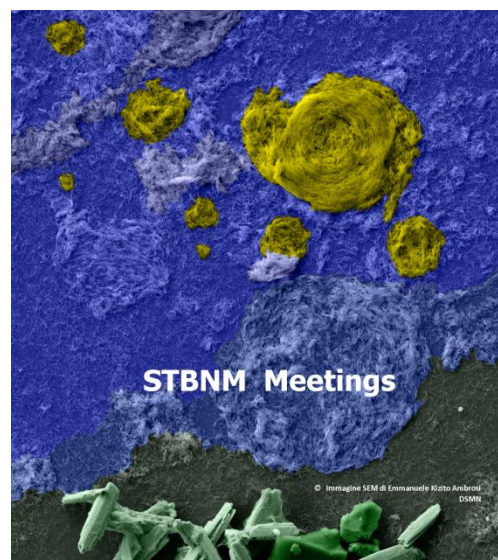




Università
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**Department
of Molecular Science
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**PhD Programme
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of Bio and Nanomaterials**



Nano-Bio Workshop
December 11th, 2020

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BOOK OF ABSTRACTS

Multifunctional materials for emerging technologies

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Abstract

This presentation focuses on structure property/relationships in advanced materials, emphasizing multifunctional systems that exhibit multiple functionalities. Such systems are then used as building blocks for the fabrication of various emerging technologies. In particular, nanostructured materials synthesized via the bottom–up approach present an opportunity for future generation low cost manufacturing of devices [1]. We focus in particular on recent developments in solar technologies that aim to address the energy challenge, including third generation photovoltaics, solar hydrogen production, luminescent solar concentrators and other optoelectronic devices. [2-37].

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Biographical details

Federico Rosei received MSc (1996) and PhD (2001) degrees from the University of Rome “La Sapienza”. He held the Canada Research Chair (Junior) in Nanostructured Organic and Inorganic Materials (2003–2013) and since May 2016 he holds the Canada Research Chair (Senior) in Nanostructured Materials. He is Professor at the Centre Énergie, Matériaux et Télécommunications,

Institut National de la Recherche Scientifique, Varennes (QC) Canada, where he served as Director from July 2011 to March 2019. Since January 2014 he holds the UNESCO Chair in Materials and Technologies for Energy Conversion, Saving and Storage.

Dr. Rosei's research interests focus on the properties of nanostructured materials, and on how to control their size, shape, composition, stability and positioning when grown on suitable substrates. He has extensive experience in fabricating, processing and characterizing inorganic, organic and biocompatible nanomaterials. His research has been supported by multiple funding sources from the Province of Quebec, the Federal Government of Canada as well as international agencies, for a total in excess of M\$ 17. He has worked in partnership with over twenty Canadian R&D companies. He is co-inventor of three patents and has published over 365 articles in prestigious international journals (including *Science*, *Nature Photonics*, *Proc. Nat. Acad. Sci.*, *Adv. Mater.*, *Angew. Chem.*, *J. Am. Chem. Soc.*, *Adv. Func. Mater.*, *Adv. En. Mat.*, *Nanolett.*, *ACS Nano*, *Biomaterials*, *Small*, *Phys. Rev. Lett.*, *Nanoscale*, *Chem. Comm.*, *Appl. Phys. Lett.*, *Phys. Rev. B*, etc.), has been invited to speak at over 330 international conferences and has given over 240 seminars and colloquia, over 60 professional development lectures and 40 public lectures in 48 countries on all inhabited continents. His publications have been cited over 15,300 times and his H index is 64.

He is Fellow of numerous prestigious national and international societies and academies, including: the Royal Society of Canada, the European Academy of Science, the African Academy of Sciences, the World Academy of Art and Science, the World Academy of Ceramics, the Academia Europaea, the American Physical Society, AAAS, the Optical Society of America, SPIE, the Canadian Academy of Engineering, ASM International, the Royal Society of Chemistry (UK), the Institute of Physics, the Institution of Engineering and Technology, the Institute of Materials, Metallurgy and Mining, the Engineering Institute of Canada, the Australian Institute of Physics, Honorary Fellow of the Chinese Chemical Society, Foreign Member of the Mexican Academy of Engineering, Foreign Member of the Bangladesh Academy of Sciences, Senior Member of IEEE, Alumnus of the Global Young Academy and Member of the Sigma Xi Society.

