Invited speakers:

Prof. Javier García Martínez, IUPAC President
University of Alicante

Javier Garcia-Martinez is Director of the Molecular Nanotechnology Lab at the University of Alicante. He has published extensively in the areas of nanomaterials and energy and is the author of more than twenty five patents. Javier is founder and President of Celera, a talent acceleration program that supports and provides resources and mentoring to young members that have resulted in more than 10 companies funded, valued at $500 million. He is also the President of the Young Academy of Spain. Javier is currently the President of the IUPAC. Javier received the Europe Medal in 2005, the Silver Medal of the European Young Chemist Award in 2006, the TR 35 Award from MIT's Technology Review magazine, in 2009 he was selected as a Young Global Leader, the King Jaime I Award in 2014, the Kathryn C. Hach Award for Best Entrepreneur in the Chemical Sector by the American Chemical Society in 2018. Javier is a Fellow of the Royal Society of Chemistry and a member of the Global Young Academy and since 2010 he is a member of the World Economic Forum Council on Emerging Technologies.
More at: http://nanomol.es/en/home/

Prof. Katherine Villa, Group Leader
Institute of Chemical Research of Catalonia (ICIQ)

Dr. Villa obtained her PhD in Chemistry from the UAB. Then, she worked at the Catalonia Institute for Energy Research (IREC) and at the Institute for Bioengineering of Catalonia (IBEC). In 2018she joined the Advanced Functional Nanorobots center at the University of Chemistry and Technology (Czech Republic). Since 2021, she is leading a research group on advanced photocatalytic materials for energy and environmental applications at the Institute of Chemical Research of Catalonia (ICIQ). She has received important recognitions such as the RSEQ Award 2023 for Young researchers (group leader) as well as competitive funding including an ERC Starting Grant 2022. Her research interests include photocatalysis, nanomaterials, renewable energy, micro/nanomotors, and environmental remediation.
More at: https://www.iciq.org/research/research_group/dr-katherine-villa/

Prof. Ben Feringa, Nobel Prize in Chemistry
University of Groningen

Ben L. Feringa obtained his PhD degree at the University of Groningen in the Netherlands under the guidance of Professor Hans Wynberg. After working as a research scientist at Shell in the Netherlands and the UK, he was appointed lecturer and in 1988 full professor at the University of Groningen and named the Jacobus H. van't Hoff Distinguished Professor of Molecular Sciences in 2004. In 2008 he was appointed Academy Professor and was knighted by Her Majesty the Queen of the Netherlands. Feringa's research has been recognized with a number of awards including the Koerber European Science Award (2003), the Spinoza Award (2004), the Norrish Award of the ACS (2007), the Paracelsus medal (2008), the Nagoya gold medal (2013), ACS Cope Scholar Award 2015, Chemistry for the Future Solvay Prize (2015), The 2016 Nobel prize in Chemistry and the Euchems gold medal. Feringa's research interest includes stereochemistry, organic synthesis, asymmetric catalysis, molecular switches and motors, self-assembly, molecular nanosystems and photopharmacology.
More at: http://www.benferinga.com/

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 event aims to strengthen the links between the research groups of the programme, with the ultimate goal of promoting interdisciplinary and more ambitious research projects. In this edition, 26 young researchers will have an excellent opportunity to share their projects. The Doctoral Workshop will also include an exciting series of plenary lectures given by international experts.

Organizing, Scientific and Awards Committee:

- Prof. Gregori Ujaque, Dept. of Chemistry, UAB.
- Prof. Félix Busqué, Dept. of Chemistry, UAB.
- Prof. Xavier Sala, Dept. of Chemistry, UAB.
- Prof. Daniel Maspoch, Catalan Institute of Nanoscience and Nanotechnology (ICN2)
- Prof. Mireia Baeza, Dept. of Chemistry, UAB.
- Prof. Rosario Núñez, Institute of Materials Science of Barcelona (ICMAB-CSIC)
- Arnau Comajuncosa, PhD Student.
- Jewel Ann Marie Xavier, PhD Student.

