DOCTORAL WORKSHOP

PhD in Chemistry

Scientific Programme

May 20th-21st, 2026

Sala d'Actes

Faculty of Science

Organised by the Department of Chemistry

Sponsored by:

RSEQ Real Sociedad Española de Química

RSEQ Secció Territorial Catalana

SCQ Societat Catalana de Química

UAB Universitat Autònoma de Barcelona

Facultat de Ciències UAB

WELCOME TO THE XV DOCTORAL WORKSHOP OF THE PhD PROGRAMME IN CHEMISTRY

May 20-21, 2026

It is our great pleasure to welcome you to the new Edition of the Doctoral Workshop of the PhD programme in Chemistry that is organized by the UAB's Department of Chemistry.

This year's workshop continues its tradition of providing supportive environment for doctoral students to present and discuss their dissertation with peers, members of the program and other experienced reserchers, with the aim to strengthen the links and facilitating the exchange of research experiences and new ideas in the fields of entrepreneurship and small business.

During the event, 24 students, mostly on their third year will have an excellent opportunity to share their research. The Doctoral Workshop will also include an exciting series of plenary lectures given by international experts.

All the members of the PhD program in Chemistry and related programs, as well as other members of the research community are more than welcome.

We look forward to your participation in this event.

The Organizing Committee

ORGANIZING, SCIENTIFIC AND AWARDS COMMITTEE

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. Xavier Solans Monfort, Secretary of the academic committee of the PhD in Chemistry
Judit Prat Trunas, PhD Student
Mercè Alemany, PhD Student

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Event sponsored by:

Real Sociedad Española de Química (RSEQ) – Secció Catalana de la RSEQ
Societat Catalana de Química (SCQ) – GEQO – Seminarios Itinerantes

RSEQ Real Sociedad Española de Química El Sitio de la Química en España

RSEQ Secció Territorial Catalana www.rseq.cat

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INVITED SPEAKERS

Prof. Federico Bella
Politecnico di Torino

Federico Bella is Full Professor of Chemistry at Politecnico di Torino, where he leads research on materials chemistry for energy conversion and storage, with a focus on electrochemical nitrogen reduction, batteries, photovoltaics, and sustainable materials. He obtained his PhD in Electronic Devices from the Italian Institute of Technology and built his academic career at Politecnico di Torino, becoming Full Professor in 2022. His research combines electrochemistry, materials science, photochemistry, chemometrics, and green chemistry to develop more sustainable energy technologies. He has been the Principal Investigator of the ERC Starting Grant SuN2rise, devoted to solar-driven electrochemical nitrogen fixation for ammonia production. His group works on nitrogen and nitrate electroreduction, with particular attention to electrolyte design, interface control, analytical reliability, and process sustainability. He has authored more than 130 peer-reviewed papers, collecting over 12,500 citations and reaching an h-index of 81 according to Scopus. He serves on the editorial boards of leading journals including Energy Storage Materials, Chemical Engineering Journal, ChemSusChem, and ACS Sustainable Chemistry & Engineering. Among his recognitions are the ISE Prize for Electrochemical Materials Science, the ISE-Elsevier Prize for Applied Electrochemistry, the ACS Sustainable Chemistry & Engineering Lectureship, and the ChemComm Emerging Investigator Lectureship.

Prof. Jesús Campos
Instituto de Investigaciones Químicas (IIQ), Universidad de Sevilla and Consejo Superior de Investigaciones Científicas (CSIC)

Jesús Campos obtained his PhD (2012) in organometallic chemistry at the University of Sevilla (E. Carmona), including a visiting stay at the University of North Carolina (M. Brookhart). He developed his postdoctoral research at the universities of Yale (R. Crabtree) and Oxford (S. Aldridge). Since 2017 he is CSIC tenured scientist and group leader at the Institute for Chemical Research. During that time, he has been awarded with ERC Starting and Consolidator Grants to develop bimetallic cooperative systems from different perspectives. His work has been recognized with several distinctions, including the Premio a la Excelencia Investigadora from RSEQ or the Premio Nacional de Investigación Joven. His interests include all aspects of organometallic chemistry, particularly on the study of cooperative mechanisms for bond activation and catalysis.

Prof. Carme Rovira
Universitat de Barcelona

Carme Rovira is an ICREA Research Professor at the University of Barcelona. She obtained her PhD in Chemistry from the University of Barcelona and carried out research stays in Germany, at the Max Planck Institute for Solid State Research, and in the UK, at the University of York. Her research focuses on modelling enzyme catalytic mechanisms through computer simulations, with a special emphasis on carbohydrate-active enzymes. She has received several awards, including distinctions from the Generalitat de Catalunya, the Barcelona City Council, and the European Carbohydrate Organization (*Emil Fischer* award). In 2020, she was awarded an ERC Synergy Grant, and in 2025 she received the National Research Award “Enrique Moles” in Chemistry and Chemical Technology. She currently serves as President of the Computational Chemistry Group of the Spanish Royal Society of Chemistry and as Associate Editor of *ACS Omega*

SCIENTIFIC PROGRAM

May 20th

08:45—09:00 Welcome and opening

Prof. Ramon Alibés, Head of the Department of Chemistry
Mrs. Beatriz Ferrus Anton, Head of the Doctoral School

