Curriculum vitae
Giuseppe Brancato

EDUCATION

. 2011-Present, Assistant Professor, Classe di Scienze, Scuola Normale Superiore, Pisa, Italy
. 2009-2011, Senior Postdoc at the Italian Institute of Technology, NEST Laboratory, Pisa, Italy
. 2004-2009, Postdoc at the University of Neaples "Federico II" in the group of prof. Vincenzo Barone
. 2002-2003, Postdoc at the New York University, New York - NY, USA, in the group of Prof. Mark E. Tuckerman
. 1999-2003, PhD in Chemistry at the University of Rome "La Sapienza", Italy.
Supervisors: Prof. Di Nola and Dr. Amadei
. 1994-1999, Undergraduate degree in Chemistry at the University of Bologna, Italy.
Supervisor: Prof. F. Zerbetto

MEMBERSHIPS

. 2016, Associated to the Italian Biophysical Society
. 2016, Associated to GSGI consortium
. 2008-Present, Associated to the Interuniversity Consortium on Materials Science and Technology (INSTM)
. 2012-Present, Associated to the National Institute of Nuclear Physics (INFN)
. 2012-2013, Member of the board of directors of CASPUR computing center (Rome, Italy)

PROJECTS

. 2016-2018, SNS Internal project. Funding agency: SNS. Research Role: PI. Project title: “Self-Propelled Molecular Machines in Solution and Lipid Bilayers: A Combined Theoretical and Experimental Investigation”.
. 2016-2018, FAS SALUTE 2014. Funding agency: Regione Toscana. Research Role: PI of a network node including 5 national research groups. Project title: “DIAMANTE: Diagnostica molecolare innovativa per la scelta terapeutica personalizzata dell'adenocarcinoma duttale pancreatico”.
. 2014-2017, PRIN Funding agency: MIUR. Research Role: PI of a network node including 3 national research groups. Project title: “Innovative Chemical Tools For Improved Molecular Approaches in Biomedicine”.
. 2014-2016, SNS Internal project. Funding agency: SNS. Research Role: PI. Project title: “Lights on Membrane: A Theoretical and Spectroscopic Investigation of Lipid Diffusion and Self-Organization”.
. 2016-2018, INFN Biophys project. Funding agency: INFN. Research Role: PI of a network node including 10 national research groups.
. 2012-2015, FIRB2010 program. Funding agency: MIUR. Research Role: PI of a network node including 4 national research groups. Project title: “Supramolecularly Templated Synthesis of Homochiral Carbon Nanotubes for Photovoltaic Applications”.
. 2006-2007, PRIN program. Funding agency: MIUR. Role: Member of PI Unit. Project title: "Study of the influence of molecular architecture on the structure, reactivity and physico-chemical properties of POSS by an integrated computational approach".

RESEARCH INTERESTS AND ACTIVITY

. Scientific interests: Theoretical development of molecular dynamics methodologies; Computational study of optical and magnetic properties of molecular probes; Computational study of biological channels and lipid membranes; Modeling of molecular machines and rotors.
. 51 papers on peer-reviewed journals (23 as corresponding author).
. Co-organizer of 1 national and 3 international CECAM conferences
. >20 invited lectures in national and international conferences
. Peer-reviewer of JACS, JPC Letters, Comput. Phys. Comm.
. Reviewer for University of Turin, MIUR National projects, Member of PRACE Prioritisation Panel

TEACHING

. Professore aggregato since academic year 2013/2014.
. Co-lecturer of the course “*Fundaments of Quantum Mechanics and Statistical Mechanics*” (Academic Year 2011/2012, 2012/2013)

. Co-lecturer of the course "*Molecular Modeling of Bio and Nano Systems*" (Academic Year 2011/2012, 2012/2013)
. Lecturer of the course "*Frontiers in Chemistry*" (Academic Year 2013/2014)
. Lecturer of the course "*Methods and Models for Molecular Sciences*" (Academic Year 2014/2015, 2015/2016)
. Co-lecturer of the course "*Astrobiology*" (Academic Year 2013/14, 2014/15, 2015/16, 2016/17)
. Lecturer of the course "*Computational Life and Material Sciences*" (Academic Year 2016/2017)

OTHER SNS INSTITUTIONAL ACTIVITIES

. 2012-Present, Research Fellow Representative at Consiglio di Classe di Scienze, Scuola Normale Superiore.
. 2015-2017, Member of Comitato Unico di Garanzia (CUG) at the Scuola Normale Superiore.
. 2016, Member of the Research Commission for the attribution of the research fellowships.
. 2016, Member of the Electoral Commission for the election of the Director of the Scuola Normale Superiore.

SELECTED PUBLICATIONS

Brancato G.(*); Di Nola A.; Barone V.; Amadei A., *A mean field approach for molecular simulations of fluid systems*, J. Chem. Phys., **122**, 154109 (2005).