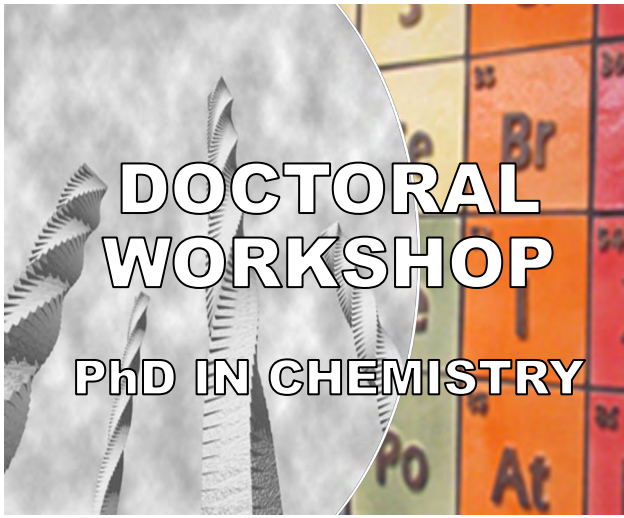
Contact:

Dr. Gregori Ujaque
PhD Coordinator of PhD studies in Chemistry

Elena Jiménez
Administrative Assistant PhD Studies in Chemistry
Telf.: 935811997, E-mail: gestio.postgrau.quimica@uab.cat
More information: https://www.uab.cat/ca/quimica

Where?

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).



29th - 30th of May
2nd of June
2023

Sala d'Actes
Faculty of Sciences

Departament of Chemistry

Facultat de Ciències UAB

Universitat Autonoma de Barcelona

May 29th

09:30 - 09:45 Welcome and opening

09:45 - 10:45 Plenary Lecture

Chair: Gregori Ujaque

Title: Chemistry beyond the Valence Shell
Prof. Javier García Martínez

10:45 - 11:45 Poste's session

11:45 - 13:00 Presentation's Session I

Chair: Xavier Sala

11:45-12:00 Machine Learning to Predict Adsorption Energies and Interatomic Potential Development. **Usuga, Andrés Felipe** 1.1
12:00-12:15 New plant-based nanovesicles based on alkyl polyglucosides surfactants and β-sitosterol as topical drug delivery Systems. **Alcaina Hernando, Marta**. 1.2
12:15-12:30 Polymerization of Porous Molecular Cages Through Covalent Chemistry: Synthesis, Functionalization, and Applications. **Khobotov Bakishev, Akim**. 1.3
12:30-12:45 Metal-Based Nanomaterials as Photo/Electro-Catalysts for Hydrogen Evolution Reaction and Intracellular Catalysis. Hou **Heting**. 1.4
12:45-13:00 Industrial Process Development to Manufacture a Highly Potent Active Pharmaceutical Ingredient. **Miranda Salinas, Ronnie Andres**. 1.5

13:00 - 15:00 Break

15:00 - 16:00 Presentation's Session II

Chair: Mireia Baeza

15:00-15:15 Computational studies and developments for chemical glycobiology: an overview of results and current developments. **Fernández-Luengo Flores, Xavier**. 2.1
15:15-15:30 Cerium-doped Magnetite Nanoparticles: Synthesis, Characterization and Catalytic Activity. **Mejía Carmona, Karen Stefanie**. 2.2
15:30-15:45 Functionalized silica nanostructures and cotton fabrics for topical biomedical applications. **Liu, Ming**. 2.3
15:45-16:00 New sensors based on microelectronic technologies for cell culture monitoring. **Moreno Díaz, Alexandre**. 2.4

