PhD Programme in Chemical Sciences

A PhD Programme of the Dipartimento di Chimica, Biologia e Biotecnologie (DCBB) of the Università degli Studi di Perugia

Research Seminars Offered for the Academic Years
2020/2021
2021/2022
2022/2023
2023/2024

Coordinator: Prof. Luigi Vaccaro
Seminars will be held in room A and/or at the dedicated MicrosoftTeams room and the exact time will be updated on the webpage and communicated via email to all PhD students. Final schedule will be also advertised on the screens in the main entrance.

February 12, 2021 VISPEC online: [https://indico.chem.polimi.it/event/26/](https://indico.chem.polimi.it/event/26/)

*Wavelength dependence of the enhancement in SERS substrates*  
Prof. Roberto Pilot, Università di Padova e Consorzio INSTM

*Label-free SERS and metabolomics*  
Prof. Alois Bonifacio, Università di Trieste

*SERS methodologies and practical considerations for analyses in cultural heritage*  
Dr. Brenda Doherty (CNR Perugia)

February 18, 2021

*Introduction to theoretical methods for solid state modelling* (0.25 CFU)  
*Dr. Daniele Meggiolaro, Institute CNR-ISTM – Perugia*

February 19, 2021 VISPEC online: [https://indico.chem.polimi.it/event/26/](https://indico.chem.polimi.it/event/26/)

*Recent advances in Synchrotron UV Resonance Raman spectroscopy for exploring small and large molecules*  
Dr. Barbara Rossi, Elettra-SincrotroneTrieste

*Dry-state SERS for the "in-situ" identification of natural textile dyes*  
Prof. Margherita Longoni, Università di Milano
**Manipulation of optical nanoantennas for nanospectroscopy (SERS) and nanoscale imaging (TERS)**
Dr. Pietro Gucciardi, IPCF CNR Messina)

March 12, 2021 VISPEC online: [https://indico.chem.polimi.it/event/26/](https://indico.chem.polimi.it/event/26/)

**The investigation of stereospecific intermolecular interactions through Vibrational Circular Dichroism (VCD) in the IR and in the NIR**
Giovanna Longhi (Università di Brescia)

**3D structures of (Ac-Phe-OMe)1,2 peptides by DFT-MD: Graph Theory for the assignment of far-IR gas phase IR-UV ion dip spectra**
Daria Ruth Galimberti (Radboud University, Nijmegen, The Nederlands)

- **How many water molecules are needed to solvate one?**
Riccardo Conte (Università di Milano)

April 9, 2021, 15:00 Microsoft Teams

**Development of sustainable and green methodologies for homogeneous gold catalysis: the key role of the counterion** (0.25 CFU)
Dr. Daniele Zuccaccia, Università degli Studi di Udine

19 April 2021

**X-Ray based synchrotron spectroscopies for Environmental and Cultural Heritage sciences** (0.25 CFU)
Dr. Marine Cotte del ESRF Grenoble (F)

April 23, 2021 VISPEC online: [https://indico.chem.polimi.it/event/26/](https://indico.chem.polimi.it/event/26/)

**Broadband stimulated Raman scattering for non-linear label-free microscopy of cells and tissues**
Dario Polli, Politecnico di Milano
Raman spectroscopy of carbon atomic wires
Carlo Casar, Politecnico di Milano

Sub-Surface Molecular Investigation in Turbid Art Materials using Raman Spectroscopy
Claudia Conti, CNR-ISPC

May 22, 2021
*Cationic gold(I) diarylallenylidene complexes: bonding features and ligand effects* (0.25 CFU)
Prof. Johannes E.M.N. Klein, University of Groningen - NL

June 8, 2021
*Computational aspects of molecular dynamics: Hardware/hands on* (0.25 CFU)
Dr. Daniele Mosconi, Institute CNR-ISTM – Perugia

July 2, 2021
*Supramolecular Medicine crossing the gap between the fundamental research and biomedical applications* (0.25 CFU)
Prof. Veronica Dodero, Bielefeld University, D.

July 10, 2021
*Application of molecular dynamics to cultural heritage* (0.25 CFU)
Dr. Simona Fantacci, Institute CNR-ISTM – Perugia
November 10, 2021

**Modelling the Transport of Platinum-Based Drugs through Lipid Membranes by Quantum and Classical Approaches** (0.25 CFU)

Dr. Juan J. Nogueira, Universidad Autónoma de Madrid, ES

April 12, 2022

**Data-based accelerated excited-state dynamics** (0.25 CFU)

Prof. Dr. Shirin Faraji, University of Groningen, NL.

February 2, 2022

**Quantum effects in IR spectroscopy by semiclassical molecular dynamics simulations** (0.25 CFU)

Prof. Michele Ceotto, Università Milano Statale

February 7, 2022

**In Silico Drug Discovery Using Molecular Interaction Fields** (0.25 CFU)

Dr. Simon Cross, Molecular Discovery, UK

February 9, 2022,

**Introduction to hybrid/organic photovoltaics: understanding the mechanism, improving the efficiency** (0.25 CFU)

Prof. Filippo De Angelis, Università degli Studi di Perugia

March 15, 2022

**Resonant Raman spectroscopy: a valuable tool to unveil the structure and function of heme proteins**

Prof. Giulietta Smulevich, Università degli Studi di Firenze
May 2, 2022  
*Intermolecular interactions in van der Waals aggregates: determination and analytical representation*  
Dr. Massimiliano Bartolomei, CSIC Madrid, ES

May 19, 2022  
*Brillouin scattering as a probe for mechanical and morphological characterization of materials* (0.25 CFU)  
Dr. Lucia Comez, IOM-CNR, Italy

June 6, 2022  
*Recent advances in Synchrotron UV Resonance Raman spectroscopy for exploring small and large molecules* (0.25 CFU)  
Dr. Barbara Rossi, Elettra Sincrotrone Trieste, Italy

May 25, 2023  
*Circular dichroism signals: a unique probe of the secondary structure of biosystems* (0.25 CFU)  
Dr. Lucia Comez, IOM-CNR, Italy

Additional seminars given by the guests of the Department of Chemistry, Biology and Biotechnology will be announced and the list updated accordingly.

On average, each year over 30 research seminars are organized and the PhD students are strongly encouraged to attend all of them. It is mandatory to attend a minimum of 16 seminars (4 CFU, 0.25 CFU per seminar) over the entire PhD course.