

It is our great pleasure to welcome you to the XIV Doctoral Workshop organized by the PhD Chemistry and the Chemistry Department. This event aims to strengthen the links between the research groups of our Department, with the ultimate goal of promoting interdisciplinary projects. During the event, 20 students will have the opportunity to present and discuss their research work, interact and receive feedback from experienced researchers.

Prof. Mircea Dincă
Princeton University

Mircea Dincă is the Alexander Stewart 1886 Professor of Chemistry at Princeton University. He grew up in Romania and moved to the United States to pursue his Bachelor's degree in Chemistry at Princeton University. Graduate studies in Inorganic Chemistry at UC Berkeley were followed by a postdoctoral appointment at MIT. He started his independent career in 2010 at MIT and moved his research group to Princeton in 2025. His group focuses on the synthesis of new multifunctional materials for applications in electrical and electronic devices, heterogeneous catalysis, and various uses in clean and renewable energy. In recognition of his group's research, Dincă has been awarded the Alan T. Waterman Award from the NSF in 2016, the ACS Award in Pure Chemistry in 2018, and the Blavatnik National Award in Chemistry in 2021, among several others. He has been named to the Thomson-Reuters/Clarivate Analytics Highly Cited Chemists List yearly since 2014.

Prof. Géraldine Masson
ICSN-CNRS/Paris-Saclay University

Géraldine Masson received her Ph.D. in organic chemistry from Joseph Fourier University (Grenoble, France) in 2003, under the supervision of Dr. Sandrine Py and Prof. Yannick Vallée. That same year, she joined the University of Amsterdam (Netherlands) as a Marie Curie postdoctoral fellow, working with Prof. Jan van Maarseveen and Prof. Henk Hiemstra.

In 2005, she became a CNRS researcher in the group of Prof. Jieping Zhu at the Institut de Chimie des Substances Naturelles (ICSN). She launched her independent research career in 2011 and has led the POWER group (Photocatalysis and Organocatalysis With Efficient Reactivity) since 2012. She was promoted to CNRS Research Director (DR2) in 2014 and to DR1 in 2020. In 2021, she became Co-Director of Labcom HitCat, a joint laboratory between SEQENS and the CNRS. Her research focuses on the development of innovative catalytic methodologies for the synthesis of optically active, biologically relevant molecules, with particular emphasis on asymmetric organocatalysis and photoredox catalysis.

Prof. Charles Machan
University of Virginia

Charles Machan (muh-hahn) was born in Madison, WI and grew up in Wauwatosa, WI where he attended Marquette University High School before going to Washington University in St. Louis (WashU). While at WashU he played football for four years as a defensive tackle and majored in Chemistry and German (B.A. 2008). Charles attended Northwestern University and completed a Ph.D. in Inorganic Chemistry (2012) under the supervision of Chad A. Mirkin. At Northwestern he served as President of the Alpha Gamma Chapter of Phi Lambda Upsilon, a co-ed chemistry honors fraternity, and received the Edmund W. Gelewitz Award for Outstanding Senior Graduate Student (2012). From 2013-2016 he was a postdoctoral researcher with Clifford P. Kubiak at the University of California, San Diego. Charles joined the Department of Chemistry at the University of Virginia in 2016 as an Assistant Professor. Since 2022, he has been an Associate Professor in the Department, where his research program currently receives funding from NSF and DOE. He received the Bessel Research Award from the Alexander von Humboldt Stiftung in 2024. His research covers energy-relevant catalysis involving abundant small molecules like carbon dioxide, dioxygen, dihydrogen, and water as reagents at the interface of molecular electrochemistry and materials. The approach focuses on developing new inorganic complexes and materials which incorporate co-catalytic moieties, non-covalent secondary sphere interactions, and substrate relays as catalysts to store electrical energy in chemical bonds

Organizing and Scientific Committee:

Dr. Xavier Sala, Coordinator and president of the academic committee of the PhD in Chemistry
Dr. Rosario Núñez, Vocal of the academic committee of the PhD in Chemistry
Dr. Daniel Maspoch, Vocal of the academic committee of the PhD in Chemistry
Dr. Xavier Solans, Secretary of the academic committee of the PhD in Chemistry
Dr. Maria Jesús Sánchez, Vocal of the academic committee of the PhD in Chemistry
Dr. Carolina Gimbert, Vocal of the academic committee of the PhD in Chemistry

Awards Committee:

Dr. Xavier Sala, Coordinator and president of the academic committee of the PhD in Chemistry
Dr. Carolina Gimbert, Vocal of the academic committee of the PhD in Chemistry
Dr. Heber, Eduardo Andrada, postdoctoral researcher
Dr. Roberto Sanchez Naya, postdoctoral researcher ICN2
Alvaro Lozano, PhD Student
Anna Vidal López, PhD Student

Venue:

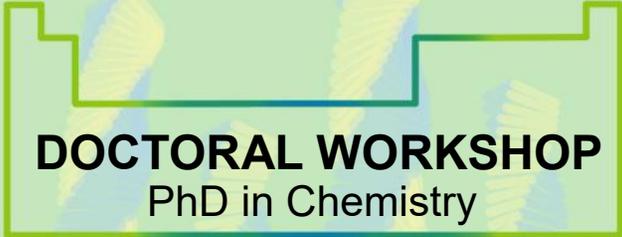
Plenary Lectures and PhD students' presentations: Auditorium of the Faculty of Sciences (Sala d'Actes).
Posters' Exhibition: Hall on the ground floor of the Faculty of Sciences (in front of Sala de Graus I).

