giorgi, P. Baglioni

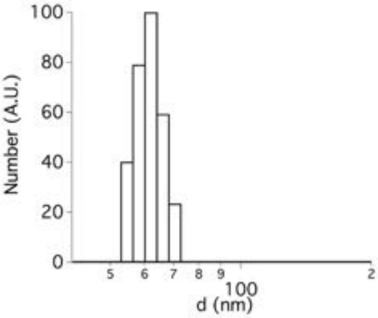
Aims

The acid-catalyzed hydrolysis of glycosidic bonds, that is the most important degradation pathway of paper, 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 paper, both a deacidification and a consolidation treatment are required.

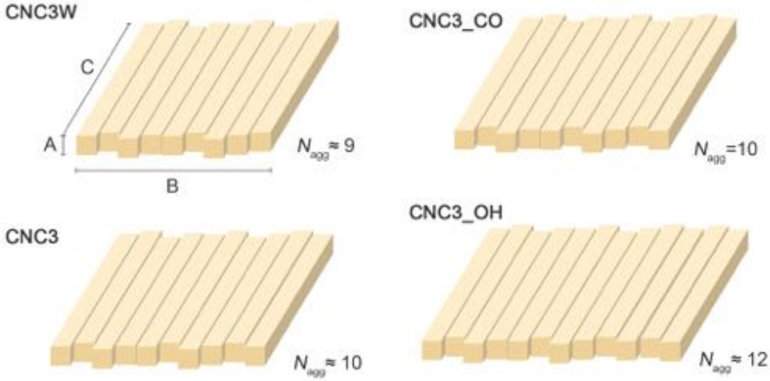
Results

In the framework of the EU project NANORESTART, hybrid systems for the concomitant neutralization of acidity and the improvement of the mechanical resistance of paper have been developed. 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. 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 CaCO3 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.





The mechanical response of CNCs dispersions was studied with rheological measurements. The presence of ethanol in CNCs aqueous dispersion resulted in the overall increase in the viscosity of the system. This behavior is probably due to a decrease in the Debye length, triggered by the lowest permittivity of ethanol with respect to water that allows for stronger interactions between particles. A similar effect, even more pronounced, was obtained after the addition of calcium hydroxide nanoparticles. In fact, the Debye length is also a function of the ionic strength and divalent ions screen the superficial charges of cellulose nanocrystals, favoring their interactions and resulting in the formation of a strong gelled system. A less pronounced effect on the screening of the crystal repulsive forces was displayed after the addition of calcium carbonate, which is significantly less soluble than Ca(OH)2. SAXS measurements confirmed the increase in cellulose interactions after the addition of ethanol and alkaline nanoparticles. In fact, the changes in the aggregation number of CNCs clusters follow the same trend displayed by the mechanical response, i.e., bigger clusters were found in the more gelled system.



After characterization, hybrid systems were applied on aged paper. Mechanical tests, pH and colorimetric measurements were used to evaluate their efficacy. Hybrid systems resulted highly effective in the strengthening and deacidification of acidic and mechanically-degraded cellulosic material, without significant alterations in the visual aspect of samples.

We are currently working on the surface modification of CNC with carboxyl acids, so as to produce nanocellulose derivatives that can be dispersed in pure ethanol. The aim is to formulate hybrid systems to be used on paper artifacts that are highly water-sensitive.

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2A – Inorganic nanoparticles and hybrid nano-composites for the consolidation of stone materials

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Aims

Consolidation of stone artworks with compatible strategies based on nano-materials.

Results

The consolidation and protection of immovable works of art, such as wall paintings, plaster and stone artworks, can be successfully achieved by using dispersions of alkaline-earth metal hydroxide nanoparticles. Inorganic nanoparticles can also be combined with organic compounds to obtain tailored and versatile hybrid formulations. Before the introduction of nanotechnology in the conservation field, synthetic organic materials were widely applied by conservators for consolidation purposes. Unfortunately, their presence on artistic substrates was shown to be detrimental due to the different physico-chemical properties of polymers with respect to the materials constituting the original artworks. On the other hand, inorganic nanoparticles exhibit high compatibility with many artistic and architectonic substrates and thus represent a valid alternative to the organic coatings. The nano-size of the particles, together with the dispersing medium, influences their reactivity and penetration through porous matrices. Furthermore, particles polydispersity greatly affects their performance on stone substrates, as matrices to be consolidated can exhibit wide pores size distributions. It appears thus evident that the processes involved in the preparation of nanoparticles and their dispersion in carrier media play fundamental roles in determining the final effectiveness for specific consolidation issues and the applicability of these conservation tools.

After the disastrous flood of Florence, in 1966, the first compatible consolidation method for wall paintings was developed by Enzo Ferroni. The so-called Ferroni–Dini method, designed for the conservation of sulfate polluted wall paintings, consists in applying ammonium carbonate and barium hydroxide aqueous solution loaded on poultices, in a two-step procedure.

An improvement of this method is represented by the usage of a dispersion of hydroxide nanoparticles, or, in other words, of a colloidal system instead of a solution. Recently, new formulations of barium and calcium hydroxide nanoparticles have been successfully used for consolidation of degraded wall paintings, even in presence of large amount of salts.

These methodologies are currently used for the consolidation of wall paintings in Italy and other countries, including Mexico, Sweden, Israel, and Denmark.

"Nanorestore®" and "Nanorestore Plus®" are two chemical products based on nanotechnology, made available specifically to the conservator community. They are calcium hydroxide nanoparticles dispersed in short-chain alcohols, such as ethanol and 2-propanol, produced at the CSGI laboratory and distributed by CTS company (Italy).

Siliceous compounds are also largely employed, mainly for treatments of silicate-based stones. Recently, colloidal silica was introduced in traditional formulations for the development of crack-free composite materials for stone consolidation, so to overcome the known drawback of the more popular alkoxysilanes.

In this view, hybrid nanotechnologies are providing candidate materials to improve compatibility and versatility of existing products, for specific case studies. For instance, the combination of silica and calcium hydroxide, in the form of nanoparticles, to obtain the in situ formation of calcium silicate hydrate phases, was studied for surface consolidation treatments of earthen masonry (the so-called adobe bricks). Moreover, the presence of cellulose additives in the formulation allowed to stabilize the system and regulate water release during the formation of the new cementing phase.

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2A – Investigation of atmospheric emission profiles of geothermoelectric plants in Italy: a life cycle approach for the analysis of sub-regional environmental footprint

M.L. Parisi, N. Ferrara, R. Basosi

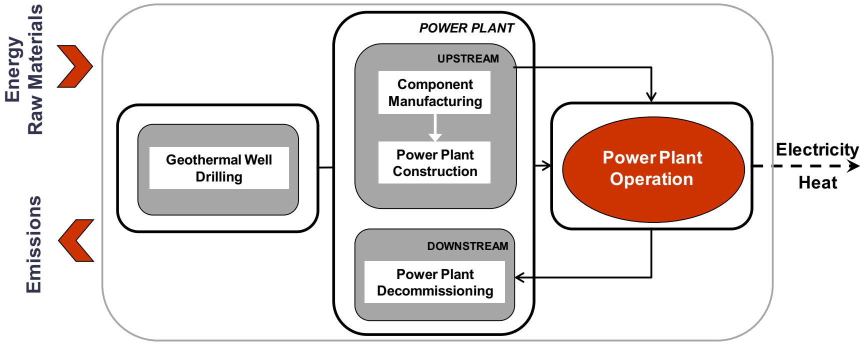
Aims

Geothermal energy is a resource of natural and renewable energy and its exploitation in the Italian Tuscany Region contributes significantly to the regional share of electricity generation from renewable sources. The energy produced by geothermal source, such as that produced by any energy source, generates non-negligible impacts on the environment, closely related to the site-specificity of the source itself. The aim of this project is the assessment of the environmental performances of geothermal power plants in relation to the geomorphological characteristics of the sites and the technologies used to exploit the resource.

Results

To date, in Tuscany there are 36 hydrothermal flash plants managed by Enel Green Power, located in the four territorial areas of Larderello, Travale-Radicondoli, Bagnore and Piancastagnaio on Monte Amiata belonging to the provinces of Pisa, Siena and Grosseto, with an electricity generation in 2016 equal to about 2% of the national electricity production and 35.6% of the total regional production.

The assessment of the atmospheric emission profiles of the geothermoeletcric activity is performed with a gate-to-gate approach focusing on the operational phase of power plants and considering all the components working during the geothermoeletcric cycle, such as the AMIS (the abatement system for mercury and hydrogen sulphide). The study is focused on the potential environmental impact associated with the emission of non-condensable gases (NGCs) that are found in greater concentration in the geothermal fluid (CO2, CH4, NH3, H2S) and gaseous Hg which, despite lower concentration, gives appreciable contribution on the impact categories.



The results of this study are expected to contribute to the wider debate concerning whether or not geothermal energy can contribute to decarbonise the European energy system in a sustainable way, to secure energy supply and to complete the energy internal market in line with the objectives of SET-Plan and of the related energy legislation (Renewable Energy and CCS Directives) and energy policies designed to deliver the 2020 targets and to shape energy market frameworks for 2030 and 2050. By focusing the attention on emissions into the atmosphere, it is possible to show that there are various factors responsible for variations in the composition and mass of NCGs and metals that are released from the cooling towers of the various plants: location and depth of the reservoirs, characteristics of the technology used (flash, dry steam, binary cycle, combined cycle, etc.) and the abatement systems adopted. In this context, the extensive assessment made on all the power plants operating in the Tuscany region allowed to draw sub-regional profiles distinctive of the various geothermal areas, by pointing out¸ in details, the contributions of each technological component or treatment system involved in the geothermoelectric cycle.

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2A – Microplastics modify microbial release of marine Chromophoric Dissolved Organic Matter

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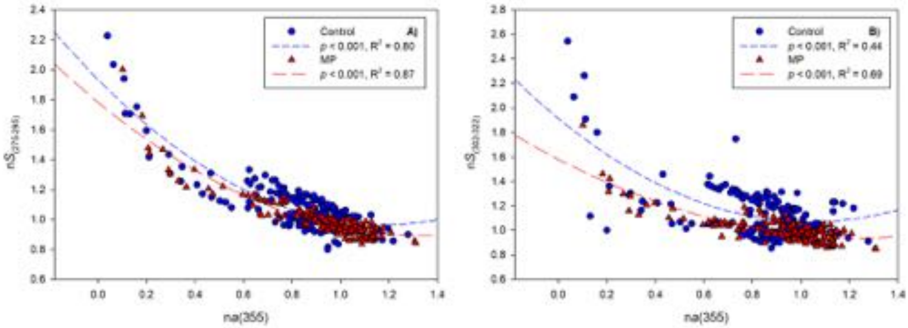
for Ocean Research Kiel, Germany)

Aims

About 5 trillion plastic particles are present in our oceans, from the macro to the micro size. Like any other aquatic particulate, plastics and microplastics can create a micro-environment, within which microbial and chemical conditions differ significantly from the surrounding water. Despite the high and increasing abundance of microplastics in the ocean, their influence on the transformation and composition of marine organic matter is largely unknown.

Results

Chromophoric dissolved organic matter (CDOM) is the photo-reactive fraction of the marine dissolved organic matter (DOM) pool. Changes in CDOM quality and quantity have impacts on marine microbial dynamics and the underwater light environment. One major source of CDOM is produced by marine bacteria through their alteration of pre-existing DOM substrates. In a series of microcosm experiments in controlled marine conditions, we explored the impact of microplastics on the quality and quantity of microbial CDOM. In the presence of microplastics we observed an increased production of CDOM with changes in its molecular weight, which resulted from either an increased microbial CDOM production or an enhanced transformation of DOM from lower to higher molecular weight CDOM. Our results point to the possibility that marine microplastics act as localized hot spots for microbial activity, with the potential to influence marine carbon dynamics.



Exponential decay of the spectral slopes of CDOM absorbance a(355) for C (blue dots) and MP samples (red dots) for control and microplastics treatments

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2A – Nanocomposites for the strengthening and deacidification of canvases

G. Poggi, R. Giorgi, P. Baglioni

Aims

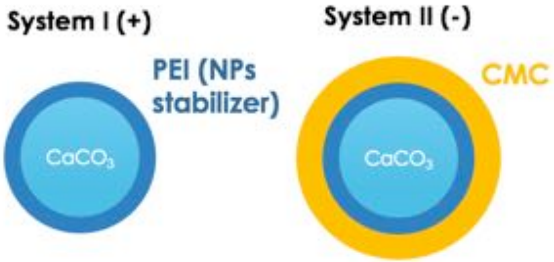
Lignocellulosic canvases, used as support in paintings, are progressively degraded by acidity originating from the application of primers, paints, glues or from absorption of acidic gases from the environment. Canvases' degradation causes a decrease in the mechanical properties and may ultimately affect the integrity of the paint layer. Therefore, new materials for the strengthening and deacidification of canvases are needed to grant the preservation of paintings and artworks featuring canvases.

Results

The acidity of canvases made of natural materials is generally of concern as it can lead to loss of mechanical properties and deterioration in less than 100 years. The stability of synthetic canvases is even less known than that of canvases of natural origin. This problem dramatically concerns also jute, which becomes quite acidic in a faster way than linen, and paintings done on this type of canvas become more brittle.

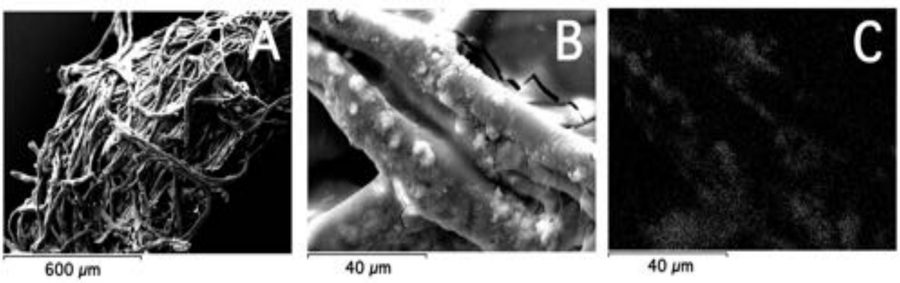
The lining, that is the gluing of a new canvas on the back of the painting, is traditionally used for the consolidation of canvases. However, although inevitable for the most degraded canvases, lining should to be avoided due to its invasiveness, because it hides the original canvas and is very resource-intensive.

The goal within the EU Project NANORESTART was to develop materials for the mechanical strengthening of canvases of modern/contemporary paintings to be mixed with alkaline nanoparticles to hamper the depolymerization of cellulosic fibers.



One of the most interesting strategy we designed to this aim 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.
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.
The effect of the treatments on cotton fibers was also assessed using Scanning Electron Microscopy. Canvas fibers display several clusters of nanoparticles (B), as clearly shown by EDX map of calcium reported in C.



On the basis of the experimental test, the most promising systems were sent to conservators belonging to the Consortium of the NANORESTART project, to be tested on real samples.