He has received several awards and honours, including the FQRNT Strategic Professorship (2002–2007), the Tan Chin Tuan visiting Fellowship (NTU 2008), the Senior Gledden Visiting Fellowship (UWA 2009), Professor at Large at UWA (2010–2012), a Marie Curie Post-Doctoral Fellowship from the European Union (2001), a junior Canada Research Chair (2003–2013), a senior Canada Research Chair (2016–2023) a Friedrich Wilhelm Bessel Award (von Humboldt foundation 2011), the Rutherford Memorial Medal in Chemistry (Royal Society of Canada 2011), the Herzberg Medal (Canadian Association of Physics 2013), the Brian Ives lectureship award (ASM international 2013), the Award for

Excellence in Materials Chemistry (Canadian Society for Chemistry 2014), the NSERC EWR Steacie Memorial Fellowship (2014), the José Vasconcelos Award for Education (World Cultural Council 2014), the IEEE NTC Distinguished Lectureship 2015–2016, the Lash Miller Award (Electrochemical Society 2015), the Chang Jiang Scholar Award (China), the Khwarizmi International Award (Iran), the Recognition for Excellence in Mentorship (American Vacuum Society 2015), the Selby Fellowship (Australian Academy of Sciences 2016), the John C. Polanyi Award (Canadian Society for Chemistry 2016), the Outstanding Engineer Award (IEEE Canada 2017), the President's Visiting Fellowship for Distinguished Scientists (Chinese Academy of Sciences 2017), the Sigma Xi Distinguished Lectureship (2018–2020), the Sichuan 1000 talent (short term) award, the Lee Hsun Lecture Award (2018), the Changbai Mountain Friendship Award (2018), the IEEE Montreal Gold Medal (2018), the APS John Wheatley Award (2019), the Blaise Pascal Medal (European Academy of Science 2019), the IEEE Photonics Society Distinguished Lectureship (2020–2021) and the TMS Brimacombe Medal (2021).

Raman spectroscopy in virology: decrypting the hidden language of the Raman light

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Abstract

The Raman spectrum of living cells and microorganisms contains highly specific fingerprint-like signatures, which can be used to unequivocally identify them and to interpret their physiological and metabolic responses to environmental stress conditions. Viruses are not exceptions to this approach. In situ Raman imaging with dedicated instruments of high sensitivity can translate selected spectroscopic fingerprints into vivid snapshots of molecular species or specific biological reactions. Raman imaging is compatible with life and allows time-lapse experiments, a crucial condition in characterizing growth-dependent phenomena and metabolic responses to different drugs or substrates. This presentation will illustrate examples of Raman analyses of viruses in their infectious and inactivated states, as well as following up their inoculation into cells. Tasks covered here include: (i) identification of different species of viruses through vibrational fingerprints of their Raman spectra; (ii) spectroscopic characteristics of virion inactivation; and, (iii) time-lapse analyses of cells metabolic reactions upon viral inoculation. The shown spectroscopic findings demonstrate the invaluable contribution of Raman spectroscopy in virology and, more generally, in biophysics research.

Giuseppe Pezzotti is Vice President of the Kyoto Institute of Technology Director of the International Center since the year 2017, and a full tenured professor and leader of the Ceramic Physics Laboratory since the year 2000. He graduated summa cum laude in mechanical engineering from Rome University “La Sapienza”, Italy, in 1984 and holds four doctoral degrees in Engineering (Materials Science; Osaka

University), Science (Quantum Chemistry; Kyoto University), Medical Science (Orthopedics; Tokyo Medical University), and Medical Science (Immunology; Kyoto Prefectural University of Medicine), all obtained in Japan, the country where he has been living for the past 34 years. Fluent in Japanese, and capable to read and write it at a nearly native level, he was one of the first foreign nationals to obtain a tenured full professor position in a Japanese Government University and is now the first and only western-born Vice President in a National Japanese University. From 2002 to 2012, Professor Pezzotti served as the director of the Research Institute for Nanoscience at the Kyoto Institute of Technology. From 2005 to 2015, he has been an adjunct professor at the Department of Orthopaedic Research of Loma Linda University, Loma Linda, California. Since 2009, he obtained an Invited Professorship from the Department of Medical Engineering of Osaka University, from 2010 to 2017 he has been a Visiting Professor at the Department of Molecular Cell Physiology of Kyoto Prefectural University of Medicine, since 2016 he is a Guest Professor at the Department of Orthopedics of the Tokyo Medical University, since 2018 he serves as an Adjunct Professor at the Department of Immunology of the Kyoto Prefectural University of Medicine, and from 2020 he is a Honorary Fellow of the Ca' Foscari university of Venice. Professor Pezzotti has published about 680 scientific papers, 1 book as a single author, 15 book chapters, and holds 12 patents, including a world patent regarding nanoscale stress microscopy in the scanning electron microscope. He has licensed his intellectual properties to more than 20 major industrial firms around the world and served as their consultant. His book entitled "Advanced Materials for Joint Implants" (published in 2013) has quickly become a landmark for scientists and medical doctors working in the field of joint arthroplasty. In 2013, Professor Pezzotti became a Fellow of the Academy of Science (Bologna Institute) in appreciation of his advanced studies of Raman spectroscopy, linking quantum mechanics to medical sciences. In 2015 and 2016, the City of Kyoto awarded him with a City Prize for two years consecutively for his contribution to developing and progressing the internationalization of the City of Kyoto. In 2017, he has been awarded of the prestigious Prize for Scientific Research of the Ministry of Education of Japan (MEXT) for his invention of the nanoscale stress microscope and his fundamental contribution to the Japanese industrial world (first foreigner as an individual recipient).