16:00 - 16:30 Break and poster's session

16:30 - 17:30 Presentation's Session III

Chair: Félix Busqué

16:30-16:45 Synthesis of phosphorus dendrimers for applications in green solvent catalysis. **Cejas Sánchez, Joel**. 3.1
16:45-17:00 DELOS nanovesicles-based hydrogels as promising subcutaneous drug delivery systems. **Castellar Alvarez, Carla**. 3.2
1:00-17:15 7Microanalyzers' development for tracking key compounds in biotechnological processes for contaminants revalorization. **Paré Estalella, Franc**. 3.3
17:15-17:30 Multiscale Modelling of Heterogeneous Catalysts for CO2 Conversion. **Díaz López, Estefanía**. 3.4

May 30th

09:30 - 10:45 Presentation's Session IV

Chair: Jose Maria Muñóz

09:30-09:45 Screening of a Feasible Synthetic Route for an API-A. **Fazio Zalányi, Zeno**. 4.1
09:45-10:00 Catalytic activity of Cu/Mo2CTx: hydrogenation of CO2 and CO to methanol. **Vidal López, Anna**. 4.2
10:00-10:15 Towards the photocontrol of biological activity under two-photon excitation with near-infrared light. **Gómez Ventura, Marc**. 4.3
10:15-10:30 Selenium biofortification of Wheat Plants by Foliar Application of liposomes. **Viltres Portales, Marcia**. 4.4
10:30-10:45 Development of a Portable Paper-Based Electrophoretic Bioassay with Simultaneous Electrochemical Readout. **Maroli , Gabriel**. 4.5

10:45 - 12:00 Poster's session

12:00 - 13:15 Presentation's Session V

Chair: Rosario Núñez

12:00-12:15 Catalysis in supercritical CO2 with asymmetrically functionalyzed phosphorous dendrimers. **Petriccone, Massimo**. 5.1
12:15-12:30 Switchable MOP solubility through surface chemistry: engineering molecular self-sorting systems. **Hernández López, Laura**. 5.2
12:30-12:45 Green synthesis and processing of CaSyr-1 bioMOF: a potential drug delivery system with intriguing triple bioactivity. **Rosado Morente, Albert**. 5.3
12:45-13:00 Dithienylethene-based photoswitchable phosphines for in situ modification of catalysts. **Sherstiuk, Anastasiia**. 5.4
13:00-13:15 Novel bifunctional ligand scaffolds for stable and inert complexes as PET imaging contrast agents. **Torralba Maldonado, Daniel**. 5.5

13:15 - 15:30 Break

15:30 - 16:15 Presentation's Session VI

Chair: Carolina Gimbert

15:30-15:45 Se-biofortified microgreens as functional foods: phytochemical profile, bioactive properties, and Se speciation. **García Tenesaca, Marilyn Mishelle**. 6.1
15:45-16:00 Application of scale-up methodologies into industrial pharmaceutical processes. **Suriñach Ros, Amando**. 6.2
16:00-16:15 Theoretical Investigation on the Catalytic Performance of Pt3Mn Alloys in Propane Dehydrogenation to Propylene. **Zhang, Wenjuan**. 6.3

16:15 - 16:45 Break and poster's session

16:45 - 17:45 Plenary Lecture

Chair: Jose Peral

Title: Light-driven photocatalytic micromotors based on single-component semiconductors
Prof. Katherine Villa

17:45 - 18:00 Awards ceremony
Doctoral Workshop 2023 distinguished Diploma, along with a gift, will be given to the two best Poster & Presentation.

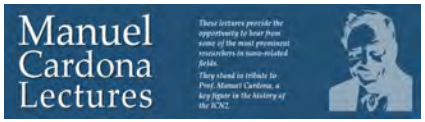
June 2nd

12.00 - 13:00 Lecture

Chair: Daniel Maspoch

Title: The Art of Building Small
from molecular switches to motors
Prof. Ben Feringa

Included within 2023 Manuel Cardona Lecture Series organized by the Catalan Institute of Nanoscience and Nanotechnogy (ICN2).



ICN2

13:00 - 13:15 Closing ceremony

Sponsored by:

RSEQ-Cat
Secció Territorial Catalana

SCQ
Societat Catalana de Química

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