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2A – Nanofluids and chemical hydrogels for the selective removal of overpaints and graffiti from murals

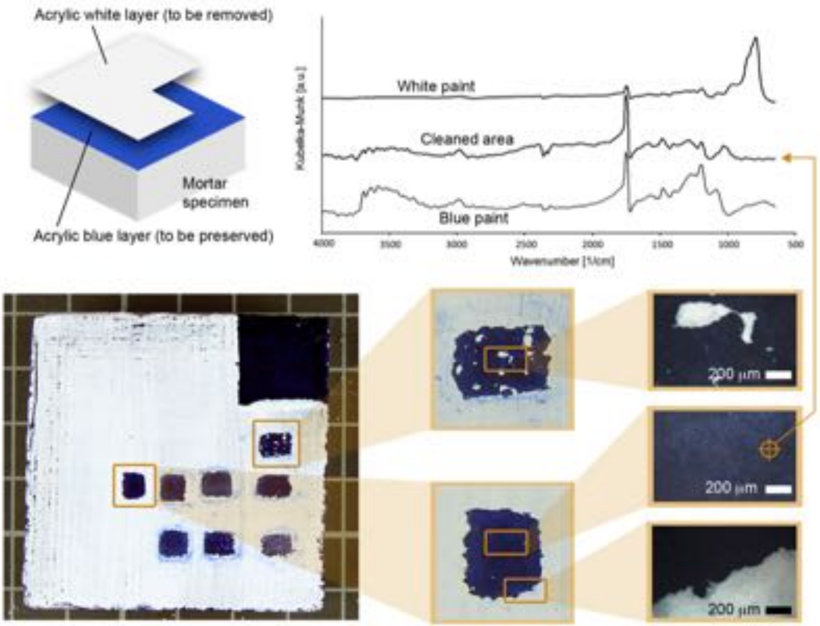
R. Giorgi, M. Baglioni, P. Baglioni

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.

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, in the frame of the Horizon 2020 EU-funded project NANORESTART, the use of nanostructured fluids, such as micelles and microemulsions, either neat or combined with highly retentive chemical hydrogels, was proposed and it is here reported as a selective and controllable cleaning system for the removal of graffiti and overpaints from street art. The highly water-retentive hydrogels, above mentioned, are semi-interpenetrated polymer networks (SIPN) 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). These hydrogels were shown to be particularly suited to limit the cleaning action to the surface layers of the treated area. These hydrogels can be loaded with water, some polar solvents, or with aqueous nanostructured fluids (hereafter, shortly, "nanofluids"), composed by eco-friendly, volatile or auto-degradable compounds, which ensure a residue-free and environmentally compatible cleaning intervention.

Setting up application times and performing careful and delicate mechanical action were found to be key factors when removing overpaints having the same binder as the original paint layer. In fact, the removal of acrylic (or vinyl) paints from other acrylic (or vinyl) paints was achieved with minimum stress for the original paint layer. Microscopic observation and FT-IR analysis of the treated areas confirmed the good results of the cleaning tests.

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2A – Nanostructured fluids for the conservation of cultural heritage – Understanding the mechanism of organic coatings removal

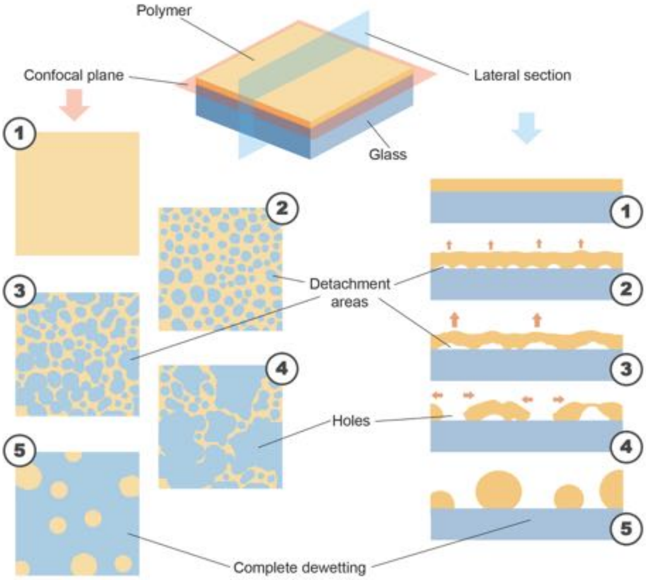
M. Baglioni, D. Berti, C. Montis, T. Guaragnone, M. Raudino,
M. Bonini, D. Chelazzi, R. Giorgi, P. Baglioni

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. 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).



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2A – New challenges in the study of lithic raw materials in central Italy at the dawn of metal working societies: pXRF analysis of the radiolarite artifacts in Tuscany

V. Volpi, A. Donati, S. Scaramucci

Aims

In central-southern Tuscany radiolarite has been used as a lithic raw material throughout prehistory. During the Copper Age it was selected for the local production of leaf-shaped artefacts.

Within this context, the discovery and recent investigation of the large radiolarite quarry of La Pietra (Roccastrada, Grosseto) and of the related workshops is of great interest.

The geological, chemical and archaeological data coming from the quarry-workshops will be used, in a future stage of research, to source the radiolarite artefacts found in Copper Age graves of Central Italy. The Copper age armatures are valuable artefacts mostly kept in museums and fully non-destructive analyses must be applied to them.

To tackle these challenges we followed a methodological approach which integrates field surveys, the individuation of petrographic markers of the most exploited radiolarite horizons and geochemical analyses. For geochemical characterization we made use of pXRF portable spectrometer and here we present some preliminary results.

Results

Geochemical characterization for the sourcing of sedimentary siliceous rocks has been a fundamental scientific tool in much research on prehistoric life-ways based on the study of lithic assemblages. This research has been successful only in as much as it was integrated with other techniques and as far as it was able to bring together different levels of analyses, from the macroscopic downwards. Sourcing of radiolarite artefacts at the site of Krems-Wachtberg (Austria) was done by LA-IPC-MS analyses. This proved to be a valid tool for distinguishing radiolarite of different geological regions. Variations in light elements Ba and Mg were found to be the most diagnostic for distinguishing between the Northern Alpine and Carpathian sources, although it was not possible to make well distinct groups within the same regions. Also Sr, Rb and V allowed some distinctions to be made between the two main regions.

In our own research we made use of pXRF for a preliminary characterization of radiolarite samples and archaeological artefacts from the central-southern Tuscany.

Portable X-ray fluorescence spectrometry (pXRF) allows non-destructive analyses of the elemental composition of archaeological artefacts also outside the labs (e.g.: in museums) and is thus very useful when it comes to analyse valuable archaeological collections, as in the here presented case of the Copper Age arrowheads.

Our Laboratory pXRF analyses on radiolarite was performed using an Olympus DELTA-Premium handheld pXRF analyzer, equipped with a 40kV tube, a “large area SDD detector", accelerometer and barometer for atmosphere pressure corrections of light elements measurements. The laboratory measurements were done with the instrument mounted on the fixed station. pXRF analyses are aimed at:

-characterizing radiolarite of different geological sources in the region to see if it is possible to make distinct groups between Ligurian and Tuscan Domain radiolarite and between different outcrops within each of the two domains.

-assign archaeological radiolarite arrowheads to the different radiolarite groups.

We took as starting point for our geochemical characterization the work by Brandl and colleagues (2014) where variations in trace elements Ba, Mg and, to some extent, Sr, Rb and V were found to be the most diagnostic for distinguishing between radiolarite outcrops of different geological areas. We focused on Sr and Rb only as Ba could not be detected by the pXRF device we employed and Mg was detected only in a small number of our samples. V, although present, was not found to vary significantly across the different samples we measured, whereas a good response was observed for Zr. For these preliminary analyses we simply plotted in scatter diagrams the variations of the couples Sr vs Rb and Rb vs Zr. In the first place we verified the possibility of distinguishing between different radiolarite outcrops of the same geological domain. This is especially important for Ligurian Domain radiolarite as the outcrops of this rock have yielded most of the evidence for Copper Age raw material exploitation.

The attempt of distinguishing geochemically the radiolarite of the Ligurian Domain from that of the Tuscan one was done in this preliminary analysis only with samples coming from the outcrop of Poggio Mutti. The green type radiolarite of Poggio Mutti, the only one on which traces of exploitation were found, was compared with green radiolarite samples of La Pietra. These radiolarites are macroscopically similar. The results of these measurement are quite encouraging as it is possible to distinguish that elemental values of the green radiolarite of the two different Domains fall quite apart and tend two form two distinct groups.

As the final scope of these analyses is the sourcing of archaeological artefacts made of radiolarite we performed pXRF measurements also on the above mentioned Copper Age arrowhead.

The raw material of this artefact is macroscopically very similar to the radiolarite of La Pietra and Albatreti. The pXRF results show how its Rb/Sr and Rb/Zr values fall within the lower range of the Ligurian radiolarites group of La Pietra and Albatreti type, and very distant from the range of the Petorsola group.

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2A – Organogels for the cleaning of artifacts

P. Ferrari, D. Chelazzi, R. Giorgi, P. Baglioni

Aims

Synthesis and characterization of chemical organogels with tunable properties for the cleaning of artworks.

Results

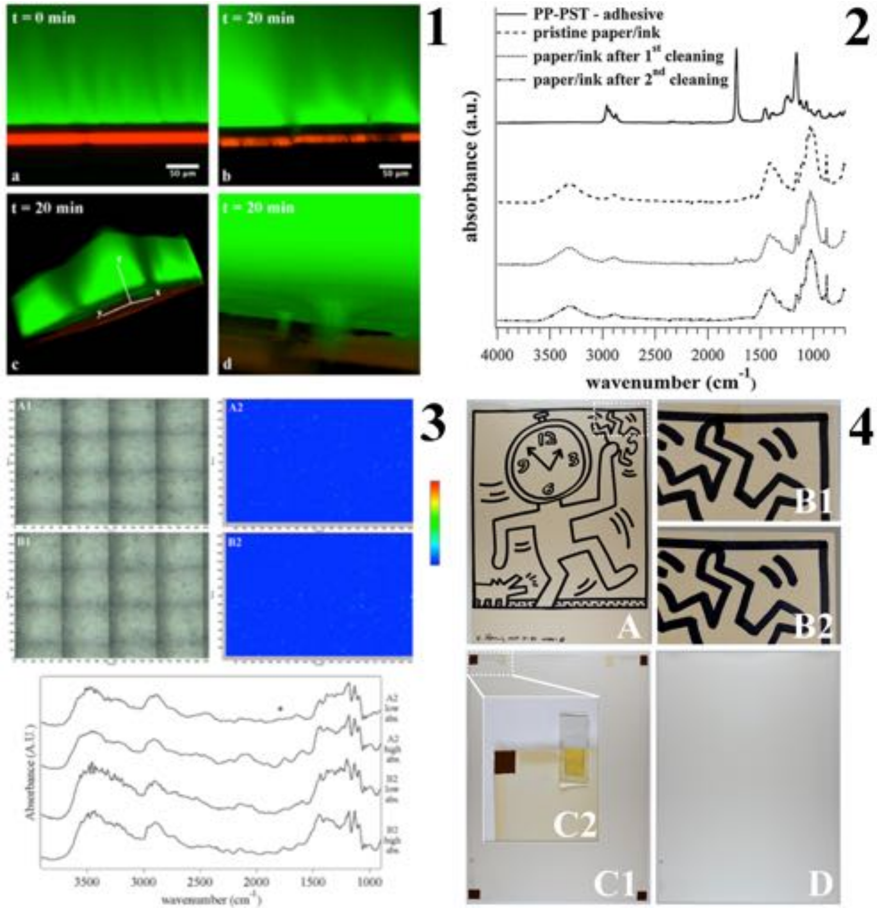
Gels are particularly useful for the cleaning of works of art as they allow the controlled delivery of cleaning fluids on solvent-sensitive substrates. Owing to the covalent cross-links between polymer chains, chemical gels exhibit mechanical properties that allow their easy handling and their residue-free removal from artistic surfaces after the cleaning intervention.

Poly methyl methacrylate (PMMA) organogels obtained by solubilizing MMA together with a dimethacrylate cross-linker in organic solvents, e.g. ethyl acetate (EA), butyl acetate (BA), and metyl ethyl ketone (MEK), were prepared for the removal of aged varnishes from canvas paintings.

In order to achieve successful organogel applications also to the cleaning of solvent-sensitive paper artworks, more retentive systems were developed. Specifically a PMMA-MEK organogel was designed for the selective removal of aged wax from inked paper. As compared to previous formulations, the larger amount of cross-linker and the different solvent-monomer ratio actually 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 in order 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 in poly ethyl methacrylate (PEMA) 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 (see figure 1), the embedment of the solvent into the gel network allows a feasible intervention by applying the gel directly on the top surface of PSTs (e.g. a poly propylene PST, PP-PST, is shown in figure 1): 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 effectiveness in removing also adhesive residues after a second gel application performed directly on the paper support was assessed by ATR-FTIR measurements on paper mock-up samples (i.e. PP-PST on paper, see figure 2). Furthermore the absence of gels residues on mock-ups after the cleaning intervention was verified by 2D FTIR Imaging (figure 3). 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.

Overall, this work validated the use of poly methacrylate organogels as versatile cleaning tools useful for cleaning intervention on different artistic surfaces, furthermore minimizing the risks of altering the original properties of the artifacts.



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2A – PVA-based cryogels for the cleaning of Modern and Contemporary Art

R. Mastrangelo, D. Chelazzi, G. Poggi, E. Fratini, P. Baglioni

Aims

Removal of undesired materials from rough painted layers, like the ones characterizing Modern and Contemporary Art. Formulation of cryogels composed by one or more polymer types.

Results

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. Unwanted materials can be solubilized in proper media, like microemulsions, swollen micelles or free solvents. 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 restriction of human intervention on invaluable masterpieces is, then, necessary to transfer Cultural Heritage to the future generations.

Poly(vinyl) alcohol-based cryogel are obtained through a freeze-thawing (FT) process, applied on PVA aqueous solutions. The freezing step induces a water-polymer phase separation. When water freezes, the polymer chains are pressed together until PVA crystallites form. Crystallites act as junctions, conferring to the hydrogel cohesion and elasticity closer to those of chemical gels. Ice crystals act as templates in the formation of a ubiquitous porosity. Free water content and water retentiveness are far higher than the ones characterizing traditional gels used in restoration.

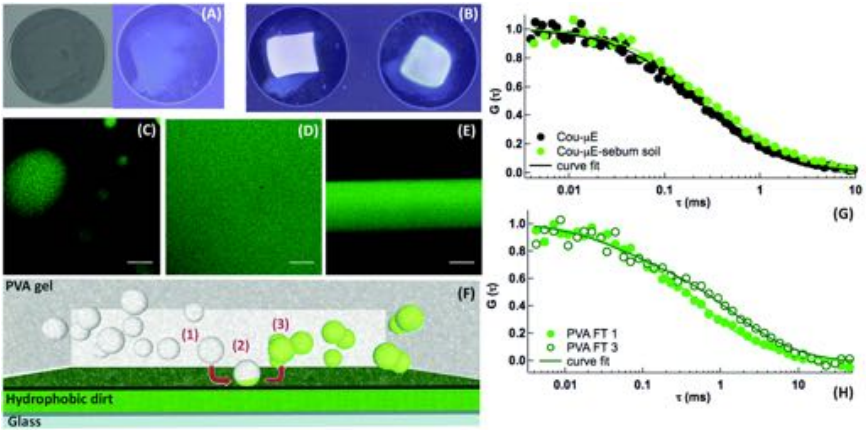
PVA-based cryogels have been prepared with procedures involving up to 7 FT cycles.

