UNIVERSITY OF NAPLES "FEDERICO II"
Department of Chemical Sciences

Ph.D. School in Chemical Sciences

PhD Course in the frame of the arCHIMede project of the Department of Chemical Sciences

***Venue*: Department Conference room**

***Date:* May 8th, 2024**

10:30 Prof. Manuel COIMBRA
Department of Chemistry, University of Aveiro, Portugal.
Brewer's spent yeast polysaccharides – structural features and applications.

14:30 Prof. Marco FRAGAI
Department of Chemistry 'Ugo Schiff' and Centro di Risonanze Magnetiche
University of Florence, Italy.
NMR characterization of biological therapeutics and nanosystems

16:00 Prof. Laura RUSSO
School of Medicine and Surgery, University of Milano-Bicocca, Italy.
University of Galway, Department of Chemistry, Ireland.
Biomaterials in clinical translation: from synthesis of 3D tissue mimetics to AI-assisted synthesis strategies

***Date:* May 15th, 2024**

15:30 Prof. Valerie GAUCHER,
UMET University of Lille, France
Effect of macromolecular orientation on the mechanical properties of polylactide and thermomechanically induced crystalline phase transitions in polyamides

***Date:* May 16th, 2024**

10:00 Prof. Carlo ADAMO
Institute of Chemistry for Health and Life Sciences, Chimie ParisTech, Paris, France
There and back again: from applications to theoretical modeling in Chemistry.

Prof. Manuel COIMBRA
Department of Chemistry, University of Aveiro, Portugal

Seminar Summary

Brewer's spent yeast polysaccharides – structural features and applications

Yeast cell walls undergo modifications during the brewing process, leading to a remodeling of their architecture. One significant change is the increased insolubility of the cell wall glycogen pool, due to the formation of covalent bonds between glycogen and cell wall polysaccharides. The combination of multiple enzymatic approaches and NMR methods shed light into the role of yeast cell wall glycogen as a structural core covalently linked to other cell wall components during the brewing process. Microcapsules derived from brewer's spent yeast can be used as oral carriers for food and biomedical applications. Under a circular economy for promotion of sustainability, the thickening and emulsifying properties of brewer's spent yeast mannoproteins can be used as a source of ingredients for the replacement of food additives and protein from animal origin.

Short biography

Manuel A. Coimbra is Full Professor at the Department of Chemistry of University of Aveiro, Portugal. Graduated in Biochemistry at the University of Porto and PhD in Chemistry at the University of Aveiro, in a collaboration with the Institute of Food Research, in Norwich, UK.
Professor of Food Chemistry and Biochemistry and Director of the BSc graduation in Biochemistry. Scientific expertise and interests are focused on carbohydrate chemistry, polysaccharide structure and applications, food chemistry, and industry by-products valuation under a circular economy.
Co-author of 8 patents, 340 research peer-reviewed papers, and supervised 28 PhD thesis (+9 running) and 13 post-Docs.
Editor in Chief of Elsevier journal Carbohydrate Polymers (IF2022= 11.2), President of the Scientific Panel of Food Additives and Food Chain Contaminants of ASAE, the Portuguese Food Safety Agency, and Former President of the Carbohydrate Group of the Portuguese Society of Chemistry (2001-2003 & 2017-2019) and Member of the Executive Board of the Portuguese Society of Biotechnology (2011-2019).

Prof. Marco FRAGAI
Department of Chemistry 'Ugo Schiff' and Centro di Risonanze Magnetiche
University of Florence, Italy.

Seminar Summary

NMR characterization of biological therapeutics and nanosystems

Thanks to advances in the instrumentation and in sample preparation, solid-state NMR has reached sufficient maturity to start tackling systems of outstanding complexity, which are challenging for the other structural biology techniques. Immobilized enzymes, fibrils, vaccine formulation, and biological drugs, can be characterized at the atomic level, allowing a deeper understanding of these systems.