Topological defects & self-assembly of filamentous viruses

Eric Grelet

Centre de Recherche Paul-Pascal, CNRS & University of Bordeaux, France

Abstract

Topological defects are ubiquitous in Nature, from condensed matter and geophysics to cosmology. In ordered systems, defects mediate phase transitions, and determine many distinctive features of materials, from crystal growth to mechanical properties in metals. However, despite theoretical predictions, the detailed structure of defects remains largely elusive, especially close to their core with the presence of a singularity. By using a model system of colloidal rod-shaped particles, the fd filamentous viruses, enabling improved resolution and contrast by optical microscopy, in situ visualization and quantitative characterization of elementary linear defects - dislocations - has been performed in colloidal smectic liquid crystalline phases. We will also show how topological defects can drive the chirality transfer from particle to supramolecular structure level during self-assembly processes.

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Eric Grelet is Research Director at Centre de Recherche Paul-Pascal, CNRS & University of Bordeaux, France

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CURRICULUM

2012: Habilitation to conduct research, HDR (University of Bordeaux)

Since 2002: CNRS researcher at CRPP

2001-2002: Postdoctoral fellow at Brandeis University (USA) in Seth Fraden's group

1998-2001: PhD under the supervision of Brigitte Pansu at Laboratoire de Physique des Solides (Orsay, France)

1997-1998: Internship in nuclear physics at CEA (Saclay, France)

Awards and distinctions

2009: CNRS Bronze Medal

2002: Glenn Brown prize from the International Liquid Crystal Society

RESEARCH INTEREST

SOFT CONDENSED MATTER and Materials Science

Liquid Crystals / Colloids & Nanoparticles / Complex Fluids

We aim at elucidating rules that govern self-assembly, especially focusing on the role of particle's shape, interaction (entropy vs. enthalpy), chirality and activity (self-propulsion).

We are currently working on the dynamics, the phase behavior and the functionalization of complex fluids with a particular interest for filamentous bacteriophages (fd and M13).

We have been also involved on the use of self-assembled discotic molecules as active layers in organic solar cells.

Our group is currently a member of the Soft Matter team (M2SD : "Matière Molle, Structure et Dynamique") at the Centre de Recherche Paul-Pascal.

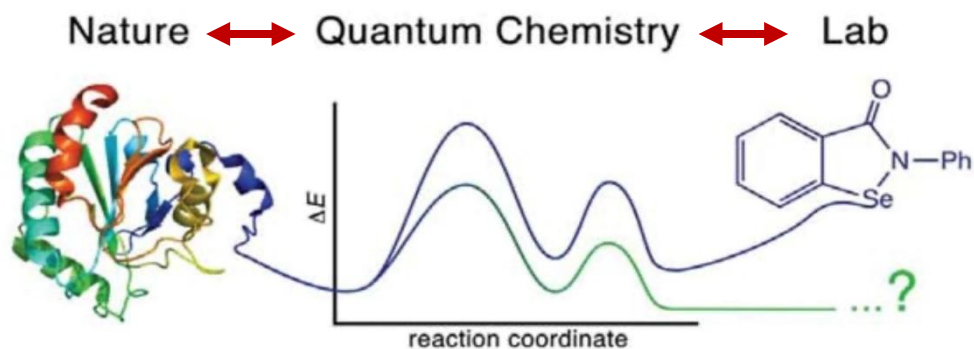
Website: <http://www.crpp-bordeaux.cnrs.fr/spip.php?article929>

Rational design of functional molecules: lessons from enzymes

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In the last few decades, the progress in silicon technology has impacted positively on all fields of science, including chemistry, allowing atomistic simulations of large and complex biomolecules, nanoscale systems and materials as well as very accurate quantum mechanical calculations of molecular structures, properties and reactivity. Particularly, the idea of designing *in silico* molecules with tailored functions strongly attracts the interest of scientists, also with the aim of reducing the costs, the work and the risks in the lab. Computational protocols can thus be set up for very different applications, including the synthesis and repurposing of drugs, the planning of novel catalysts, the development of new materials and nano-systems, the *de novo* design of enzymes, and so on.