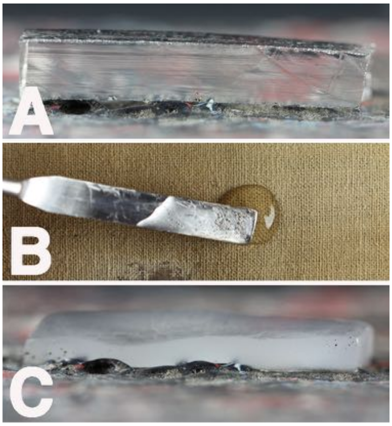
The number of FT cycles influences physico-chemical and viscoelastic properties, as proven by rheology, thermic, microscopy and scattering measurements. Moreover, pore diameter increases with the number of FT cycles.

The diffusion of cleaning systems through the gel pores, such as oil-in-water microemulsions, was investigated in pure PVA systems through Fluorescence Correlation Spectroscopy. The results show that the pores' size allows the free diffusion of 16 nm droplets in the FT3 hydrogels, while some trapping effects arise in the case of FT1 gels, i.e. when the pores size is smaller. The embedded microemulsion was able to remove hydrophobic dirt (sebum soil) from a glass surface and to retain it inside the hydrogel.

An oil-in-water microemulsion embedded in PVA FT1 and PVA FT3 hydrogels can capture hydrophobic dirt from a model surface (glass) and retain it inside the gel matrix.

Properties of PVA cryogels strongly changes when a second polymer (like polyvinylpyrrolidone or a different type of PVA) is added to the formulation: the resulting semi-interpenetrated network shows higher porosity and water retentiveness. The ability to clean surfaces is strongly enhanced, especially if compared to gels traditionally used in restoration. In this sense, the high adaptability to rough surfaces and the absence of residues after the treatment play a fundamental role.





Gels used in conservation: (A) a rigid gel – gellan gum 3%; (B) a soft gel - Klucel™4%; (C) a PVA/PVP hydrogel. The rigid gellan gum does not adhere as homogenously as a PVA/PVP hydrogel to a rough painted layer that mimics a modern/contemporary painting.

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2A – Recent perspectives in electronic wearable textiles: carbon nanotube-doped hybrid silica coatings for heart rate monitoring

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Aims

Recently, the interest in the real-time monitoring of parameters related to both human health and the environment has grown rapidly focusing the attention of scientific research towards the development of innovative technologies for the design of "stimuli-responsive coatings". A new category of smart textiles, able to sense, respond and react to external stimuli thanks to the integration of sensing coatings has been developed. In order to design stimuli-responsive coatings, the sol-gel process represents a simple, versatile, efficient and environmentally sustainable route largely investigated. The so-resulting hybrid thin films are characterized by nano or mesoporous structures with fascinating properties as optical transparency, excellent chemical stability, no cytotoxicity, in which several sensing molecules can be immobilized. The integration of electronic devices, the deposition of carbon nanotubes (CNTs) tracks, and the simultaneous maintenance of the most fascinating properties of textile fabrics represent the main challenges in the design of wearable smart textiles. The aim of this study is to demonstrate the efficacy and reliability of sol-gel CNT-based coatings for cotton textiles in the real-time monitoring of heart rate using photoplethysmography (PPG) and electrocardiography (ECG).

Results

To obtain electroconductive CNT-based cotton fabric, a sol-gel synthesis was followed to disperse multiwalled carbon nanotubes (MWCNTs) in a water-based polymeric matrix. With this goal, an amino-terminal silica precursor and a thermo-sensitive surfactant were simultaneously used for their role in the π-π stacking CNT-interactions providing a stable and homogeneous nanotube dispersion and by preserving nanotube-electroconductive properties. These latter were mainly ensured by the chemical nature of the surfactant able to evaporate during the curing process without interfering with the CNT-CNT electrical connections. The CNT-coating was firmly linked to the cellulose surface since retention over to 99% of the starting electrical surface resistance of coated fabric was measured after one washing cycle. Developed textiles were tested as conductive elements in the heart rate (HR) monitoring by PPG (Figure 1) and ECG. The CNT-textiles demonstrated to be reliable in the transmission of the electrical signal since they were able to detect a different amplitude in the systolic peaks.

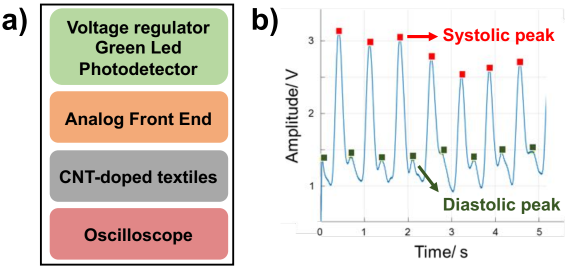

Fig. 1.a) Schematized setup for PPG analysis; b) Systolic and diastolic peaks in PPG.

In Figure 2, a prototype of smart textile (ELECT) for the real-time monitoring of the heart rate by ECG is provided. Using a specific app, it is possible to display the collected data in an easy and rapid way.

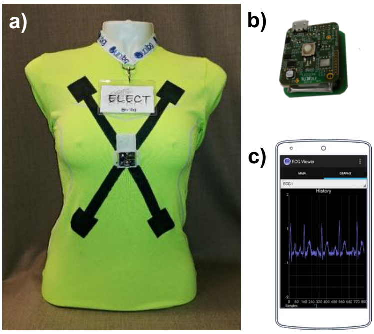

Fig. 2. a) ELECT smart textile; b) electronic device; c) App for HR monitoring.

Experimental findings demonstrated the potentiality of the sol-gel developed CNT-conductive textiles in both PPG and ECG techniques for heart rate long-term monitoring in a non-invasive way with interesting applications in wellness, healthcare, medical and fitness fields.

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2A – Study of the efficiency of the visible light activated Carbon doped Titanium Dioxide as photocatalyst

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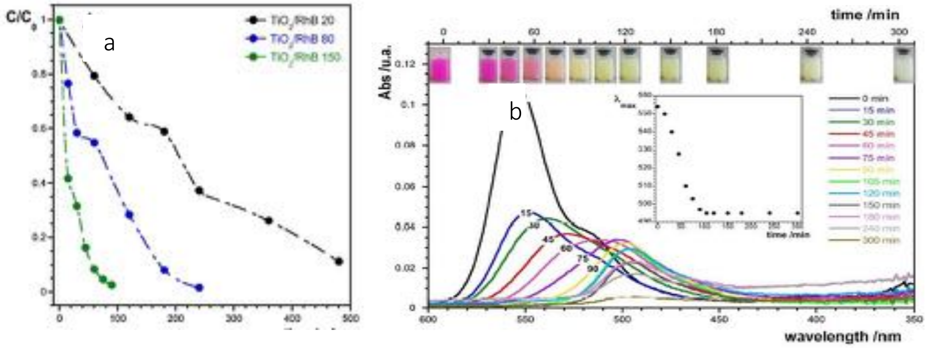
Aims

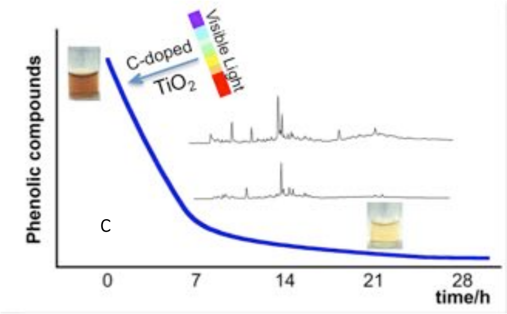
The use of titanium dioxide as heterogeneous photocatalyst is drawing considerable attention for water and air purification and remediation. With the aim to eliminate Rhodamine B (RhB), a dye widely used in the textile manufacturing that contributes with other dyes to harm the environment, and phenolic compounds of olive mill wastewater (OMW) glucose-doped titanium particles (CDT) through a photocatalysis process activated by visible light were used. In the present research project, the CDT catalyst effectiveness for the photodegradation of different compounds was tested on systems containing RhB, caffeic acid or total phenols.

Results

First, whit the final goal to provide new tools for the removal of dyes from water CDT was used to investigate on the decolourization and the photocatalytic degradation of RhB dye from water solutions. For this purpose a suitable parameter was introduced namely the ratio between the amount of catalyst and the amount of the target called TiO_2/RhB (a). It was demonstrated that the proposed degradation method could be scaled up without losing its effectiveness and the important role played by doped TiO_2 particles is demonstrated by the highly efficient color removal obtained during the visible light-induced photocatalysis (b).



In addition, UV−Vis absorption spectroscopy and gas chromatography−ion trap mass spectrometry analyses revealed a substrate concentration dependence of the removal of caffeic acid from a water solution and to evaluate the photodegradation event. The effect of the adsorption process on the whole degradation was also monitored in the absence of light. The positive effects of the visible light activated CDT on the removal of caffeic acid from aqueous solutions highlighted the potential application of this technology for the elimination of phenolic compounds from olive mill wastewater. By the way, the cleaning effectiveness of this catalyst towards the polluted wastewater from olive oil industry was demonstrated by means of HPLC and UV-visible spectroscopy combined with phenol compound determination. The OMW decolorization occurring in the presence of CDT particles under visible light radiation is marked enough to be directly appreciated with the naked eye (c). The decolorization is strongly associated with the removal of phenols and in fact, while bleaching the solutions, CDT successfully removed 70% of the phenols in 24 hours. HPLC analysis demonstrates that CDT was effective in degrading the higher part of the phenols present in olive mill wastewaters.



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2B – Environmental Assisted Cracking of High Strength Steels for Energy Industries

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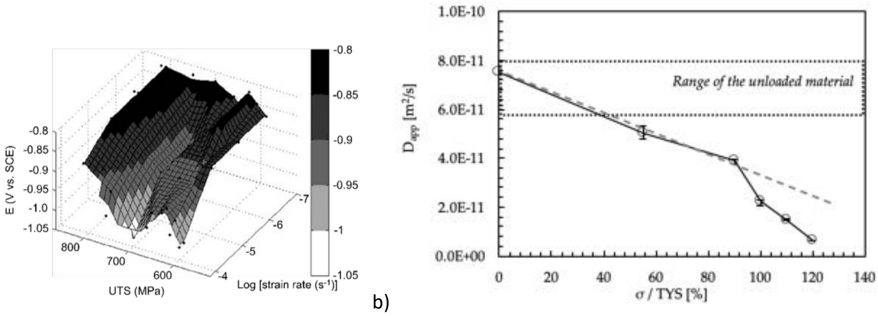
Aims

This research project studies the Environmentally Assisted Cracking (EAC) phenomena of different steels using in the industry of extraction, transport, conversion and storage of oil, gas, biofuel, and geothermal steam. The world consumes massive quantities of energy prevalently coming from fossil fuels. The increasing of demand of oil and gas industry has witnessed a significant transition to more severe downhole operating conditions and environments that involve higher pressures and temperatures along with increased well depths. On the other hand, the progressive increase in the use of fossil fuels as energy sources and the simultaneous increasing deforestation are the main causes of global warming. Both the carbon capture transport and storage and the increasing of renewable energy, like geothermal and biofuels, are middle time solutions to reduce the CO_2 emissions. Actually, there is a lack of knowledge on the corrosion resistance of traditional materials in these extreme environmental conditions.

Results

EAC takes place for the simultaneously action of aggressive environment and mechanic loading. In all the considered environments, the EAC mechanism is related to a hydrogen embrittlement mechanism. Hydrogen cathodic evolution takes place as complementary reaction of the generalized corrosion of the steel or by means of cathodic polarization. In the presence of external stresses, atomic hydrogen can migrate to regions of high stress concentration causing failures (Hydrogen Embrittlement – HE). In absence of H_2S, the considered steels are immune to HE, on the contrary HE effects can be observed during continuous plastic straining, like SSR tests, depending from applied cathodic potential and strain rate (figure 1a).

Applying a cyclic load up to yield strength, it is possible to observe a slight decrease in apparent hydrogen diffusion coefficient (D_{app}). Exceeding such value - i.e. at 110% TYS - D_{app} marked decreases due to the creation of a large quantity of new reversible and irreversible trapping sites (figure 1b). Applied cyclic load causes a very small decrease in the hydrogen permeation current at the steady state, mainly hindered by the increase in the passive current. This is slight as the cycle frequency decreases and it significantly increases as the load amplitude increases. Increase in the maximum load causes a temporary decrease in the permeation flux, which becomes larger and larger as applied load increases. Once the new traps generated are saturated with diffusible hydrogen, the steady state current returns to the value prior to the load increase. No transient reductions in the permeation flux are detected after subsequent load variations on specimens already subject to the same load variation (already strain-hardened), probably because of the local strain-hardening of the material and no creation of new trapping sites.



a) b)

Fig. 1: a) Critical potential for HE as a function of strain rate and ultimate tensile strength of laminated steels (hot rolling, controlled hot rolling, controlled hot rolling with accelerated cooling) b) Apparent diffusivity (Dapp) as a function of maximum stress and loading condition

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2B – Microstructure, Properties and Corrosion Resistance of Light Alloys Produced by Innovative Processing

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Aims:

This research aims on the evaluation of the relations between microstructure and corrosion behavior of light alloys obtained by means AM or jointed by FSW. The characteristics of high strength and stiffness, low weight, good formability, good corrosion resistance, and recycling possibility make aluminum, magnesium and titanium alloys ideal candidate to replace heavier materials (steel or copper) in many items, like transport, to satisfy the weight reduction demand. Recent examples of aluminum applications in vehicles cover power trains, chassis, body structure and air conditioning; there are strong predictions for aluminum applications in hoods, trunk lids and doors hanging on a steel frame. Nowadays new manufacturing technologies have been developed in order to improve design possibilities, of main interest are the Additive Manufacturing (AM). The term Additive Manufacturing refers to all the techniques to produce almost finished products starting from a three-dimensional CAD model directly by building the material layer by layer. Materials made through this technology have unique macrostructure and microstructures, characterized by the presence of porosities, traces left by the laser source during the process and very rough surface finishing which can lead to different corrosion morphologies compared to alloys manufactured with traditional solidification processes. In addition, to avoid the difficult of welding light alloys, Friction Stir Welding (FSW) technology, has been successfully used. The technique is now widely used in naval application, aerospace, automotive and railway applications, on the other hand, FSW may result in remarkable local microstructural modifications which can also affect the corrosion behavior.

Results:

Microstructural and corrosion behavior have been studied on AlSi10Mg produced by laser powder bed fusion technique, considering several operating parameters such as stress relieving temperatures, heat treatments, and different surface finishing. **T**he aluminum oxide film on the AlSi10Mg after production and standard stress relieving at 300 °C for two hours, is less protective than that formed spontaneously in air. The corrosion behavior of the alloys can be improved by considering the mechanical removal of the film formed at high temperature, i.e. by polishing the surface with abrasive paper and alumina (Fig. 1a). A further improve of the corrosion resistance was obtained by means of a subsequent application of a conversion treatment with cerium. The morphology of the attack evidences a selective penetrating dissolution in correspondence of the border of the melt pools generated by laser scanning. It is strictly dependent upon the subsequent heat treatment, which causes a different distribution of second phase precipitates (Fig. 1b).