Contact details:

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DOCTORAL WORKSHOP

PhD in Chemistry

May 22nd - 23rd 2025

Sala D'Actes

Faculty of Sciences

Chemistry Department

UAB



May 22nd

08:45—09:00 Welcome and opening

Prof. Lluís Escriche, Head of the Department of Chemistry
Prof. Rosa Maria Sebastian, Vicerector for Innovation, Transfer and Entrepreneurship

09:00—10:00 Plenary Lecture

Chair: Daniel MasPOCH

Title: From electrically conductive MOFs to sustainable batteries
Prof. Mircea Dincă

10:00—10:45 Poster session + Coffee Break

10:45—12:00 Presentations I

Chair: M^a Jesus Sánchez

- 10:45 - 11:00 Clip-Off chemistry as a synthetic tool towards unprecedented reticular and molecular materials. **Sara Ruiz Relaño. P1.1**
- 11:00 - 11:15 A Ni based OER photoanode working in CO₂RR conditions. **Aureliano Macili. P1.2**
- 11:15 - 11:30 Design of low-powered electrochromic devices using quasi-solid matrices on ionic liquids. **Tehreema Naeem. P1.3**
- 11:30 - 11:45 Light-induced HER using 2D-COF in multicomponent systems. **David Reyes Mesa. P1.4**
- 11:45 - 12:00 Atomistic modelling of corrosion inhibition: the role of oxides. **Mazhar Iqbal. P1.5**

12:00—13:00 Plenary Lecture (GEQO Seminarios Itinerantes)

Chair: Xavier Sala

Title: Metal-Free Molecules as Electrocatalysts and Co-electrocatalysts
Prof. Charles Machan

13:00—15:15 Break

15:15—17:15 Presentations II

Chair: Xavier Solans

- 15:15 - 15:30 Sol-gel materials based on 1st row metals for water oxidation photoelectrodes. **Axel Guinart Guillem. P2.1**
- 15:30 - 15:45 Modelling Metals in Supramolecules – Proteins and Metalloccages. **Mercè Alemany Chavarria. P2.2**
- 15:45 - 16:00 Process development towards Bismuth Subsalicylate. **Rubén Doblaz Perez. P2.3**
- 16:00 - 16:15 Molecular modelling for the design of metal-containing biosystems: cytochrome P450 CYP19A4. **Laura Martínez Castro. P2.4**
- 16:15 - 16:30 Development of quantitative point-of-care devices for detection of infectious diseases. **Judit Prat Trunas. P2.5**
- 16:30 - 16:45 New azobenzene derivatives for selective light-modulated COX-2 inhibition. **Amanda Morales Jiménez. P2.6**
- 16:45 - 17:00 From Inflammation to Cancer: Computational modelling of key systems of interest. **Álex Pérez Sánchez. P2.7**
- 17:00 - 17:15 Polyethylene terephthalate microplastics staining with iDye Poly Pink: staining optimization and toxicity evaluation. **Uma Maheswari Mariappan. P2.8**

May 23rd

09:15—11:00 Presentations III

Chair: Rosario Núñez

- 09:15 - 09:30 Scalable Synthesis of Organic Molecules via Clip-off Chemistry from Covalent Organic Frameworks. **Juan Pablo Cavalieri P3.1**
- 09:30 - 09:45 Inside-out functionalization of Rh(III)-Based MOPs. **Xiang Zhang. P3.2**
- 09:45 - 10:00 Absorption and reactivity in interstellar refractory materials: a quantum-mechanical study. **Niccolo Bancone. P3.3**
- 10:00 - 10:15 Synthesis of metal-organic nanosheets via clip-off chemistry. **Pilar Marina Fernández Serifán. P3.4**
- 10:15 - 10:30 Design of 2D Germanene nanoarchitectonics for implementation in energy and biosensing systems. **Yiming Lei. P3.5**
- 10:30 - 10:45 Synthesis of Spirooxazines with long lifetime of Merocyanine Form. **Mila Miroshnichenko. P3.6**
- 10:45 - 11:00 A novel nanotheranostic approach for glioblastoma based on nanocarriers and immune-PET radiopharmaceuticals (nanothera-PET). **Emily Betancourt Fernandez. P3.7**

11:00—12:00 Poster session + Coffee Break

12:00—13:00 Plenary Lecture

Chair: Carolina Gimbert

Title: Combined Asymmetric and Photoredox Catalysis for the Efficient Synthesis of Chiral Amines
Prof. Géraldine Masson

13:00—13:15 Award and Closing Ceremony

Doctoral Workshop 2025 distinguished Diploma, along with a gift, will be given to the two best Poster & Presentation.

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