The topic of this lecture is the multiscale computational description of selenoenzymes. These are important proteins mainly involved in the regulation of oxidative stress,¹ which is connected to severe pathologies like cancer and neurodegenerative diseases, but also to chronic inflammatory states and even mental disorders. The thorough comprehension of their mechanism, pursued via a combined classic and quantum mechanical approach,² has provided important hints and elements for an improved design of selenium-based mimics^{3,4} to be used as antioxidant drugs, and has recently led to the synthesis of the selenium-based analogue of a popular antidepressant.⁵ Fully exploiting an intuitive and accurate computational approach, known as activation strain analysis, combined with the rigorous molecular orbital theory, it emerges that the chemistry of selenium fully justifies the presence of this oligo-element in biology, despite the complex machinery for its insertion in proteins.

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SHORT C.V. – Laura Orian

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Laura Orian is currently Associate Professor of Physical Chemistry at the University of Padova. She graduated in Chemistry in 1997 and got her PhD (2001) at the University of Padova; then, she moved abroad for her post-doctoral experience, to Lisbon (Portugal) and to Leuven (Belgium). She became permanent researcher at the University of Padova in 2006. Since the same year, she has been regular (almost yearly) visiting scientist in the Theoretical Chemistry group at the VU of Amsterdam (The Netherlands), coordinated by Prof. F. M. Bickelhaupt, with whom she maintains a strong collaboration and shares PhD students and post-docs. L.O. has participated as speaker at more than 40 national and international conferences, she has given more than 10 invited/keynote lectures at conferences and at foreign universities, she is currently member of four editorial boards and has co-authored more than 80 peer-reviewed publications and two book chapters. In 2018, L.O. has obtained the National Scientific Habilitation as Full Professor in the disciplinary area 03-A2 / Models and methodologies for chemical sciences.

Her main research interest is the theoretical rationalization of the chemical bonding and reactivity, particularly of metal-based catalysts, biological and bioinspired systems, for a rational design of functional molecules assisted by computer, aiming at reactivity prediction in advance of the experiment.

Laura Orian is also active in scientific divulgation in the schools for pupils and in STEM activities for the Secondary school students and shares numerous chemistry projects with their teachers.

An atomic description of nanomaterial surfaces using NMR

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Abstract

Nanomaterials are increasingly used in a wide range of applications, including optoelectronics, sensors, drug delivery and catalysis. Understanding the atomic-scale structure of their surfaces and interfaces is essential in order to design nanomaterials with targeted properties. Solid-state NMR can provide unique information on the local atomic-level structure for materials. Nevertheless, the characterization of surfaces and interfaces remains challenging owing to the lack of sensitivity of NMR and the need to distinguish the signals of surface and interface regions from those of the nanoparticle core

We have recently developed novel solid-state NMR methods to characterize the surfaces and interfaces of nanomaterials. In particular, we have introduced methods to probe the local environment of quadrupolar nuclei in those regions. These nuclei with spin $I \geq 1$ represent 75% of isotopes detectable by NMR. These methods have notably been applied to investigate the atomic-level structure of surfaces and interfaces in dendritic silica colloidal nanoparticles coated with boron nitride and oxide, which are promising catalysts for the conversion of propane to propene, an important building block in chemical industry, used for the production of polypropylene [1]. In particular, innovative NMR experiments have shown the anchoring of boron nitride and oxide phases on the silica surface (see Fig. 1). We have also demonstrated the possibility to observe the local environment of surface atoms, which can only be detected via insensitive quadrupolar nuclei having low natural abundance, such as ^{17}O , or low gyromagnetic ratio, such as ^{67}Zn [2]. These experiments have been employed to identify the phases at the surface of Al-doped ZnO nanoparticles employed in various optoelectronic devices.

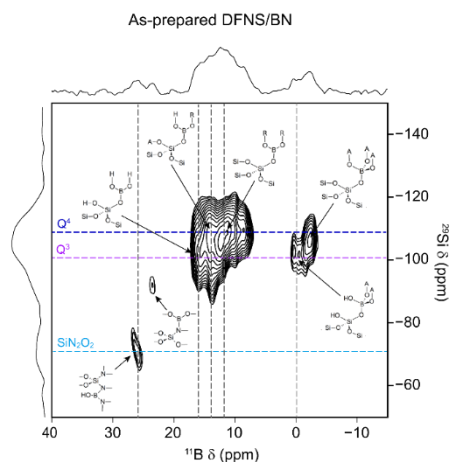


Figure 1 2D Correlation NMR spectrum between ^{11}B and ^{29}Si NMR signals showing the anchoring of BN and B_2O_3 phases on the surface of silica nanoparticles.