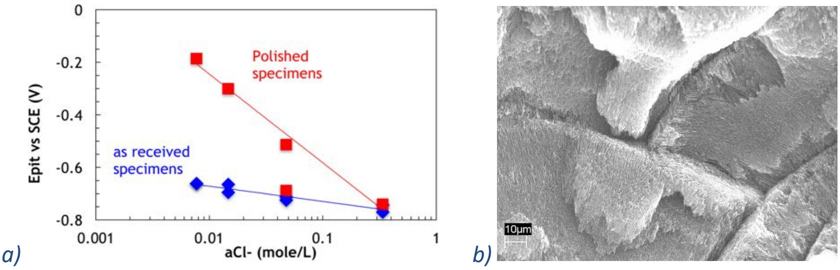
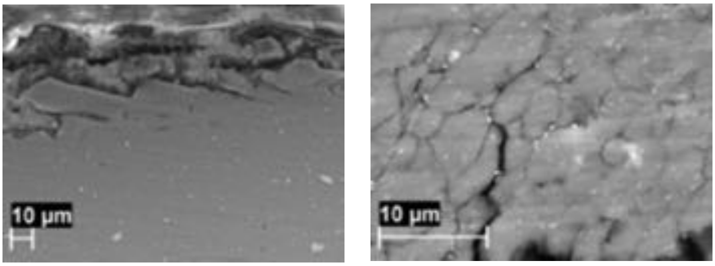


Fig. 1: a) pitting potentials as a function of chlorides ions activity for as received and polished specimens of alloy AlSi10Mg b) preferential corrosion of the border of the melt pool

Stress corrosion cracking tests carried out FSWed AA 2024T3 showed the presence of a Stress Enhanced Intergranular corrosion attacks in the central zone of the weld (Fig. 2). The preferential attack of the weld with respect to the parent material can be attributed to the alteration of the microstructure due to the thermomechanical action during FSW that provokes the precipitation of copper rich second phases at the grain boundaries that depletes the aluminium matrix and stimulates corrosion in these zones.



a) b)

Fig. 2: metallographic section of un-loaded (a) and loaded (b) and (c) 4PBB after 1400 hours of immersion in aerated 0.6M NaCl solution (a and b specimen welded with S 1000 rpm and F 10 mm/min, c specimen welded with S 1500 rpm and F 10 mm/min)

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2B – New materials for electrochemical applications

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Aims

Characterization and optimization of the physico-chemical properties of materials for electrochemical applications, to put into evidence the relationships among crystal structure, properties, synthesis method, doping and electrochemical performances. The investigated cathodes, anodes and electrolyte materials point at obtaining more performing rechargeable batteries for demanding applications (automotive, smart grids) in Li-ion batteries (LIBs), the energy storage system that actually dominates the market.

Results

1) Cathodes for LIBs.

Li2(Mn,Fe)SiO4 – The lithium transition metal ortho-silicates Li2MSiO4 (M = Co, Mn, Fe), offer a suitable high capacity cathode material for application in LIBs, thanks to the possible extraction of two Li ions per formula-unit and a particularly stable anionic framework. It has been demonstrated in our previous works that the defects formation, the easy segregation of impurity phases during the synthesis, and the polymorphism influence the electrochemical performances of Li2MSiO4. Our recent studies demonstrate that paramagnetic Solid-State NMR is a powerful tool to address polymorphs speciation of the Li2(Mn,Fe)SiO4 system. In fact, it displays extended polymorphism and similarities between the crystal phases, implying ambiguous and non-unique phase attribution by conventional structural techniques.

LiNi0.5Mn1.5O4 – The Si doped LiNi0.5Mn1.5O4 spinel compound has been prepared and characterized, and applied as high-voltage cathode material for LIBs. The study demonstrates the silicon substitution is an effective way to improve the structure stability and lithium diffusion, and to optimize both charge-discharge capacities and cycling performances of the cell.

2) Anodes for LIBs.

Ca- and Al-doped ZnFe2O4 – The spinel ZnFe2O4 compound is a promising anode material for LIBs, thanks to the low price, abundance, environmental benignity and high theoretical specific capacity. Nevertheless, it suffers for fast capacity fading and poor rate capability. Ca- and Al-doped samples (doping levels up to 25 atom%) have been prepared and characterized by several techniques (XRD, FTIR, TGA-DSC, SEM-EDS), and the doping cations distribution on the cationic framework is addressed. In the case of Al doping, improved electrochemical performances, especially at high C rate, are observed, thanks to the increased structural stability during charge-discharge processes and to Al ions contribution to the redox process.

FeNb11O29 – It is a new emerging anode material: thanks to the possibility to exchange up to 23 electrons per formula unit in the involved Fe3+ and Nb5+ ions redox reactions, it reaches a theoretical capacity value of 400 mAh/g. The monoclinic and orthorhombic polymorphic structures of the pure and V- and Mn-doped FeNb11O29 compound have been synthesized and characterized. The structural, spectroscopic and magnetic investigation put into evidence the presence of edge and corner-sharing

Nb octahedra with different distortion levels, especially in the monoclinic crystal form. The EPR and magnetic measurements confirm the presence of Fe3+ in high-spin configuration, Mn3+, and both diamagnetic V5+ and non-Kramers V3+ ions. No antiferromagnetic ordering occurred up to 2K. The electrochemical tests on the FeNb11O29 anode have been carried out on both polymorphs (monoclinic and orthorhombic) changing the carbon type to prepare the anode ink. The best performances (high and stable value of 250 mAh/g at 10C after 100 cycles) are obtained for the orthorhombic crystal form and Super C65 carbon source.

3) Electrolytes

Li7La3Zr2O12 – We investigate the Li7La3Zr2O12 garnet, a ceramic electrolyte that finds application in all solid-state lithium batteries, thanks to its high conductivity at room temperature. The investigated compound displays different structural modifications (High-Temperature cubic, tetragonal, Low-Temperature cubic) that play a relevant role in the optimized application of the solid electrolyte. Our study points at describing the relationship between the selected experimental synthesis condition and the obtained crystalline structure and stoichiometry, by investigating the LT-cubic phase stability in different temperature (25-750°C) and atmosphere conditions (air or Ar). In Ar flow, the LT-cubic structure is stable up to 750°C, then transforms into the tetragonal one on cooling to room temperature. In air, the garnet undergoes lithium loss above 250°C, as confirmed by ICP-OES analysis, and partially decomposes to La2Zr2O7; Li2CO3 and La2(CO3)3 formation is observed due to CO2 absorption on cooling in air.

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2C – Characterization of nutraceutical components in tomatoes pulp, skin and locular gel

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Aims

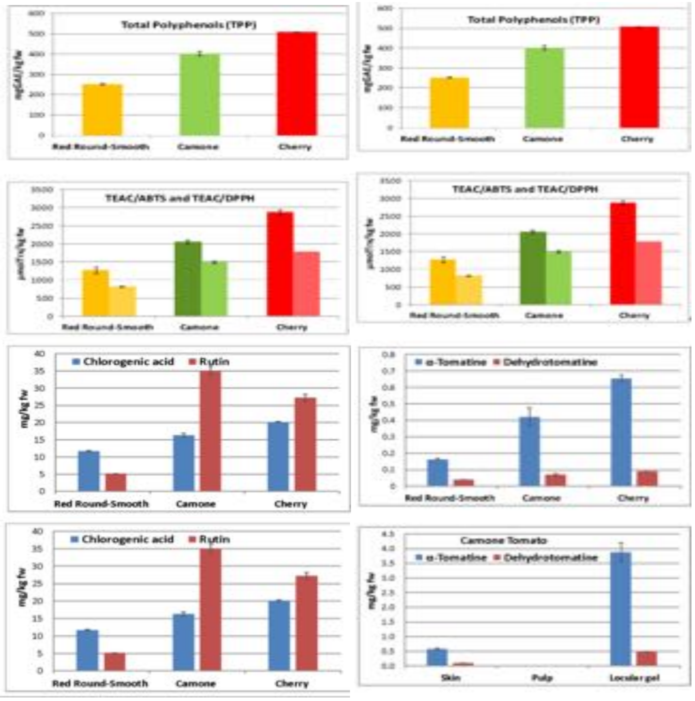
Nutraceutical properties of tomato fruits (Solanum lycopersicum L.) were investigated, focusing on selected secondary metabolites: glycoalkaloids and polyphenols (hydroxycinnamic acids and flavonoids). Three tomato varieties were studied: Red Round-Smooth, Cherry, and Camone (as whole fruits), and portions of Camone fruits (skin, pulp and locular gel) were characterized. Particular attention was devoted to the locular gel portion, a by-product material in the tomato processing industry. Quantifications of α-tomatine, dehydrotomatine and selected targeted polyphenols were carried out by reverse-phase liquid chromatography coupled with electrospray ionization tandem mass spectrometry (HPLC-ESI-MS/MS). Samples were also assayed for antioxidant activity, via ABTS and DPPH radicals quenching.

Results

Tomatoes, like many plants belong the Solanaceae family (including potatoes, peppers and eggplant) produce secondary metabolites, known as steroid glycoalkaloids. Tomatoes contain α-tomatine and dehydrotomatine, and commonly, the sum of the two compounds is reported as tomatine. The α-glycosidic triterpenoid, α-tomatine is a steroid, formed by the aglycone, called tomatidine, and a tetrasaccaride residue composed of a galactose, two glucose and a xylose unit. The dehydrotomatine is the α-unsaturated tomatine analogue (formed by the tomatidienol aglycone), and it is found in unripe tomatoes in an amount approximately 10 times lower than α-tomatine.

The antioxidant capacity of the analyzed samples was evaluated on the basis of spectrophotometric assays for total polyphenol content (TPP), and radical quenching (TEAC/ABTS and TEAC/DPPH). Cherry tomatoes revealed the best phenolic profile with respect to the Camone and Red Round-Smooth fruits, with statistically significant higher contents of TPP, as well as the highest TEAC values (both from ABTS and DPPH assays). The phenolic profile obtained via HPLC-ESI-MS/MS analyses, showed that chlorogenic acid and caffeic acid were the main hydroxycinnamic acids in all the studied varieties, while rutin was the most abundant flavonoid. On the other hand, rutin mainly occurred in the Camone skin, while chlorogenic acid was primarily in the locular gel. As regards the glycoalkaloids species, relatively low amounts were found, with the highest content in the Cherry whole fruit, while the Camone locular gel revealed higher level of tomatine with respect to pulp and skin portions.

It is interesting to note that the locular gel is usually a waste material in the tomato processing industry, and on the basis of the polyphenols and glycoalkaloids contents revealed in this study, could be recovered in order to obtain products of interest from the nutraceutical point of view, useful for fortifying foods, as diet supplements, as cosmetic ingredient, and many other applications. However, from this perspective point of view, the Cherry variety is not optimal for easily separation of the locular gel, due to its small size and relatively tender pulp, whereas the Camone fruits represent an excellent compromise between morphology of the fruit, especially in terms of separation of locular gel (and its recovery yield), and nutraceuticals profile.



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2C – Cu(I)-Glutathione derivative compound: structural characterization

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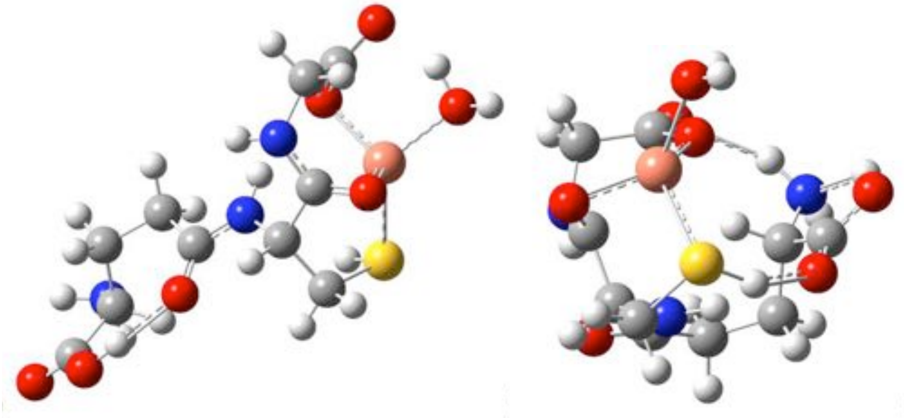
Aims

The structural investigation via density functional geometry optimization of some conformations of Glutathione (GSH), and molecular models of Cu^I-GSH binary and ternary complexes, have been studied and reported. A copper(I) compound of reduced glutathione (Glu,S;Cys,R)-(GSH) has been isolated from the reaction of Cu^ICl and zwitterionic H_3GSH^+ in acetonitrile:water medium. The complex has been experimentally characterized at solid state via infrared (ATR-FTIR) and thermogravimetric TGA analysis. The experimental results have been compared with computed data to identify the structure for the Cu^I-GSH derivative.

Results

The analytical data bring about the $Cu^I(H_2GSH)(H_2O)_2$ stucture. The characterization was carried out via infrared spectroscopy and density functional (DFT) method computations, that allowed to fully optimize structures for the free ligands and for several complex molecules of the type $[Cu^I(S,O,O\text{-}H_2GSH)(OH_2)]$ having a pseudo-tetrahedral coordination arrangement and the Gly residue deprotonated at carboxylic group. The molecules have been fully optimized at DFT-B3LYP/6-31G** (BS1) and in some cases at B3LYP/6-311++G** (BS2) and the solvent treatment (water, via PCM method) has been taken into account (BS1W). The comparative analyses between experimental and computed infrared spectra confirmed that the free ligand was reduced glutathione in the zwitterionic form at the Glu residue. The study also showed that the metal compound consisted of complex molecules of the type $[Cu^I(S,O,O\text{-}H_2GSH(Gly))_{str}(H_2O)]$ where the ligand has a stretched (str) arrangement assisted by a network of hydrogen bonds. A possible globular structure with a same coordination cannot be rejected. The analysis of computed infrared vibrations brought about results that are useful for the evaluation of force constant that are significant for building reliable force field for molecular mechanics computations for proteins and metallo-proteins.



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2C – Double Vortex Assisted Dispersive Liquid-Liquid microextraction coupled with GC Ion Trap Mass-Spectrometry for determination of Bisphenol A in hydroalcoholic matrices

G. Cinelli, F. Cuomo, F. Venditti, L. Ambrosone, F. Lopez

Aims

The aim was to validate an efficient, low cost, and time-saving method for bisphenol A (BPA) determination in red-wine beverage. BPA is an organic synthetic compound widely produced Bisphenol A (BPA) is a synthetic compound broadly used in medical devices as well as in packaging of food and drinks. Recently, BPA toxicity has become of concern to environmental public health. Red wine that is susceptible to BPA contamination is an alcoholic beverage made from yeast fermentation of grapes in the presence of grape skins so as to extract phenolic compounds. To this end, a microextraction based on a revised dispersive liquid–liquid micro-extraction (DLLME) is proposed for the determination of BPA. In particular, emphasis is given on the delicate parameters related to the pre-concentration process such as amount of extraction solvent, temperature and supplied energy.