09:00—10:00 Plenary Lecture

Chair: Xavier Sala

Title: Ammonia by Electrons: Turning Nitrogen Feedstocks into Sustainable Fuels and Fertilizers
Prof. Federico Bella

10:00—12:00 Presentations I

Chair: Xavier Sala

10:00 - 10:15 DFT study on the electrocatalytic reduction of NO3 and N2 into ammonia. **Yanis Abid Charef. P1.1**

10:15 - 10:30 Synthesis of Organic Molecules via Spray-Drying. **Gerard Pena Pozo. P1.2**

10:30 - 10:45 Recovering Copper from vineyards: Phytoremediation as a circular strategy. **Camila Cazorla Ares. P1.3**

10:45 - 11:00 Sulfanilic Acid-capped Ruthenium Nanoparticles for Enhanced HER activity in neutral media. **Matilda Kraft. P1.4**

11:00—11:45 Poster session

11:45—12:45 Presentations II

Chair: Carolina Gimbert

11:45 - 12:00 Chitin - choline bio-sourced composites for CO2 electrolysis in atmospheric conditions. **Boya Wu. P2.1**

12:00 - 12:15 Beyond Isostructurality: Controlling Function and Scale in Zr and Hf Carborane MOFs. **Shuo Zhang. P2.2**

12:15 - 12:30 Giant Unilamellar Vesicles (GUVs) for Cell Membrane mimicry. Towards Artificial red bloods cells. **Carlos Cascales Guerrero. P2.3**

12:30 - 12:45 Development of 3D-printed sensing platforms applied to pH and hydrogen monitoring. **Mingyue Pan. P2.4**

12:45 - 13:00 Selective recovery of heavy metals from wine sludge using oxidizing agents: towards sustainable waste management in viticulture. **Mónica González Quintela. P2.5**

13:00—15:15 Break

15:15—16:15 Plenary Lecture

Chair: Daniel Maspoch

Title: Cooperation, Inhibition and other Bimetallic Synergies
Prof. Jesús Campos

16:15—17:30 Presentations III

Chair: Xavier Solans

16:15 - 16:30 Plant nano-biofortification selenium release in soil systems to produce functional foods. **Alejandro Fuentes García. P3.1**

16:30 - 16:45 Molecular electrocatalysts for RedOx reactions: water oxidation and CO2 reduction using carbanionic ruthenium. **Jake Tyler Kerkhof. P3.2**

16:45 - 17:00 Developing computational tools to explore reaction pathways for periodic systems. **Andreha Gelli. P3.3**

17:00 - 17:15 Rice Husk Ash-Derived Zeolite X Supported Mn-ZIF-67 for Visible-Light-Assisted PMS Activation: From Agro-Industrial Waste Valorisation to Organic Pollutant Remediation. **Hanwen Luan. P3.4**

17:15 - 17:30 Reversible colorless-to-colored thermochromic materials based on modified. **Noel Muñoz Pérez. P3.5**

May 21st

09:00—10:30 Presentations IV

Chair: Maria Jesús Sánchez

09:00- 09:15 TT-CF3+OTf-: a bench-stable trifluoromethylation reagent with formal CF3+, and CF3• reactivity. **Xiangyu Tan. P4.1**

09:15 - 09:30 Portable electrochemical biosensing platform for point-of-need. **Juan Carlos Porras. P4.2**

09:30 - 09:45 How Multi Component Reactions simplify the synthesis of Organic Radical Dendrimers as potential MRI contrast agents? **Ehsan Shirdel Tazehkand. P4.3**

09:45 - 10:00 Toward Cu Remediation of Vineyard Soils: A Sulfonated Amide COF and COF-Based Membrane Approach. **Di Cai. P4.4**

10:00 - 10:15 Making Mesocrystals with Colloidal MOF Particles. **Amir Mohammad Ghadiri Ghehi. P4.5**

10:15 - 10:30 Development of point-of-need potentiometric devices for the monitoring of rare inherited metabolic diseases. **Laia Garrido Carretero. P4.6**

10:30—11:15 Poster session

11:15—12:15 Presentations V

Chair: Rosario Núñez

11:15 - 11:30 Development of electrochemical sensors from revalorize biomass for emerging pollutant monitoring. **Yudong Bian. P5.1**

11:30 - 11:45 Electrocatalytic ammonia synthesis via iron-based nanoparticles: mechanistic insights from computational studies. **Adenilson Felipe Sousa Silva. P5.2**

11:45 - 12:00 Synergistic Enhancement of Cu (II) Adsorption by Tannic Acid and L-Cysteine Functionalized Magnetic Chitosan Beads: Role of Structure–Function Trade-Off. **Xiaojie Sun. P5.3**

12:00 - 12:15 Towards graphene functionalization with small organic molecules for neurotransmitters detection. **Aina Galceran Sabatés. P5.4**

12:15—13:15 Plenary Lecture

Chair: Mariona Sodupe

Title: Using Computer Simulations to Understand How Enzymes Work
Prof. Carme Rovira

13:15—13:30 Award and Closing Ceremony

Doctoral Workshop 2026 distinguished Diploma, along with a gift, will be given to the two best Poster & Presentation.

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