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- [2] "Observation of Low- γ Quadrupolar Nuclei by Surface-Enhanced NMR Spectroscopy"; Nagashima, H.; Trébosc, J., Kon, Y. et al; *J. Am. Chem. Soc.* **142**, 10659 (2020) <https://dx.doi.org/10.1021/jacs.9b13838>

Biographical sketch:

Olivier Lafon graduated from ENS Lyon in 2002 and obtained his PhD at the University of Paris-Saclay in 2006. He then worked as a postdoc at CEA. In 2007, he became assistant professor at ENSCL and obtained his habilitation in 2010. In 2011, he was recruited as professor at the Univ. of Lille. The focus of his research is to push the frontiers of solid-state NMR spectroscopy in order to gain unique insights into the structure-property relationships of materials used in the field of bio-economy, energy and health. He has published more than 120 articles in peer-reviewed international journals. He was admitted as a junior member of Institut Universitaire de France in 2016. He has also received the Magnetic Resonance in Chemistry award for young scientist in 2013 and the Chinese Academy of Sciences President's international fellowship in 2015. He is the PI in charge of 1.2 GHz NMR equipment to be installed in Lille, which will offer unparalleled resolution and be one of the first equipment of this type at international level for the characterization of materials. He is also responsible of transnational access to spectroscopy within European EUSMI infrastructure. He coordinates a MOOC on NMR and belongs to the editorial board of Solid-State Nuclear Magnetic Resonance since 2017. He has been member of review panels of ANR, the French research funding agency and expert for various foreign research funding agencies, including Marie Skłodowska-Curie individual fellowships, Department of Energy (USA) and EPSRC (UK).

Biophysical interactions with model plasma membranes

Dr. Loredana Casalis

NanoInnovation Lab at Elettra Sincrotrone Trieste

Abstract

Cell membrane is a very complex and highly dynamic structure made by thousands of different lipids with a variety of saturation and length of acyl chains. Membrane proteins and sugars are also key components of the structure.

The plasma membranes of eukaryotic organisms contain functional, highly dynamic nano-domains called "lipid rafts" enriched in cholesterol, sphingolipids and GPI-anchor proteins, involved in several biological processes as protein trafficking, intra-extracellular cell signalling, chemotaxis and cell polarity. In order to highlight the structural role exerted by the different membrane lipid component in the interaction with proteins and protein containing vesicles, in health and disease, supported lipid bilayers (SLB) of variable composition can be employed. We will present here a multiscale investigation platform made of atomic force microscopy, neutron scattering and infrared spectroscopy to highlight structural details of SLB endowed with raft-like microdomains in interaction with alpha synuclein (α S), whose aggregation is a hallmark of Parkinson's disease, and with natural extracellular vesicles, a potent intracellular communication system. Such studies are ultimately critical for developing therapies targeting the right membrane components.

Dr. Loredana Casalis



1989-MsC. in Physics at the University of Pisa
1990-1993 - PhD Fellow at the University of Trieste, Physics Dept.
1991-1992 – Visiting Scientist at the Ludwig Maximilian University, München
1994-Ph.D. in Condensed Matter Physics
1994-2000 - Researcher (Beamline Scientist) at the ESCA Microscopy Beamline of Elettra Sincrotrone Trieste
2000-2002 – Visiting Research Fellow at Princeton University (Chemistry Dept.)
2003-Present - Coordinator of the NanoInnovation Lab at Elettra Sincrotrone Trieste; Member of the Board of Experts of the PhD course in Nanotechnology, University of Trieste and of the PhD Course in Neurobiology at SISSA, Trieste

Brief Research profile

Expertise: surface functionalization and bio-functionalization; self-assembling; surface bio-recognition; cell biomechanics; single molecule atomic force microscopy imaging in liquid environment; nanolithography; fluorescence microscopy; X-ray photoemission.

Publications and Dissemination:

About 90 articles in reviewed journals, over 40 invited talks and lectures at International Congresses, Schools, Universities and Research Centers. Organization of 4 International Schools in Nano-Biophysics and 2 International Workshops. 23 PhD students supervised and a number of undergraduate students in Physics, Biology, Biotechnology, Chemistry and Engineering. PI of several national and international projects.