Results

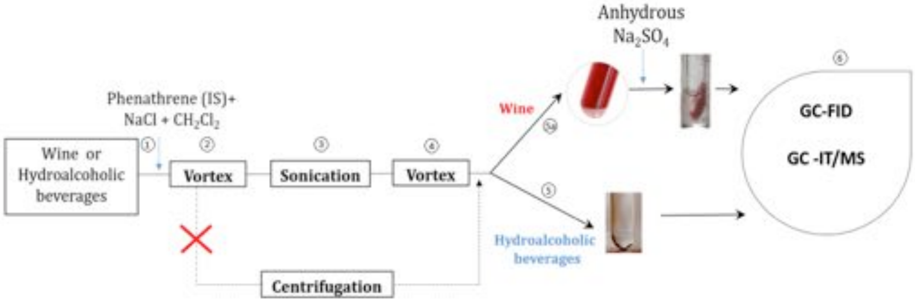

FIG. 1 Schematic representation of the vortex–ultrasound–vortex-assisted microextraction procedure for determination of BPA in wine and hydroalcoholic solutions

A rapid and simple microextraction method is here proposed consisting in liquid–liquid separation assisted by a vortex–ultrasound–vortex procedure combined with gas chromatographic analysis (GC-Fid or GC-IT/MS). By means of a comparative study between real red-wine matrix and synthetic hydroalcoholic solutions, different parameters related to the microextraction steps were investigated. The minimal amount of extraction solvent for a given volume of sample was calculated for both the systems. It was demonstrated that for red-wine matrix, the extent of phase separation is strongly affected by some wine constituents and that separation can be tuned by varying the amount of the extraction solvent. The amount of solvent to supply is strongly dependent on the matrix used. This double vortex–ultrasound-assisted method achieved high recovery of BPA and enrichment factor compared with other microextraction methods.

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2C – Graphene/Nanoparticles hybrid system for the controlled immobilization of biomarkers for early diagnosis of neurodegenerative diseases

G. Caminati, C. Lofrumento, M.R. Martina

Aims

We propose a sensing platform based on arrays of silver nanowires and nanostars (AgNPs), both naked or veiled by graphene oxide (GO), for the detection of subnanomolar concentration of amyloid fibrils of Lysozyme and toxic oligomers of the Aβ peptide (1-42). Amyloid biomolecules with high beta-sheet content are regarded as biomarkers of the early onset of neurodegenerative disorders as Alzheimer's and Parkinson's diseases

Results

Ordered arrays of nanoparticles were obtained by Langmuir-Blodgett assembly of the silver nanowires on the transducer surface or by direct electro-deposition of Ag nanostars. The morphology of the compact arrays at water-air interface was monitored with Brewster Angle Microscopy whereas the structure of the transferred layers was revealed by Atomic Force Microscopy (AFM) and UV-Vis spectroscopy.

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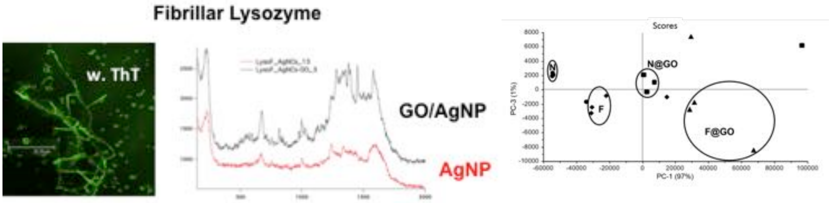
The adsorption of oligomeric Aβ peptide and fibrillar lysozyme onto the outer surface of the nanoconstruct was followed by means of Quartz Crystal Microbalance (QCM), the measurements provided the mass density and thickness of the amyloid aggregates as well as their detection limit.

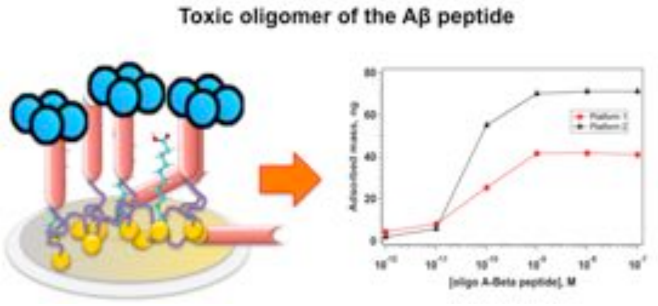
AgNPs and GO/AgNPs arrays covered with a saturated layer of the protein were prepared also on quartz surfaces and further characterized by Confocal Laser Scanning Microscopy experiments.



Parallel Surface Enhanced Raman Spectroscopy (SERS) combined with Principal Component Analysis (PCA) studies showed a remarkable uniformity in the distribution of the signal and that the presence of hot spots in the AgNP array and GO coating supplies additional signal amplification.

The QCM detection limit found for fibrillar lysozyme on GO/AgNp was of 3x10-10 M, in the case of toxic oligomers of the Aβ peptide, thanks to the functionalization of the

AgNP surface with an oligomer-specific receptor, a detection limit as low as 5x10-11 M could be assessed.



The body of the results paves the way for the construction of an efficient sensing device with high selectivity and low detection limit for toxic fibrillar aggregates.

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2C – Identification and characterization of a different oxidation site in the LRET pathway of a novel DyP

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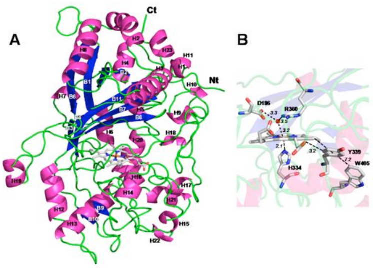
Aims

A dye-decolorizing peroxidase (DyP) from *Pleurotus ostreatus* (*Pos*DyP4) is able to oxidize Mn(II) in the presence of H_2O_2 with an efficiency similar to the classical MnP and Versatile Peroxidase. Crystal structure, molecular simulation, EPR and site-directed mutagenesis allowed to identify the residues (three aspartates and one glutamate) involved in the Mn(II) oxidation and present on the surface of the protein. As the Mn(II) is not in direct contact with the heme propionates, a tyrosine is involved in the electron transfer. For the oxidation of aromatics and dyes a second electron transfer takes place and it occurs at the surface of the protein on a tryptophan.

Results

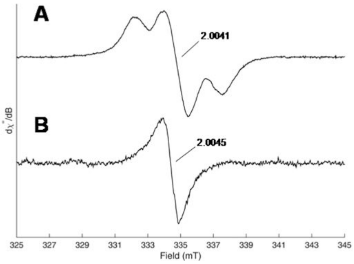
The crystal structure of *Pos*DyP4 shows the overall topology of the DyP family.



*Pos*DyP4 crystal structure. (A) Ribbon representation of the overall fold with α-helices in magenta (H1 to H28), β-strands in blue forming two β-sheets (B1–B6 and B7, B8 and B11), random coil in green, C and N termini of the solved structure (Ct and Nt) included, and the heme cofactor as CPK-colored sticks (PDB: 6fsk). (B) Detail of the heme pocket with His334, Asp196, Arg360, and water134 (at the sixth coordination position of heme iron), and Trp405 and Tyr339 at 7.2 and 3.2 Å from the heme cofactor.

In contrast with class-II peroxidase, which have a main heme access channel and a small second channel in front of one of the heme propionates, *Pos*DyP4 has only a narrow access channel connecting the solvent with the upper side of the heme pocket and lacks the channel in proximity of the heme propionates. Asp196 and Trp405 are homologous to residues involved in the catalysis by other fungal DyPs and the first residue placed over the heme plane is essential for activity, whereas Trp405 is involved in VA oxidation and other substrates with the exception of Mn(II) whose oxidation is not affected. QM/MM calculations showed that: Trp405 is the residue with the highest tendency to form a radical at the heme neighborhood, predicted that this tendency would pass to Tyr339 in the W405S variant. According to the computational data, four aminoacids (Asp215, Glu345, Asp352, Asp354) could be involved in the binding of Mn(II) with Tyr339 located at the cation vicinity. To confirm the role of the above residues seven mutated variants were characterized. All the variants had a reduced Mn(II) oxidation activity, confirming the role of the residues in Mn(II) binding and oxidation with Tyr339 the most important residue.

EPR spectrum of native *Pos*DyP4 after the addition of H_2O_2 showed the presence of a Trp radical in combination with other minor radical species. The EPR spectrum of the W405S variant, inactive for all substrate oxidation except Mn(II), showed the presence of a tyrosyl signal being absence the Trp contribution.



Twenty mT scan width X-band EPR spectra of 0.25 mM native PosDyP4 (A) and W405S variant (B) in tartrate buffer, pH 3, after the addition of 8 equiv of H_2O_2. Conditions were 5 mW microwave power, 0.2 mT modulation amplitude, and ν= 9.39 (A) or 9.38 (B) GHz.

For the first time the oxidation of Mn(II) (in *Pos*DyP4) implies a LRET pathway. Four residues coordinate the metal ion at this position. One of these residue (Glu345) would receive the electron from Mn(II) transferring it to the neighbor Tyr339 necessary for the oxidation reaction to take place. QM/MM predicted the involvement of Tyr339 in the electron transfer from Mn(II) to the heme and EPR confirmed this residue contribution for the W405S variant.

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2C – Interaction of the anti microbial peptide LL-37 with lipid membranes

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Aims

The aim of this work is to study the interaction of bioactive antimicrobial peptides with phospholipids membranes combining several spectroscopic techniques (i.e. Circular Dichroism, Fluorescence Emission, Site Directed Spin Labeling – Electron Paramagnetic Resonance) in order to clarify various features that regulates the mechanism of this interaction.

Results

LL-37, a cationic peptide belonging to the cathelicidins, is the only peptide of this group expressed in humans. In addition to its bactericidal activity, LL-37 exerts immunomodulatory functions and forms, along with other peptides, the first line of defence againts infections. The formation of LL-37 aggregates in the presence of neutral membranes, promotes a lack of cell selectivity, which could explain the presence of citotoxicity when the peptide reaches high concentrations. While cationic amino-acids such Arg and Lys are known determinants of these amphipathic molecules for bacterial killing, little is known how lysine-arginine exchange can influence peptide biological activity. Since we consider antimicrobial peptides promising candidates for the development of novel anti-infective agents, we have compared the biocidal effects and citotoxicity of five different LL-37 variants with wild type peptide. The antimicrobial activity was tested against *Escherichia coli* and *Streptococcus agalactiae*, while citotoxicity was measured with A549, a human bronchoepithelial cell line. There are clear differences in bacterial killing kinetics towards both pathogens when central Arg are mutated in Lys, with Arg more efficient than Lys in bacterial membrane permeation. Of interest the Arg in position 34 can compensate the absence of the Arg in position 19 and 23 and the presence of Lys at the other positions results in a diminished toxicity to eukariotic cells. Our study sheds new light on key amino-acid residues of LL-37 and should be considered when novel cationic amphipathic peptides, LL-37 derived, are designed.

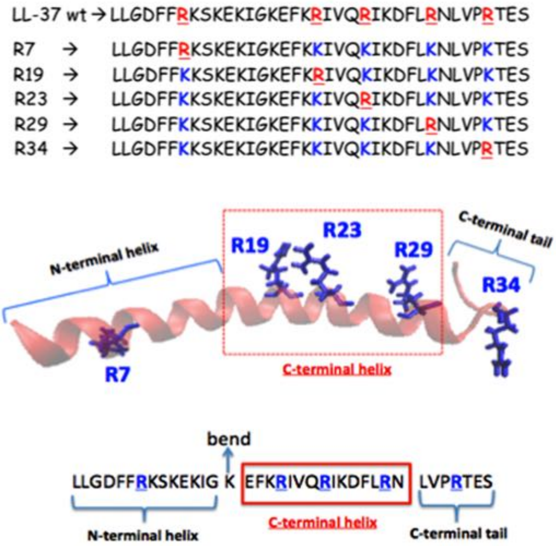

Figure 1 Amino acid sequences and secondary structure of LL-37. The amino-acid sequences of native LL-37 and variants and the mutated amino-acids are represented in the upper panel. In the lower panel is represented the secondary structure of LL-37 with the key Arg in blue. The structure was obtained with Visual Molecular Dynamics and Discovery Studio tools (LL-37 2K6O pdb code).

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2C – Mechanism of phospholipid transport across biological membranes mediated by P4-ATPases (phospholipid flippases)

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Aims

Phospholipid flippases (P4-ATPases) utilize ATP to translocate specific phospholipids from the exoplasmic leaflet to the cytoplasmic leaflet of biological membranes, thus generating a transmembrane lipid asymmetry, which is essential for a variety of cellular processes [1]. Central aspects of the translocation pathway and flipping mechanism of P4-ATPases remain elusive, including electrogenicity of the phospholipid flippases. It is unknown whether lipid transfer between membrane bilayer leaflets can displace charge across the membrane. Using an electrophysiological method based on solid supported membranes (SSM) we investigated the electrogenic properties of the mammalian flippase ATP8A2. The SSM method (Fig. 1) has been used to study the ion transport mechanism and identify electrogenic steps of P-type ATPases, such as sarcoplasmic reticulum Ca2+-ATPase [2] and Cu+-ATPases [3]. Activation of ATP8A2 by an ATP concentration jump generates an electrical current which is related to the movement of a charged lipid head group between the membrane bilayer leaflets. Electrogenicity of phospholipid transport represents an unexplored key feature of the flipping mechanism of P4-ATPases.

Results

Current measurements were performed on reconstituted proteoliposomes containing purified ATP8A2. The proteoliposomes were adsorbed to the surface of a SSM electrode (Fig. 1) [4]. We activated the adsorbed membrane-bound ATPase by an ATP concentration jump, and detected the related current signal [2,3]. It is shown in Fig. 1 that a 100 µM ATP jump on ATP8A2 reconstituted into proteoliposomes consisting of a mixture of 90% phosphatidylcholine (PC) and 10% phosphatidylserine (PS) induced a current transient, which was not observed following addition of ATP to control liposomes devoid of ATP8A2 (data not shown). To confirm that the measured current was actually due to ATP8A2 activity, we performed an ATP jump in the presence of the ATPase inhibitor orthovanadate, which caused complete suppression of the current transient (Fig. 1).

