



# 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 (XXXVI cycle ongoing and previous ones)**  
**2021/2022 (XXXVII cycle and previous ones)**  
**2022/2023 (XXXVIII cycle and previous ones)**  
**2023/2024**  
**2024/2025**

*Coordinator: Prof. Luigi Vaccaro*



DIPARTIMENTO **2018**  
di **ECCELLENZA** **2022**  
progetto AMIS



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Seminars will be held in room A and/or at the dedicated Microsoft Teams 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/>

***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/>

***Recent advances in Synchrotron UV Resonance Raman spectroscopy for exploring small and large molecules***

Dr. Barbara Rossi, Elettra-Sincrotrone Trieste

***Dry-state SERS for the "in-situ" identification of natural textile dyes***

Prof. Margherita Longoni, Università di Milano



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**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/>

**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)<sub>1,2</sub> 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 Netherlands)

**- 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/>

**Broadband stimulated Raman scattering for non-linear label-free microscopy of cells and tissues**

Dario Polli, Politecnico di Milano



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## **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 Doderò, Bielefeld University, D.*

July 10, 2021

### ***Application of molecular dynamics to cultural heritage*** (0.25 CFU)

*Dr. Simona Fantacci, Institute CNR-ISTM – Perugia*



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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

28 gennaio 2022 | 14:30 VISPEC on line (<https://indico.chem.polimi.it/event/26/>)

***Organic molecular materials: insight from low frequency Raman scattering***

Matteo Masino, (Dipartimento di Scienze Chimiche, della Vita e della Sostenibilità Ambientale | Università di Parma)

***Probing Deep inside Turbid Materials using Spatially Offset Raman Spectroscopy (SORS)***

Pavel Matousek, (Central Laser Facility, STFC Rutherford Appleton Laboratory, Harwell Oxford)

7 March , 2022

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

Dr. Simon Cross, Molecular Discovery, UK

March 10, 2022

***Li-rich layered oxides (LRLO) for lithium cells: pushing positive electrodes to their limits (0.25 CFU)***

Prof. Sergio Brutti dell'Università di Roma La Sapienza

March 17, 2022

***In operando X-ray Absorption Spectroscopy for the study of charge transfer in electrodes for photoelectrochemical water oxidation.***

Dr. Francesco d'Acapito - CNR-IOM e ESRF Grenoble



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18 March, 2022

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

Prof. Michele Ceotto, Università Milano Statale

April 12, 2022

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

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

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



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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.*



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