Short biography

Marco Fragai is Associate Professor of Chemistry at Department of Chemistry and Magnetic Resonance Center (CERM), University of Florence. His research focuses on NMR methodologies for structural biology He has also focused on the development of solution and solid-state NMR for the characterization of nanoparticles, immobilized enzymes and biological therapeutics. He is co-author of 152 research articles in international peer-reviewed journals, and of 4 book chapter (h-index=34, Scopus). He holds 4 patents on drug design. He has been visiting research fellow at National Institute for Medical Research (MRC), London (UK) (2008); Laboratory of Biomolecular Mass spectrometry and Proteomics - University of Utrecht (NL) (2006); Sanford Burnham Prebys Medical Discovery Institute (SBP), San Diego (USA) (2003). He is/has been Member of the scientific committee of Giotto Biotech; Member of the scientific committee of the Magnetic Resonance Center (CERM), University of Florence (2017 - 2020); Member of the academic board of the International Doctorate in Structural Biology (2009 - 2012), and of the Doctorate in Chemical Sciences (2013 - present) at the University of Florence; Tutor of 4 PhD students of the International Doctorate in Structural Biology, 1 PhD student of the Doctorate in Chemical Sciences, and 3 PhD students in the frame of Marie Skłodowska-Curie grant agreement N°. 813239, and N°. 956758; Scientific director of the joint research laboratory "Recombinat protein JOYNLAB" (2017 - present), Department of Chemistry, University of Florence. Active corporate collaborations include Dompé Farmaceutici S.p.A; Merck Serono S.p.A.; GSK Vaccines S.r.l.; Abiogen S.p.A.

Prof. Laura RUSSO,
School of Medicine and Surgery, University of Milano-Bicocca, Italy.University of Galway, Department of Chemistry, Ireland.

Seminar Summary

Biomaterials in clinical translation: from synthesis of 3D tissue mimetics to AI-assisted synthesis strategies

The development of human tissue mimetics is crucial for the advancement of healthcare management through the generation of in vitro organs for drug screening and tissue engineering. To this purpose biomatetials mimicking the Extracellular Matrix (ECM) morphology and signaling capacity must be generated. The ECM has a key role in the cell fate modulation, which is mediated by specific interactions with cell receptors. The synthesis of multifunctional materials employable in the design of functional organ-like constructs still represents an open challenge in the field. With the advent of Artificial Intelligence (AI) algorithms and automated manufacturing systems like 3D printing and 3D bioprinting, it is now possible to control the generation of biomaterials with tailored biomolecular and physical properties, limiting the combinatorial and artisanal chemical approach still utilized. Here in this talk, I will present my recent efforts to generate smart multifunctional biomaterials with patient required properties using also AI algorithms.

Short biography

Laura Russo is Associate Professor at University of Milano-Bicocca, Adjunct Lecturer at University of Galway and Visiting Scientist at Imperial College of London. Her research is focused on biomaterials for the development of multifunctional medical devices, including 3D in vitro tissue models, regenerative medicine and patient-personalized biosensors. Her research experience dates to 2010, as PhD student in the BioOrganic research group of the University of Milano-Bicocca, developing n a multidisciplinary project exploiting glycoscience in the field of nano- and biomaterials for tissue engineering. In 2010 LR was Visiting Researcher at Imperial College of London, studying hybrid bioglass based biomaterials for osteochondral tissue regeneration. From 2013 to 2015, as Post Doc Fellow, at University of Milano-Bicocca, she was unit coordinator of a research project on smart biomaterials for organoid cell cultures for cardiac tissue engineering. In October 2016 LR awarded a SFI Starting Investigator Research Grant (SIRG) at Cùram, National University of Ireland - Galway – where she started her research as Principal Investigator on Glycoconjugates biomaterials for tissue engineering applications and cell biology studies. In March 2017 she got a position of Assistant professor at the University of Milano – Bicocca and maintained the position of visiting researcher at Cùram. She was also appointed Adjunct Lecturer at the National University of Ireland - Galway. LR has awarded the prestigious Junior Research Award for Organic Chemistry in Life Science of the Italian Chemical Society for her scientific contribution on organic chemistry applied to the life science field. From 2022 LR is Associate Professor at University of Milano-Bicocca, Member of the Scientific Advisory Board of Biocompatibility Innovation (BCI) and founder of Resyde srl – start-up companies in the field of implantable medical devices. LR is member of the Editorial Advisory Board of Chemistry Europe – Wiley; the Board of Assistant Editors of Journal of Materials Science: Materials in Medicine – Springer Nature; the Editorial Board of Organic Materials - Thieme Verlag KG and Carbohydrate Polymers – Elsevier.