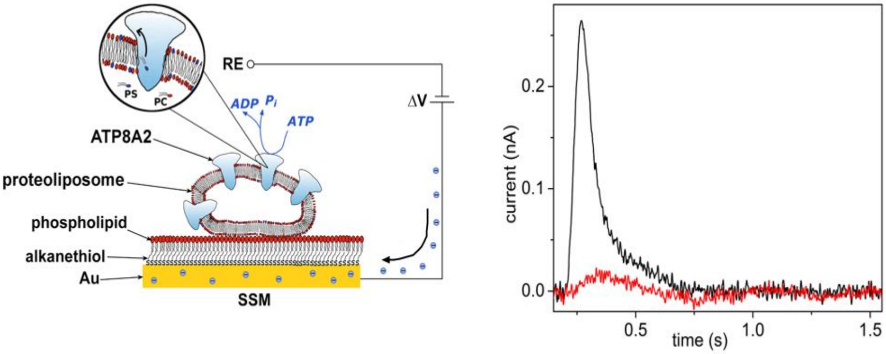

Fig. 1 - *Left Panel*: Reconstituted proteoliposome containing ATP8A2 adsorbed on the SSM surface and subjected to an ATP concentration jump. If the ATP concentration jump induces net charge displacement, i.e., displacement of negatively charged PS, across the ATPase, a current signal is detected along the external circuit (the blue spheres represent electrons) to keep constant the potential difference (ΔV) applied across the whole system. PS: phosphatidylserine; PC: phosphatidylcholine; RE: reference electrode. *Right Panel*: Current transients observed following 100 µM ATP concentration jumps on proteoliposomes containing ATP8A2 in the absence (black line) or in the presence (red line) of 50 µM orthovanadate.

PS possesses a net negatively charged head group and is a substrate of ATP8A2, whereas PC, also present in the proteoliposomes, is not a substrate and possesses an electrically neutral head group. Thus, the ATP8A2 current signal may be attributed to the displacement of negatively charged PS across the vesicle membrane in connection with ATP utilization. We are currently investigating specific steps in the ATPase reaction cycle which are directly involved in translocation of the lipid and can generate the electrogenic signal.

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2C – *N*-acetylcysteine ethyl ester as GSH enhancer in human primary endothelial cells: a comparative study with other drugs

D. Giustarini, F. Galvagni, I. Dalle-Donne, A. Milzani, F.M. Severi, A. Santucci, R. Rossi

Aims

The most common way to increase glutathione (GSH) levels in cells is to provide them with cysteine (Cys) or with a source of this molecule, since Cys is usually the limiting substrate in GSH synthesis. In the present research we study the glutathione-enhancing activity in human primary endothelial cells of the new compound N-acetylcysteine ethyl ester (NACET) in comparison with other routinely used drugs, namely N-acetylcysteine (NAC), 2-oxothiazolidine-4-carboxylic acid (OTC), glutathione ethyl ester (GSH-EE).

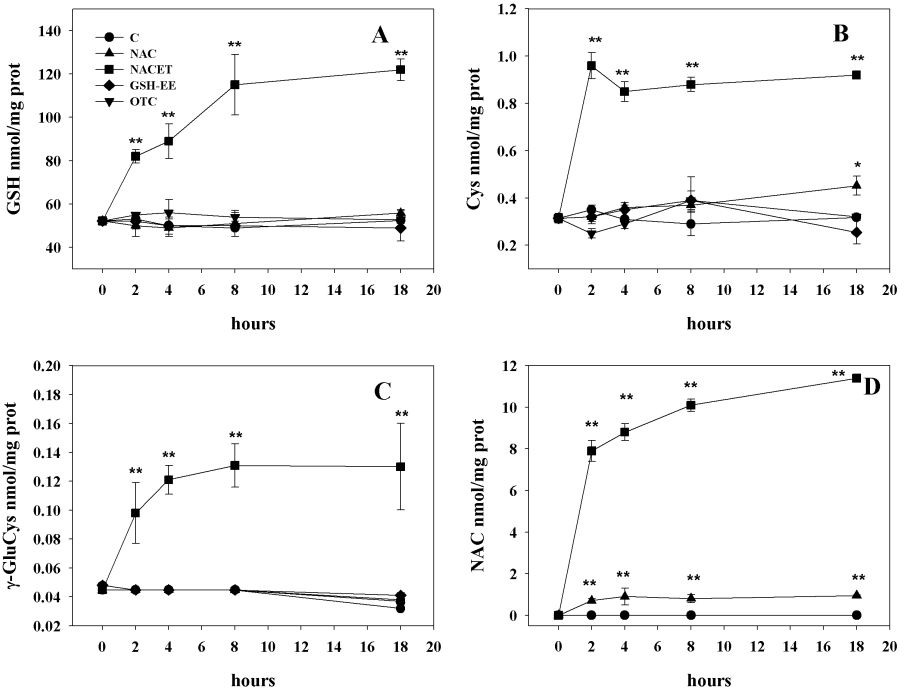
The influence of the intermediate metabolites of NACET on enzyme machinery for GSH synthesis is also investigated.

Results

We demonstrated that NACET (the ethyl ester derivative of NAC) is much more efficient than the other studied molecules in boosting intracellular GSH concentrations in HUVEC. Treatment with NACET also increased the levels of both GSH precursors, Cys and γ–glutamylcysteine (γ–GluCys). Under basal conditions, intracellular cysteine concentration is about 20 μM in HUVEC cells. Treatments with NACET raised cysteine levels up to five-fold the basal levels and this leaded to an increase in de novo synthesis of GSH, as demonstrated by the parallel dramatic augmentation of its immediate precursor, namely γ–GluCys. NACET was also able to increase the intracellular concentration of NAC more efficiently than NAC itself. NAC, in fact, is poorly membrane-permeable, having a low partition coefficient and lacking of specific transporters.

The increase in GSH concentration was not linear but peaked at 0.5 mM NACET and gradually decreased when cells were treated with higher concentrations of NACET. We demonstrated that this effect was due to the fact that NAC released from NACET turned out to be a competitive inhibitor of the enzyme glutamate-cysteine ligase, with a Ki value of 3.2 mM.

We also demonstrated that the slight increase in intracellular levels of cysteine and GSH induced by NAC in HUVEC grown in standard medium is due to the reduction of the cystine present in the medium itself there rather than to the action of NAC as Cys pro-drug. This fact may explain why NAC works well as GSH enhancer at very high concentrations in pre-clinical and in vitro studies, whereas it failed in most clinical trials.



HUVEC treatment with GSH enhancers for different times.

HUVEC at confluence were treated with 0.2 mM NAC, NACET, GSH-EE, or OTC. At the indicated times, cells were washed with PBS and lysed by TCA. Low molecular mass thiols were measured in cell lysates by HPLC. Data are the mean ± SD. Number of replicates = 3. *p< 0.05; **p<0.01 vs 0 time point.

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2C – Nanotechnology based cardiac targeting and direct cardiac reprogramming

F. Di Nezza, C. Costagliola, L. Ambrosone

Aims

The project aims to create a liposomal kit so that it can be handled easily even by non-experts.

Results

Cardiovascular diseases represent the first cause of morbidity in western countries, and Chronic Heart Failure features a significant health care burden in developed countries. Efforts in the attempt of finding new possible strategies for the treatment of CHF yielded several approaches based on the use of stem cells. The discovery of direct cardiac reprogramming has unveiled a new approach to heart regeneration, allowing, at least in principle, the conversion of one differentiated cell type into another without proceeding through a pluripotent intermediate. First developed for cancer treatment, nanotechnology based approaches have opened new perspectives in many fields of medical research, including cardiovascular research. Nanotechnology could allow the delivery of molecules with specific biological activity at a sustained and controlled rate in heart tissue, in a cell specific manner. Potentially, all the mediators and structural molecules involved in the fibrotic process could be selectively targeted by nanocarriers, but to date only few experiences have been made in cardiac research. This project highlights the most prominent concepts that characterize both the field of cardiac reprogramming and a nanomedicine-based approach to cardiovascular diseases, hypothesizing a possible synergy between these two very promising fields of research in the treatment of heart failure.

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2C – Nicotinic Acid Adenine Dinucleotide Phosphate Encapsulate in liposomes as signaling in vasculogenesis

F. Di Nezza, L. Ambrosone

Aims

The research aims to load the second messenger into liposomal nanocarriers able to permeate cell membrane.

Results

Nicotinic acid adenine dinucleotide phosphate (NAADP) has been established as a Ca^{2+} releasing intracellular second messenger in a growing number of cell types. Recent work showed that NAADP-evoked Ca^{2+} signals stimulated angiogenesis in vitro and neovascularization in vivo. An increase in intracellular Ca^{2+} concentration has been put forward as an alternative tool to improve the therapeutic outcome of regenerative medicine in ischemic patients. However, a major problem in assessing the physiological effect of NAADP and exploiting its therapeutic potential is that, just like all known second messengers, NAADP is electrically charged to prevent its leakage from the cells and is, therefore, membrane-impermeant. We describe a strategy to investigate NAADP signaling in large populations of hEPCs by exploiting liposomes to intracellularly load them with NAADP. This approach retains a significant therapeutic relevance as liposomes may be conferred a specificity towards a defined cell type, which makes the liposomal delivery of NAADP an intriguing technique to selectively promote post-ischemic neovascularization.

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2C – NMR in microtesla Field

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Biotechnology, Chemistry and Pharmacy, University of Siena)

Aims

Nuclear magnetic resonance signals are typically detected with inductive rf pickup coils, and in conventional NMR setups signals improve approximately quadratically with the magnetic field B, because both the magnetization level and the Larmor frequency increase linearly with B. In spectroscopic NMR applications the stronger the field the better is the resolution of chemical shifts. However, the spectral resolution commonly increases sub-linearly with B, because the generation of stronger fields is accompanied by larger field inhomogeneities, causing greater instrumental broadening. Conversely, in NMR spectroscopy requiring the determination of intrinsic splittings, rather than chemical shift measurements, weaker and more homogeneous fields can be used. In fact, avoiding intense magnetic fields helps to improve the instrumental resolution, although it also rapidly leads to poor signal-to-noise ratio due to the above-mentioned quadratic dependence. This negative trend can be counteracted by using magnetometers instead of inductive pickup coils, as the former make the signal strength proportional to the premagnetization field alone. Additionally, when a remote detection method is applied, a strong premagnetization field (whose homogeneity is unessential) can still be used, along with a low, homogeneous field at the detection stage. Non-inductive detectors open the way to unconventional NMR in conditions where the nuclear precession occurs at arbitrarily low frequencies, in regimes commonly known as ultralow-field (ULF-NMR) [1]. ULF-NMR includes regimes where the nuclear spin coupling becomes the dominant (or the only) term in the Hamiltonian.

Results

The magnetometer has two identical arms for differential measurements. Each arm (see Fig. 1) contains an illuminator providing lights resonant both with the D1 line of the Cs atoms (used to optically pump the atoms) and with the D2 line (used to probe the atomic precession). The two radiations are collimated into beams of 10 mm in diameter oriented along the y direction, and a specifically designed multi-order wave-plate (WP) makes the pump radiation circularly polarized, while leaving the probe one linearly polarized. Each beam crossing the vapour is monitored by a balanced polarimeter. The Cs cells contain 23 torr of N2 as a buffer gas. The Cs density is increased by warming it up to about 45 °C using an alternating current heater supplied at 50 kHz, a frequency

higher than the atomic Larmor frequency. After interacting with the atomic vapor, the pump radiation (about 1 mW of power) is blocked by an interference filter (IF), while the probe beam polarization is analyzed by a balanced polarimeter (BalPol). A trans-impedance amplifier (TIA) converts the photo-current into a voltage signal, which is then digitized by means of a 16 bit data acquisition (DAQ) card. The signal recorded is regarded as the real part of an analytic signal whose imaginary part is inferred by means of a numeric Hilbert transform. The total phase $\theta(t) = \omega_0 t + \varphi$ of that analytic signal (which corresponds to the Larmor precession angle) is analyzed with a linear regression routine. The phase u is weakly dependent upon time $(\dot{\varphi} \ll \omega_0)$ and reproduces the Faraday rotation associated with the local time-dependent magnetic field experienced by the weak and linearly polarized probe beam. The pump radiation is generated by a single-mode pigtailed distributed feedback diode laser, whose optical frequency is controlled via the junction current, and is periodically (synchronously with the Larmor precession) made resonant to the transition of Cs, at 894 nm.

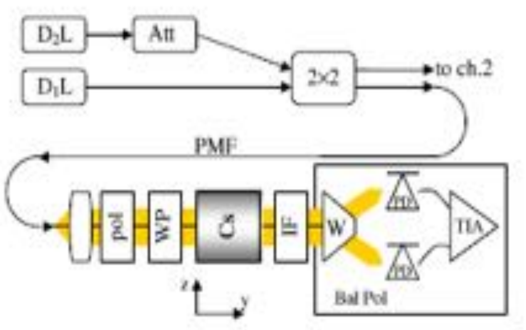

Fig. 1: Schematics of one channel of the magnetometer – D1L pump laser, D2L probe laser. The magnetometer sensor (Cs cell) is illuminated by the two fibres coupled (polarization maintaining fibres PMF) radiations mixed (at a ratio of 50%) in the 2x2 coupler. Before being mixed, the probe laser is attenuated down to lW level, while the pump is left at the mW level. After the Cs cell, the pump radiation is stopped by means of an interferential filter (IF), and a balanced polarimeter (BalPol), made of a Wollaston prism (W) and two photo-diodes (PD), measures the rotation of the probe beam polarization plane. The sample is positioned in the proximity of the sensor as depicted in Fig. 2.

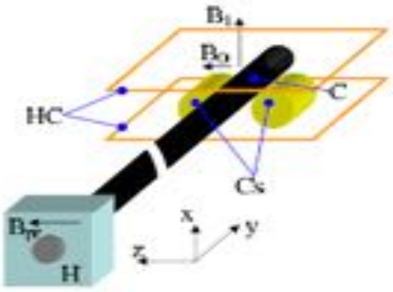

Fig. 2: Sample magnetization, shuttle and positioning. The sample is contained in a polymer cartridge (C), which is inserted in a Halbach array (H) and then pneumatically shuttled into the measurement region, 2 m away. Secondary 50 cm Helmholtz coils (HC) provide transverse B1 pulses for nuclear spin manipulation.

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2C – Physicochemical characterization of ophthalmological vital dyes and their liposomal dispersions

F. Di Nezza, C. Costagliola, G. Bufalo, L. Ambrosone

Aims

The project aims to collect chemical and physical information about vital dyes to design with less risk possible ophthalmology intervention.

Results

Vital dyes are used both in intra-operative and diagnostic ophthalmology as liquid solutions wherein dyes self-associate reducing their effects. Hence, an efficient dyes-delivery system is required to carry the maximum fraction of dye administered to the target site. Indocyanine green, patent blue V and brilliant blue G have been investigated. First, band profiles of UV–Vis absorption and emission spectra, acquired as a function of dye concentration in buffer solutions (pH = 7.4), have been analyzed to calculate the dimerization constant. Results demonstrate that their self-assembly properties have to be correlated to the molecular polarization. Second, the vital dyes have been loaded into liposomes prepared with the thin-film hydration method followed by extrusion. Encapsulation efficiency has been calculated to be 30%. Scanning electron microscopy and dynamic light scattering measurements have revealed that dye inclusion reduces the liposome diameter. Activation energy of liposome diffusion has been extracted by Arrhenius plots. Zeta potential measurements as a temperature function have been exploited to evaluate a dimensionless surface charge and prove that ratio charge(dye-loaded liposome)-to-charge(blank liposome) is always greater than unity and decreases with temperature.