Brancato G.; Tuckerman M.E., *A polarizable multistate empirical valence bond model for proton transport in aqueous solution,* J. Chem. Phys., **122**, 224507 (2005).

Brancato G.; Rega N.; Barone V., *Unraveling the Role of Stereo-electronic, Dynamical, and Environmental Effects in Tuning the Structure and Magnetic Properties of Glycine Radical in Aqueous Solution at Different pH Values*, J. Am. Chem. Soc., **129**, 15380 (2007).

Brancato G.(*); Rega N.; Barone V., *Accurate Density Functional Calculations of Near-Edge X-Ray and Optical Absorption Spectra of Liquid Water Using Nonperiodic Boundary Conditions: The Role of Self-Interaction and Long-Range Effects*, Phys. Rev. Lett. **100**, 107401 (2008).

Brancato G.; Rega N.; Barone V., *A hybrid explicit/implicit solvation method for first-principle molecular dynamics simulations*, J. Chem. Phys. **128**, 144501 (2008).

Brancato G.(*); Rega N.; Barone V., *Molecular dynamics simulations in a NpT ensemble using non-periodic boundary conditions*, Chem. Phys. Lett., **483**, 177-181 (2009).

Brancato G.(*); Rega N.; Barone V., *Uracil anion radical in aqueous solution: thermodynamics versus spectroscopy*, Phys. Chem. Chem. Phys. **12**, 10736-10739 (2010).

Brancato G.(*); Barone V., *Free Energy Landscapes of Ion Coordination in Aqueous Solution*, J. Phys. Chem. B 115, 12875-12878 (2011).

Brancato G.(*); Rega N., *Computational spectroscopy by classical time-dependent approaches*, Chapter in *COMPUTATIONAL STRATEGIES FOR SPECTROSCOPY: From Small Molecules To Nano Systems*, pp. 517-547, editor V. Barone, Wiley and Sons, New York (2011).

Koenig M.; Bottari G.; **Brancato G.(*)**; Barone V.; Guldi D. M.; Torres T., *Unraveling the peculiar modus operandi of a new class of solvatochromic fluorescent molecular rotors by spectroscopic and quantum mechanical methods*, Chem. Sci. **4**, 2502 (2013).

Zazza C.; Mancini G.; **Brancato G**; Barone V., *In silico study of molecular engineered nanodevices: a lockable light-driven motor in dichloromethane solution*, J. Phys. Chem. Lett., **1**, 3885 (2013).

Mancini G.; **Brancato G.**; Barone V., *Combining the Fluctuating Charge Method, Non-Periodic Boundary Conditions and Meta-Dynamics: Aqua Ions as Case Studies*, J. Chem. Theory Comput. **10**, 1150–63 (2014).

Koenig M., Torres T., Barone V., **Brancato G.(*)**, Guldi D. M. and Bottari G., *Ultrasound-Induced Transformation of Fluorescent Organic Nanoparticles from a Molecular Rotor into Rhomboidal Nanocrystals with Enhanced Emission*, Chem. Comm. **50**, 12955–58 (2014).

Brancato G.(*); Signore G.; Neyroz P.; Polli D.; Cerullo G.; Abbandonato G.; Nucara L.; Barone V.; Beltram F.; Bizzarri R., *Dual Fluorescence through Kasha's Rule Breaking: An Unconventional Photomechanism for Intracellular Probe Design*, J. Phys. Chem. B, **119**, 6144-54 (2015).

Chandramouli B.; Di Maio D.; Mancini G.; Barone V. and **Brancato G.(*)**, *Breaking the Hydrophobicity of the MscL Pore: Insights into a Charge-Induced Gating Mechanism*, PLoS One **10**, e0120196 (2015).

Chandramouli B., Zazza C., Mancini G. and **Brancato G.(*)**, *Boundary Condition Effects on the Dynamic and Electric Properties of Hydration Layers*, J. Phys. Chem. A **119**, 5465–75 (2015).

Di Maio D.; Chandramouli B. and **Brancato, G.(*)**, *Pathways and Barriers for Ion Translocation through the 5-HT3A Receptor Channel*, PLoS One **10**, e0140258 (2015).

Chandramouli, B.; Di Maio D.; Mancini G.; and **Brancato, G.(*)**, *Introducing an artificial photoswitch into a biological pore: A model study of an engineered α-Hemolysin*, Biochim. Biophys. Acta Biomembr. **1858**, 689-697 (2016).

Koenig M.; Storti B.; Bizzarri R.; Guldi D. M.; **Brancato G.(*)** and Bottari G., *A Fluorescent Molecular Rotor Showing Vapochromism, Aggregation-Induced Emission, and Environmental Sensing in Living Cells*, J. Mat. Chem. C **4**, 3018-3027 (2016).