Pr Valerie GAUCHER,
UMET University of Lille

Seminar Summary

Effect of macromolecular orientation on the mechanical properties of polylactide and thermomechanically induced crystalline phase transitions in polyamides.

This seminar will be divided in two parts :

The first part of this presentation will be devoted to the influence of macromolecular orientation on the mechanical behaviour of glassy amorphous polymers. The results will mainly concern Polylactide (PLA). In isotropic state, PLA exhibit a brittle behaviour under uniaxial stretching at room temperature. By contrast, ductile behaviour is observed in samples that have undergone pre-strain in the rubbery state. In order to better understand the origin of this Brittle to Ductile (B-D) transition, an in-depth structural characterisation of the pre-oriented films was carried out by Wide and Small Angle-X-ray Scattering (WAXS, SAXS) and FTIR spectroscopy.

The second part of this presentation will focus on thermally and mechanically induced crystalline phase transitions in polymorphic semi-crystalline polymers such as polyamides 11 and 6. These materials exhibit a fairly wide range of polymorphism. Initially, we will look at the thermal stability of the various crystalline phases in these materials using in-situ WAXS analyses. The evolution of these phases under uniaxial stretching will then be presented. A close link between the nature of the crystalline phases and the ability to be biaxially drawn will be shown.

Short biography
Valérie Gaucher is a full professor in the Department of Physics, at the University of Lille. She carries out her research in the Materials and Transformations Unit (UMET).
Regarding her background, Valerie Gaucher carried out a PhD thesis dealing with the study of the plasticity of polyethylenes in uniaxial tension at the University of Lille under the supervision of DR R. Seguela. Then, she spent a post-doctoral position at Case Western Reserve University in the team of E. Baer and A. Hiltner, where she studied the mechanical behaviour of multilayer films.
Valérie Gaucher teaches modules in general physics, materials science and polymer physics and rheology.
Regarding her research topics she is interested in the relationships between elaboration, structure and mechanical behaviour of polymer-based systems (petroleum-based or bio-sourced ones). In recent years, her works are devoted to (i) thermomechanically induced phase transformations in semi-crystalline polyamides and (ii) the role of macromolecular orientation on the mechanical behaviour of glassy polymers.

Prof. Carlo ADAMO
Institute of Chemistry for Health and Life Sciences, *(i-CLeHS)*, Chimie ParisTech, Paris, France

Seminar Summary

There and back again: from applications to theoretical modeling in Chemistry.

The need to understand the microscopic mechanism underlying complex chemical phenomena is a strong driving force for the development of theoretical approaches. In recent years, advanced quantum methods able to provide chemical and physical properties with accuracy comparable to that of experiments have been developed expanding their application from the purely academic world to the industrial R&D sector and even up to legislation, as in the case of the European REACH regulation. Starting from these last applications, carried out in our laboratory, the recent developments of computational methods rooted in Density Functional Theory (DFT) will be illustrated. Emphasis will be placed on the requirements that these theoretical developments should meet for R&D applications.

Short biography

Prof. Carlo Adamo is the head of i-CleHS, a joint Institute between Chimie ParisTech and CNRS, composed by about 80 researchers working at the interface between Chemistry, Life and Health Sciences. He is Full Professor in Theoretical Chemistry at Chimie ParisTech and was nominated twice senior member of the Institute Universitaire de France (2011 and 2018). He has worked at several prestigious institutions, including the Italian Institute of Technology, Rice University, University of Minnesota and CEA-Grenoble.

His main research interests concern the development of first-principles theoretical models and their application to various fields of Chemistry, from Material Sciences to reactivity. He has authored more than 400 scientific articles, which have received more than 35 000 citations. He has been Editor-in-Chief of Theoretical Chemistry Account (Spinger-Nature) from 2015 to 2023 and he is member of the Advisory Board of Physical Chemistry Chemical Physics (Royal Society of Chemistry) since 2009. In 2022 he was awarded an Advanced Grant from the European Research Council (ERC) for a project on mechanochromism in polymers.