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2C – Physico-Chemical Properties of Pharmaceutical Systems

G. Bruni, V. Berbenni, C. Milanese, A. Girella, A. Marini

Aims

The research activity in the pharmaceutical field concerns the development of methods for the resolution of problems related to the preformulation phase of active principles. The topics of interest are: polymorphism and stability of drugs in the solid state, host-guest systems, drug-excipient compatibility, crystallinity degree and phase diagrams characterization, strategies to improve the solubility and the dissolution rate of drugs. In particular, in the years 2017-2018 the efforts have been directed towards the preparation and the characterization of co-crystals and of electrospun fibers to enhance or to control the drug release and the study of polymorphism.

Results

Solubility represents an important challenge for formulation of drugs, because the therapeutic efficacy of a drug depends on the bioavailability and ultimately on its solubility. Low aqueous solubility is one of the main issues related with formulation design and development of new molecules. Many drug molecules present bioavailability problems due to their poor solubility. For this reason there is a great interest in the development of new systems able to enhance the dissolution of poorly water-soluble drugs.

Gliclazide is an oral hypoglycemic drug used to control diabetes mellitus of type 2 and in particular to prevent the increase of glucose level in blood after food intake in diabetic patients. For this action a rapid gastrointestinal absorption is required but, on the contrary, the absorption rate of gliclazide is slow because of its poor dissolution rate. Furthermore, as it is a weak acid (pKa = 5.8), its solubility is influenced by the pH values of gastric fluid and is subjected to inter-subject and intra-subject variability. Therefore, several methods have been proposed for enhancing the dissolution rate of gliclazide and the high number of research papers concerning this issue demonstrates the great interest felt in the pharmaceutical world for this molecule, and the true need for improving its pharmaceutical behaviour.

Cocrystals of gliclazide with tromethamine were successfully obtained by the methods of solvent evaporation and kneading. The same multicomponent system can be obtained also by dry grinding followed by heating, i.e. by combining the mechanical and thermal activation. The cocrystal formation was confirmed by DSC, FT-IR spectroscopy, X-ray powder diffraction, NMR and SEM-EDS. In particular, FT-IR and NMR measurements revealed that the interaction between drug and coformer takes place by considerably changing the scheme of hydrogen bonds and that almost all the functional groups of the two molecules are involved. The cocrystallization process strongly enhanced the solubility of the active and the dissolution rate of gliclazide compared to the drug alone and to the commercial formulation Diabrezide®. The molecular dispersion of gliclazide in the soluble coformer could promote the dissolution process of the active molecule by a combination of several factors: improved drug wettability and hydrophilicity, water attraction by the hydrophilic compound and prevention of aggregation and agglomeration of hydrophobic particles upon exposure to the dissolution medium.

Febantel is a broad spectrum anthelmintic used against gastrointestinal nematodes and lungworms in livestock. Although febantel is not a new molecule, it is of present great interest in the veterinary field. At present, in literature, the existence of just one polymorph is known and we choose solvent based recrystallization, thermal and mechanical treatments and spray-drying to discover new solid forms. The solids obtained were physico-chemically characterized by thermal techniques (DSC and TG), FT-IR spectroscopy, laboratory and synchrotron X-ray powder diffraction and scanning electron microscopy. Our work led to obtain a new solid form never described in literature. In particular, the new polymorph was obtained by the anti-solvent method and the crystallization from isopropanol. The new phase shows a thermal, spectroscopic and diffractometric behavior unique. Furthermore, the preliminary structure investigation suggests two possible crystal systems: an orthorhombic or a monoclinic one, with really comparable lattice parameters and cell volume. Measurements put into evidence that the new phase is a metastable polymorph that is in monotropic relationship with the stable and known form.

Metronidazole-Norfloxacin is a drug combination used in systemic treatment of infections. Metronidazole (MZ) is an antiprotozoal agent while Norfloxacin (NF) is a synthetic broad antibacterial compound active against a broad spectrum of gram-positive and gram-negative aerobic bacteria. The physico-chemical characterization of Norfloxacin commercial sample (NF), Norfloxacin anhydrous Form A (NFanh), Norfloxacin pentahydrate ($NF.5H_2O$) and MZ has been carried out. It was determined that the commercial sample is a mixture of 74% anhydrous NF and 26% NF.5 H_2O. From XRPD analysis it was observed that after the water loss, NF.5H2O undergoes a solid-solid transition and changes to NFanh. Solid-liquid equilibrium for NFanh-MZ and NF.5 H_2O-MZ binary systems has been investigated using differential scanning calorimetry (DSC) and simple eutectic point was observed, in good approximation, at 419 K for all the mixtures studied. The experimental solid-liquid phase diagram was compared with predictions obtained from available eutectic equilibrium models. The results indicate non-ideality for the mixture.

The mixing enthalpy was determined at the eutectic composition and the negative value obtained indicates that molecules of the two components form clusters in the eutectic melt. This study highlights the fact that binary mixtures NFanh-MZ and $NF.5H_2O$-MZ can be processed or stored at temperatures below the eutectic temperature. In addition, the water content from NF structure does not influence the thermal behavior of NF-MZ-MZ binary mixture.

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2C – Single molecule bio-electronic smart system array for clinical testing H2020-ICT-2018-2
GA: 824946

D. Blasi, E. Macchia, F. De Noto, N. Cioffi, G. Scamarcio, G. Palazzo, L. Torsi

Aims

Digitizing biomarkers analysis by quantifying them at the single-molecule level is the new frontier for advancing the science of precision health. The SiMBiT project will develop a bio-electronic smart system leveraging on an existing lab-based proof-of concept that can perform single-molecule detection of both proteins and DNA bio markers.

Specifically, the SiMBiT activities will develop the lab-based device into a cost effective portable multiplexing array prototype that integrates, with a modular approach, novel materials and standard components/interfaces. The SiMBiT platform exhibits enhanced sensing capabilities: specificity towards both genomic and protein markers along with single-molecule detection limits and time-to-results within two hours. This makes the SiMBiT prototype the world best performing bio-electronic sensing system ever. SiMBiT will reach these ambitious goals with a multidisciplinary research effort involving device-physicists, analytical-chemists, bio-chemists, clinicians, electronic- and system engineers. The platform is also single-use and cost effective and can work in low-resource settings. The SiMBiT field-effect sensing system will be fabricated by means of future mass-manufacturable, large-area compatible, scalable techniques such as printing and other direct-writing processes. 3D printing of a module is also foreseen. The SiMBiT prototype will demonstrate, for first time, a matrix of up to 96 bio-electronic sensors and a Si IC chip for the processing of all data coming from the matrix, multiplexing single-molecule detection. As the Si IC pins are limited the chip area is reduced and its cost minimized, enabling a single-use assay plate. SiMBiT will apply the multiplexing single molecule technology to the early detection of human pancreatic neoplasms in a well defined clinical context, performing simultaneous analysis of genomic and protein markers with a minimal sample volume, reduced costs and reduced time-to-results.

Results

The general objective of the SiMBiT project is to develop a bio-electronic smart system that can perform single-molecule detection of both proteins and DNA bio-markers. Specifically, the SiMBiT activities will develop a lab-based device into a cost-effective portable multiplexing array prototype with extremely fast time-to-results. During the first year, the programme of activities, described in the Annex 1 of the Grant Agreement, has been successfully carried out, meeting what foreseen besides few minor deviations (some foreseen and some not foreseen) that have been successfully tackled. The deliverables and the milestones have been completed and submitted on time. Only in one case a small delay was incurred and justified. Overall the SiMBiT Consortium has successfully reached the end of year one via a systematic cooperative work involving an intensive inter-sectorial research effort from academia and industrial partners, accomplishing all planned steps towards the development of a cost-effective bio-electronic smart system array.

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2C – Solution dynamics of the natural bioactive molecule capsaicin: a relaxation study

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M. Consumi, A. Magnani, C. Rossi (Department of
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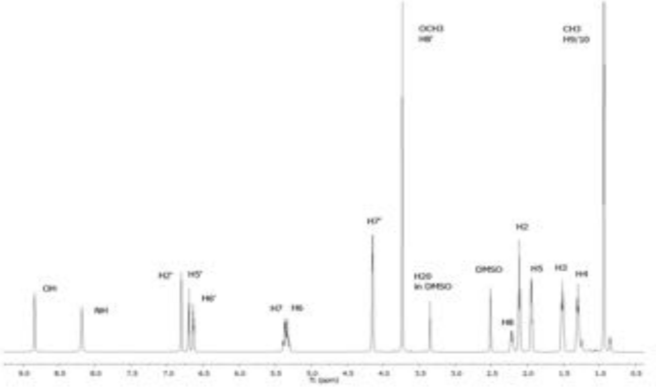
Aims

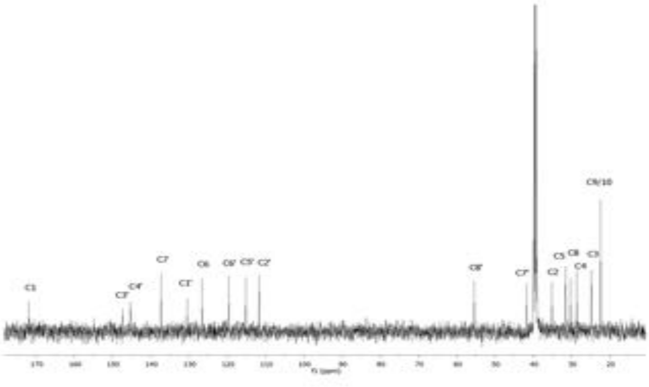
Nuclear magnetic resonance spectroscopy is a straightforward technique for studying molecular dynamics that range in timescale from picosecond (motions faster than molecular reorientation) to those that occur in real-time. This approach is important to highlight the behavior of bioactive molecules in solution, and to acquire information about action mechanisms and potential pharmacological effects. Proton and carbon-13 spin-lattice relaxation experiments were performed to calculate the reorientational correlation time for protonated carbons. Capsaicin showed complex dynamical properties and the results revealed two regions with different dynamical properties: aliphatic region with fast reorientation motions and the aromatic region with slow motions.

Results

The complete assignments of ^{1}H-proton and ^{13}C-carbon NMR spectra of capsaicin in DMSO-d_6 have been carried out, and are reported in (a).The study of the dynamic properties of capsaicin in solution was carried out using both proton and carbon-13 spin-lattice relaxation measurements. The strategy used was to study first, the proton spin-lattice relaxation rates, measured in a selective and nonselective mode, in order to obtain a preliminary evaluation of the rotational correlation times τ_c values. This analysis allowed to identify the regions of motion for capsaicin (fast motions $\omega_0\tau_c$«1 or slow motions $\omega_0\tau_c$»1), and to calculate the rotational correlation times along the aliphatic region of the molecule.

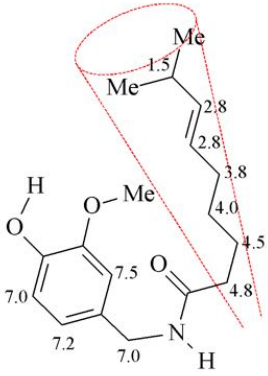
The calculation of the rotational correlation time values, for each protonated carbon along whole capsaicin molecule, was then possible by the analysis of the dipolar contribution to the spin-lattice carbon-13 relaxation rates.





(a)

The present study wishes to elucidate the dynamic behavior of capsaicin in solution. The most interesting result revealed that the capsaicin is characterized by complex dynamical properties. The molecule does not have an isotropic molecular motion, being the aromatic region subject to a restricted dynamics, within the limits of the intermediate motions ($\omega_0\tau_c$~1). The aliphatic region appears subject to free reorientation dynamics, with a dynamical gradient as indicated by (b). The slower motion of the aromatic region is probably due to its intrinsic steric hindrance and not correlated to any specific intermolecular interaction.



(b)

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2C – Streptomyces cyaneofuscatus strain: production of a novel tyrosinase and characterization of melanin obtained in the liquid and solid media

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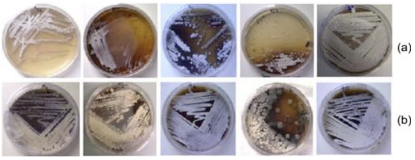
M.C. Baratto, R. Basosi, R. Pogni

Aims

Different actinomycete strains were collected and isolated from Algerian Sahara soil with the aim to select novel enzymes interesting for biotechnological applications. Ms1 strain was selected for its capability to produce melanin in different media. A tyrosinase was isolated and biochemically characterized. Synthetic melanin was enzymatically produced using *S. cyaneofuscatus* tyrosinase, from the oxidation of 3,4-dihydroxyphenylalanine (dopa) using *Trametes versicolor* laccase. The natural and synthetic pigments were characterised by UV-Vis, FT-IR, multifrequency EPR.

Results

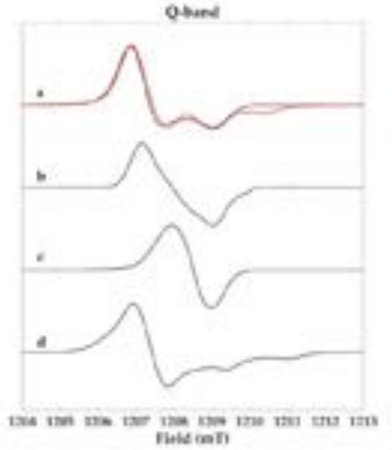
Eight actinomycete strains from Algerian Sahara soil were tested and screened for their ability to produce melanin. The strains were also investigated for extracellular tyrosinase production and the MS1 strain was selected for the highest yield of tyrosinase production.



Melanin production by tyrosinase in agar (a) and MPPM (b) (Ms1, O5, H1, M51 and 10 strains from the left

The MS1 tyrosinase showed the highest aminoacid identity with the corresponding enzyme of S. cyaneofuscatus strain (NRRL B-2570, 99.6%). The SDS-page analysis of the partially purified enzyme revealed the presence of a major protein band with a MW 30kDa. The kinetic parameters for the oxidation of L-dopa in phosphate buffer at pH=7 were determined. The tyrosinase was able to oxidise L-dopa across a range of temperature from 50°C to 70°C, with an optional temperature of 55°C. The oxidation of L-dopa was performed with high enzyme activity at neutral and basic pH with the optimal pH around 6.5-7.5. The enzyme was able to oxidase caffeic acid, p-cresol, pyrogallol while ABTS, resorcinol, guaiacol were not oxidise. The enzyme was also able to oxidise L-dopa in the presence of methanol, acetone, ethanol. Total inactivation of activity occurred in presence of L-cysteine, sodium metabisulphite, L-ascorbic acid and a limited inactivation was present with EDTA. Tyrosinase activity was enhanced in general by all the cations tested (Co(II), Cu(II), Mg(II), Mn(II), Zn(II), Ca(II), Fe(II)), apart for Ca(II) and Fe(II). The tyrosinase resulted more stable than the fungal one, retaining more than 50% of activity after incubation time up to 6 days. Finally, the enzyme was immobilised on electronspun nylon nanofiber membranes and efficiency of immobilisation, storage stability, reusability were tested.

Natural and melanin-like pigments are characterised by a persistent EPR signal due to the presence of stable free radicals. A multifrequency EPR approach is used to describe the complex pattern of MS1 natural melanin based on the synthetic dopa and cysteinyldopa melanins. Q-band spectra of MS1 natural melanin showed a signal composed of more than one radical species. The simulated spectrum has been performed taking into account a mixture of the different melanins.



