

It is our great pleasure to welcome you to the XIII Doctoral Workshop that is organized by the PhD Chemistry Program 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 and more ambitious research projects. During the event, 14 students on their third and fourth year will have the opportunity to present and discuss their research work and interact to each other, and receive feedback from more experienced researchers.

Prof. Dr. Veronique Van Speybroeck

Center for Molecular Modeling, University of Ghent.

Full Professor at the Ghent University and head of the Center for Molecular modeling (<http://molmod.ugent.be>), a multidisciplinary research center composed of about 40 researchers. She was trained as an engineer in Physics and obtained her PhD in 2001 from the Ghent University. She has a record of [significant contributions](#) in the field of modeling nanoporous materials for catalysis, adsorption; all applications are inspired and performed in close synergy with experimental groups. The research is driven by the ambition to model as close as possible realistic materials/processes and systematically pushed the limits of simulation kinetics. She developed methods to calculate chemical kinetics for reactions taking place in nanoporous materials and pioneered the simulation of complex catalytic cycles at operating conditions using enhanced sampling molecular dynamics methods. Currently, she is exploring methods to resolve complex catalytic cycles bridging length and time scales. She was recipient of two ERC grants, received numerous recognitions and prizes, such as the [Dr. Karl Wamsler innovation award in 2023](#). She is also an elected member of the Royal (Flemish) Academy for Science and the Arts of Belgium (KVAB, www.kvab.be).

Prof. Alberto Escarpa

Department of Analytical Chemistry, University of Alcalá.

His main research interests are microfluidics and micromotors for (bio) sensing. He has co-authored more than 200 articles in leading journals, books, and book chapters (h-index of 50). He has been included in the top 1% of most cited chemists worldwide (2020, 2021 by Stanford University). His works have been highlighted in top journals and social scientific media. He has given more than 50 invited lectures. He has received several awards such as the NATO Fellowship to perform postdoctoral research at the New Mexico State University (USA) in 2001, the "Young Investigator Award" by the University of Alcalá in 2003, the International Dropsens Award "Best Research Work in applied electroanalytical chemistry" (finalist) in 2015, the Excellence Award in Doctoral Thesis Direction of Sciences in 2021 at University of Alcalá, and Spanish Royal Society of Chemistry Award for Research Excellence 2024. He is currently a member of the Editorial Board of Analytical Chemistry and Editor in Chief for *Microchimica Acta*.

Dr. Beatriz Pelaz

CiQUS & Department of Inorganic Chemistry, University of Santiago de Compostela.

Beatriz Pelaz received her PhD from the University of Zaragoza in 2012. From June 2012 to December 2016, Beatriz was a member of Professor Wolfgang J. Parak's group at Philipps-Universität Marburg in Germany, first as a postdoctoral researcher and later as a Humboldt researcher. Since January 2017, she has co-lead the BioNanoTools group at CiQUS, initially as the principal investigator of a project for young researchers (JIN, MINECO), later as a Ramón y Cajal researcher (2017 call, affiliated with the Inorganic Chemistry department of the University of Santiago de Compostela). Currently, she is an Associate Professor at the USC. In 2020, the European Research Council awarded her a Starting Grant. Since 2021, she is member of the Young Academy of Spain. Her research focuses on developing remotely controllable smart materials and their interaction with biological entities.

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. Rosario Núñez, Vocal of the academic committee of the PhD in Chemistry
Dr. Maria Jesús Sánchez, Vocal of the academic committee of the PhD in Chemistry
Dr. Ruggero Bonnetto, postdoctoral researcher
Marta Alcaina, PhD Student
Albert Rosado, PhD student
Franc Paré, 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:

Prof. Xavier Sala Román
PhD Coordinator of PhD studies in Chemistry

Elena Jiménez
Administrative Assistant for PhD Studies in Chemistry

Tel.: 935811997
E-mail: gestio.postgrau.quimica@uab.cat
<https://www.uab.cat/ca/quimica>



DOCTORAL WORKSHOP
PhD in Chemistry

May 23rd-24th 2024

Sala D'Actes

Faculty of Sciences

Chemistry Department

UAB



May 23rd

May 24th

09:00—09:15 Welcome and opening

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

09:15—10:15 Plenary Lecture

Chairman: Xavier Solans

Title: Operando modelling of functional nanostructured materials for future technologies
Prof. Veronique Van Speybroeck

10:15—11:15 Poster session + Coffee Break

11:15—12:45 Presentations I

Chairwoman: Maria Jesús Sánchez

- 11:15 - 11:30 Is Size All That Matters? A Discussion on the Functionalisation of Metallic Nanoparticles. **Álvaro Lozano Roche**. P1.1
- 11:30 - 11:45 Investigating CO₂ Formation on Interstellar Water Ice: A Computational Study. **Harjasnoor Kakkar**. P1.2
- 11:45 - 12:00 Giant oligomeric porous cage-based molecules. **Alba Cortés Martínez**. P1.3
- 12:00 - 12:15 Structure-based design of serotonin 5-HT_{2C} receptor positive allosteric modulators for the treatment of obesity. **Aleix Quintana García**. P1.4
- 12:15 - 12:30 Synthesis and photochemical characterization of new Smart UV filters. **Cristina Moya Muñoz**. P1.5
- 12:30 - 12:45 Electrolyte Gated Organic Field Effect Transistors For Point-Of-Care Tests. **María Jesús Ortiz Aguayo**. P1.6

12:45—15:00 Break

15:00—16:00 Plenary Lecture

Chairman: José Muñoz

Title: Micromotors in action as smart microsensors: just a concept or a reality?
Prof. Alberto Escarpa

16:00—17:00 Presentations II

Chairwoman: Carolina Gimbert

- 16:00 - 16:15 Fluorine meets visible-light: sustainable methods and tunable materials. **Albert Gallego Gamo**. P2.1
- 16:15 - 16:30 Rapid screening test for Streptococcus agalactiae neonatal infections combining portable PCR and electrochemical. **Anaxis Del Valle Peña**. P2.2
- 16:30 - 16:45 Development of a new PEG-based biocompatible sealant for surgical applications. **Alba López Moral**. P2.3
- 16:45 - 17:00 Improvement of cocaine electrochemical detection with tailor-made polymers. **Elena Rodríguez Franch**. P2.4

09:30—10:30 Presentations III

Chairman: Xavier Sala

- 09:30 - 09:45 Engineering of Glioblastoma-derived Biomimetic Vesicles. **Noelia Hernández Lobato**. P3.1
- 09:45 - 10:00 Multivariate Metal-Organic Frameworks: Quest for Complexity. **Xiao Bao Li**. P3.2
- 10:00 - 10:15 Lignocellulosic biomass conversion into biochemicals using pyrolysis. **Mireia Mora Sanjuan**. P3.3
- 10:15 - 10:30 Co-assembly of Polyhedral Metal-Organic Framework Particles into Binary Ordered Superstructures. **Lingxin Meng**. P3.4

10:30—11:30 Poster session + Coffee Break

11:30—12:30 Plenary Lecture

Chairwoman: Rosario Núñez

Title: Development of efficient nanocarriers
Dr. Beatriz Pelaz

12:30—12:45 Award and Closing Ceremony

Doctoral Workshop 2024 distinguished Diploma, along with a gift, will be given to the two best Poster & Presentation.

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