Q-band (33.9 GHz) EPR spectra of (**a**) Sc-Ms1 natural melanin, (**b**) Sc-Ms1 tyrosinase dopa-melanin, (**c**) Tv laccase dopa-melanin, and (**d**) Tv laccase cysteinyldopa melanin samples. Spectra were recorded with 0.06 mW microwave power.

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2C – Structural study for the new binuclear cis-[RuI(CO)2(N3-MBI)(μ2-O,O-BAL)]2 sawhorse complex

G. Tamasi, C. Bonechi, A. Donati, G. Leone, M. Consumi, A. Magnani, R. Cini, C. Rossi (Department of Biotechnology, Chemistry and Pharmacy, University of Siena)

Aims

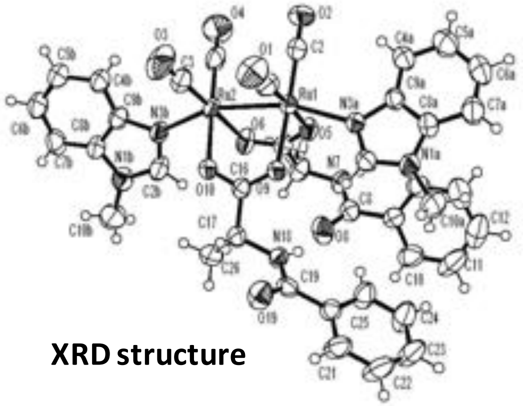
Investigating CO-Releasing Materials (CORMs) connected to their biological properties and therapeutic effects is nowadays a hot topic for the coordination/organometallic chemistry of ruthenium and other heavy metals. The reaction of *fac*-[Ru^{II}(CO)$_3$Cl$_2$($\underline{N^3}$-MBI)], (MBI=N^1-methylbenzimidazole) with HBAL (HBAL, *N*-benzoyl-DL-alanine) brought about *cis*-[Ru^{I}(CO)$_2$($\underline{N^3}$-MBI)(η^2-$\underline{O}$,$\underline{O}$-BAL)]$_2$, **2**. The new binuclear organometallic compound was structurally characterized at solid state (via X-ray diffraction and FT-IR) and in solution (via ^{1}H-NMR and UV-Vis). Simulation of the molecular structure was carried out at DFT-B3LYP/(Ru, Lanl2DZ; CHNOCl, 6-31G**) level at the gas phase, and structural parameters were compared to experimental (XRD) parameters. The absence of any other anionic/cationic molecule either as ligand or co-crystallized species, in addition to the two bridging carboxylato molecules per each dimer molecule was in agreement with the (+1) oxidation state for the two ruthenium centers.

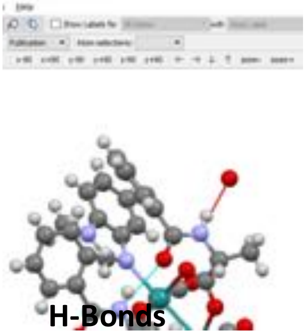
Results

The coordination sphere for each metal atom is *pseudo*-octahedral, Ru atoms being linked to two carbonyl ligands and to two bridging carboxylato groupings from BAL. These sites are considered as equatorial ones. Further coordination linkages for each Ru center are to the other ruthenium atom and to a N^3 nitrogen atom from MBI. Therefore, the metal is in the Ru^{I} oxidation status and the complex is neutral. No any other charged ligand nor cocrystallized charged or neutral particle was present in the cell. The Ru-Ru bond distance is 2.6984(4) Å. Comparing the value with data previously reported in literature for Ru-dimers it can be stated that a linking interaction between the two metal atoms is present (sum of the atomic radii is 4.26 Å, and sum of the covalent radii is 2.72 Å). The Ru^{I}-Ru^{I} interaction or d^7-d^7 one can be described as $\sigma^2+\pi^4+\delta^2+\delta^{*2}+\pi^{*4}$: in other words it is a metal-to-metal single bond.

In the case of the Ru1 center coordination environment, the MBI(A) plane is eclipsed with respect to one of CO ligand and one of the O(carboxylato) donor. The eclipsed conformation (C2A-N3A-Ru1-O9, -5.8(1)°) favors the formation of two intra-molecular H-bond type interactions: C2-H…O(carboxylato) ((C)H…O, 2.31(2) Å, Ĥ, 117(1)°) and C4-H…O(CO) ((C)H…O, 2.73(2) Å, Ĥ, 159(1)°). The staggered MBI(B) (C2B-N3B-Ru2-O10, 46.0(5)°) also gives H-bond type interactions: two (C2)H…O(carboxylato), and two (C4)H…O(CO). Regarding to the N-H…O(=C) (BAL) H-bond interactions, both intra-molecular and intermolecular are present. The one that involve two BAL ligands inside the same complex molecule has N…O contact distance and Ĥ angle by 2.98(1) Å and

157(1)°, whereas the inter-molecular one that has N…O contact distance and Ĥ angle by 2.91(1) Å and 169(1)° seems to be even stronger than the intra-molecular one.
X-Ray Diffraction data revealed a great agreement with DFT computed values, as well as spectroscopic characterization.





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2C – Synthesis and characterization of nanomaterials for biomedical applications and drug delivery

M. Bini, D. Capsoni, I. Quinzeni

Aims

Synthesis and characterization of pure and doped Zinc ferrites nanocrystals, to optimize the magnetic properties for magnetic hyperthermia application.

Synthesis and characterization of Layered Double Hydroxides (LDHs), as hosts for drugs. The obtained nanohybrids promote drug release at a predetermined time, with low undesired fluctuation of drug concentration in blood, less frequent drug administration and enhanced therapeutic response.

Results

$ZnFe_2O_4$ – Ca- and Gd-doped Zinc ferrite spinels have been synthesized by microwave assisted combustion method. The obtained samples display homogeneous nanosized particles and optimum purity levels. The structural investigation and the magnetization measurements put into evidence an enhanced superparamagnetic behavior for the Ca-doped samples, related to the complete solubility of Ca in the spinel cationic framework and to the inversion degree of the spinel, precisely determined by the Rietveld refinement of X-Ray powder diffraction data and by Raman measurements. The observed increase of saturation magnetization at room temperature is mandatory in magnetic hyperthermia applications.

LDH-Drugs hybrid compounds – The Layered Double Hydroxides (or hydrotalcites) are inorganic compounds derived from brucite. They display a positively charged two-dimensional nano-sheets structure. The counterions, located in the interlayer regions, can be exchanged with several inorganic, organic and metallo-organic molecules and, interestingly, with drugs. Moreover, the natural basic behavior of hydrotalcite makes it suitable as antiacid. Our studies points at improving the solubility in water and dissolution rate of poorly soluble drugs, such as Carprofen and Nimesulide. The Carprofen intercalation into the Zn/Al LDH was obtained by co-precipitation method. The nimesulide-Mg_3Al-LDH hybrids were successfully synthesized by both co-precipitation and reconstruction routes. In both cases, the successful insertion of the drug into the host structure is confirmed by XRD patterns displaying an increase of the interplanar distances in LDH, by FTIR spectra, and by DSC results. The LDH-drug nanohybrids display an improved drug solubility in water. The in-vitro dissolution tests demonstrate that the drug dissolved from the hybrids is much higher and much faster, compared to the drug alone and to the commercial reference.

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2C – Trodusquemine modulates the resistance of lipid membrane to the toxicity of misfolded protein oligomers

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M. Vendruscolo (Centre for Misfolding Diseases, Department of Chemistry, University of Cambridge, Cambridge, UK);
F. Chiti (Department of Experimental and Clinical Biomedical Sciences, University of Florence)

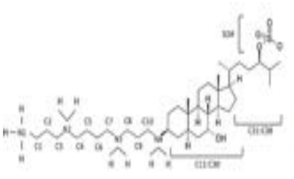
Aims

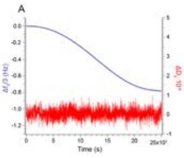
Neurodegenerative disorders include a wide range of different pathologies characterized by progressive and irreversible neuronal loss, such as Alzheimer's disease (AD) Parkinson's disease (PD). Most of these diseases originate from the conversion of peptides or proteins from their native soluble states into fibrillar aggregates, forming amyloid plaques, neurofibrillary tangles, Lewy bodies, and intracellular inclusions.

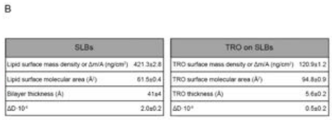
Recently, aminosterols such as squalamine and trodusquemine were found to prevent the binding of misfolded protein oligomers to cell membranes and reduce their toxicity but at present the precise mechanism of action remains unclear.

Results

The mechanism of interaction of Trodusquemine with biological membranes is studied investigating in model systems such as Large Unilamellar Vesicles (LUV) and Supported Lipid Bilayer composed of DOPC, PSM, Chol and GM1 containing raft domains. Modification of the structure and properties of the bilayer in the presence of Trodusquemine was studied combining Quartz Crystal Microbalance (QCM), fluorescence quenching and anisotropy with molecular dynamics (MD) simulations. We found that trodusquemine localises within, and partially penetrates, the polar region of the lipid bilayer. This binding behaviour causes a decrease of the negative charge of the lipid bilayer, as observed through ζ potential measurements, an increment in the mechanical resistance of the bilayer, as revealed by measurements of the breakthrough force applied with AFM and ζ potential measurements at high temperature, and a rearrangement of the spatial distances between ganglioside and cholesterol molecules in the LUVs, as determined by FRET measurements.



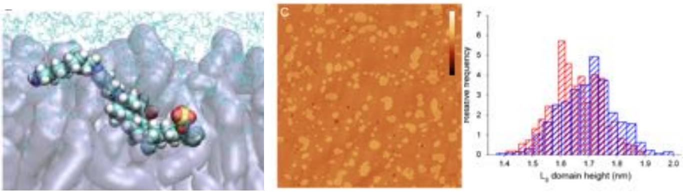



B

SLBs	
Lipid surface mass density or $\Delta m/A$ (ng/cm²)	421.3±2.8
Lipid surface molecular area (Å²)	61.5±0.4
Bilayer thickness (Å)	41±4
$\Delta D \cdot 10^{-6}$	2.0±0.2

TRO on SLBs	
TRO surface mass density or $\Delta m/A$ (ng/cm²)	120.9±1.2
TRO surface molecular area (Å²)	94.8±0.9
TRO thickness (Å)	5.6±0.2
$\Delta D \cdot 10^{-6}$	0.5±0.2

Confocal microscopy, fluorescence resonance energy transfer (FRET) and nuclear magnetic resonance (NMR) measurements also supported a strong binding of trodusquemine to large unilamellar vesicles (LUVs) and neuroblastoma cells.



These physicochemical changes are all known to impair the interaction of misfolded oligomers with lipid membranes, protecting them from their toxicity. Taken together, our results illustrate how the incorporation in cell membranes of sterol molecules modified by the addition of polyamine tails leads to the modulation of fundamental properties of the cell membranes themselves, making them resistant to protein aggregates associated with neurodegeneration.

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2C – Unconventional and sustainable nanovectors for phytohormone delivery: insights on Olea europaea

F. Menicucci, I. Clemente, C. Gonnelli, C. Giordano, C. Benelli, R. Petruccelli, S. Ristori, (University of Florence, Italy, Trees and Timbers Institute, CNR, Italy)

Aims

This research project focuses on the sustainable re-use of olive pomace employed as lipid source for the development of low-cost green-nanodevices delivering a root-promoting phytohormone (i.e. the IBA auxin). The olive-derived nanovectors were fully characterized by physicochemical techniques, such as dynamic light scattering, zeta potential and small angle scattering (SAXS, SANS) and then tested on olive cuttings. The nanovector administration was investigated both *in vitro* and *in vivo* and results showed an improvement in the rooting process due to the successful auxin delivery to the root.

Results

Olive pomace was used to obtain a starting material from which nanovectors were formulated by lipid extraction, rehydration and repeated cycles of sonication. Both entirely pomace-derived nanoformulation and pomace plus adjuvant lipid (i.e. DOPE or DOPC) were fabricated. DLS data showed that aggregates with mean size in the range 150-300 nm were formed. The polydispersity index (PDI) was in the range 0.2-0.4, indicating scattering objects with wide but controlled size distribution. These data were complemented by Zeta potential measurements, showing that all samples had negative Zeta potential (≈-23÷ ≈-13 mV). The structural properties of plain and auxin loaded nanovectors at high resolution were studied by Small Angle X-ray and Neutron Scattering (SAXS and SANS). The scattering intensity of samples made from pomace only showed unstructured profiles, confirming that very polydisperse aggregates were obtained from pure natural lipids. However, the addition of either DOPE or DOPC in small amount (10% w/w), significantly modified the SAS profiles. In the case of DOPC addition the intensity diagrams were dominated by the large oscillations pattern of monolamellar vesicles and by the typical signature of lipid bilayers. In addition, small Bragg peaks indicated that a fraction (around 12%) of bilamellar aggregates was present. When DOPE was added (10% w/w) to the pomace-derived lipids the SAS intensity diagrams showed that hexagonal arrays formed together with a smaller fraction of globular, uncorrelated aggregates. These structural features depended on the lipid composition and were substantially unaltered after auxin loading, though high incorporation rates (≈ 1 guest molecule each 3-5 lipids) could be easily obtained. The efficacy of auxin-loaded nanosystems was tested on olive trees and the results showed that the rooting process was improved both in vitro and in vivo. (Fig. 1 and 2, respectively). In all experiments the comparison was made with respect to the standard treatment, which consists in a quick immersion of the cuttings into highly concentrated hydro-alcoholic auxin solutions.

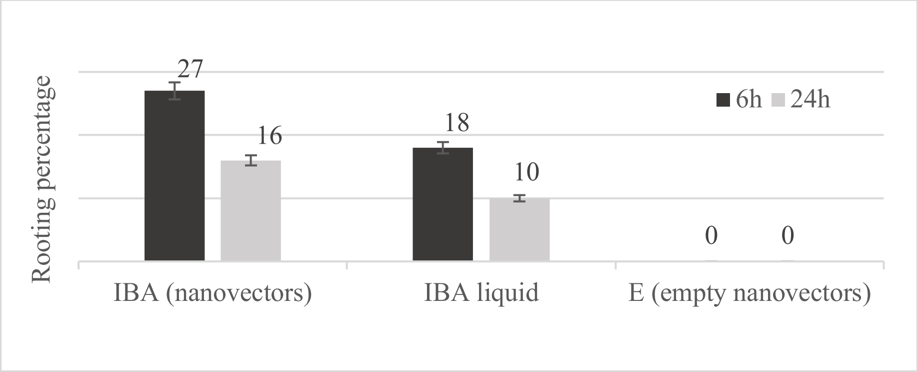

Fig. 1. Rooting percentage after treatment of 'Canino' microcuttingS

Fig. 2. Rooting after treatment of 'Leccino' cuttings with conventional treatment (a) and with IBA loaded lipid vectors(b)

Due to the alcohol added for phytohormone solubilization, the conventional procedure is not completely harmless for the plants. On the contrary, the use of lipid vectors allows a slow and sustained auxin delivery.

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