2nd Workshop for Young Researchers in Chemistry

May 19th – 20th

Faculty of Chemistry

University of València

VNIVERSITAT DE VALÈNCIA Facultat de Química

Book contents

Welcome

Dear colleagues,

The organizing committee kindly welcomes you to the second edition of the Workshop for Young Researchers in Chemistry, which is being held in the Faculty of Chemistry of the University of Valencia.

This second edition, which was originally planned to happen in 2020 but had to be postponed due to the pandemic, will be held in person and in a similar way to the first edition.

The aim of this workshop is to share the research done by PhD students in the different fields of chemistry. This workshop is thought of as an excellent opportunity for every PhD student in chemistry to practice and give an oral communication in a friendly environment and, even, open new multidisciplinary collaboration lines between the different departments of the Faculty. Although the congress has been designed by and for PhD students, undergraduate or Master's students are also welcome to present their research in the format of a poster presentation.

We hope that this workshop is of interest to you, and that you enjoy your time with us.

Organizing committee

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- Inés Adam Cervera. Institut de Ciència dels Materials de la Universitat de València - ICMUV
- María Juliana Cuéllar Zuquin. Institut de Ciència Molecular - ICMol
- Azahara Doncel Gimenez. Institut de Ciència Molecular - ICMol
- Daniel Gaviña Rueda. Departament de Química Orgànica
- Belén Lerma Berlanga. Institut de Ciència Molecular - ICMol
- Miriam Navarrete Miguel. Institut de Ciència Molecular - ICMol
- Mireia Pérez Baeza. Departament de Química Analítica
- Raquel Rubert Albiol. Institut de Ciència Molecular - ICMol
- Roberto Sáez Hernández. Departament de Química Analítica
- Paz Sebastiá Luna. Institut de Ciència Molecular - ICMol
- Ricardo Torán Muñoz. Departament de Química Orgànica

Coordination

- Prof. Dr. Begoña Milián Medina. Departament de Química Física
- Prof. Dr. Rafael Ballesteros Garrido. Departament de Química Orgànica

Workshop structure and program

19 th of May

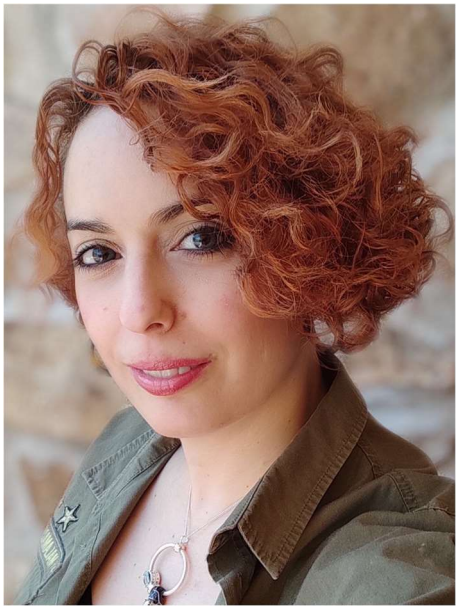
14:30 h	**Registration**	
15:00 h	**Opening**	
Session 1. Chair: Paz Sebastiá		
15:30 h	**L1**	**Johannes Gierschner: Scientific Misconduct in Current Chemistry Research: Aspects and Conditions**
16:00 h	OC1	**Alejandro Orellana:** An Excellent MOF Precursor of New Series of Spin-Crossover Clathrates via Single Crystal to Single Crystal Transformation
16:15 h	OC2	**Javier Carmona:** Photochemical reactivity of atmospheric sulfur compounds of interest in solar geoengineering
16:30 h	OC3	**Álvaro Seijas:** Covalent modification of layered double hydroxide to modulate their physical and chemical properties
Session 2. Chair: Juliana Cuéllar		
16:45 h	OC4	**Ana Rubio:** Exploring metal-based reactivity in Heterometallic Titanium-Organic Frameworks
17:00 h	OC5	**Antonio Hernández:** The role of the functional groups in the structure and properties of anilato-based Dy(III) SIMs
17:15 h	OC6	**Azahara Doncel:** Theoretical insights on self-assembling and optical properties in N-annulated perylene Bisimides aggregates
17:30 h	**Coffee break & Poster session**	
Session 3. Chair: Daniel Gaviña		
18:00 h	OC7	**Belén Lerma:** Exploiting tetrazine tags to enrich pore complexity: from pyridazine networks to fulleretic materials
18:15 h	OC8	**Cristina Rodríguez:** Batch and flow synthesis of CeO2 nanomaterials using solid state microwave generators
18:30 h	OC9	**Adrián Laviós:** Metal-free asymmetric dearomatization of 2-nitrobenzofuranes via formal [3+2] cycloaddition reactions with isocyanoacetates
18:45 h	OC10	**Paula Escamilla:** A new Zn-MOF used for catalysis and as supported to form Pd- and Ag-SACs
Session 4. Chair: Belén Lerma		
19:00 h	OC11	**Ismael Fernández:** Contactless passivation in metyalammonium lead bromide single crystal
19:15 h	OC12	**Milorad Andelkovic:** Computational Study of the Reaction Mechanism and the Active Form of Human L-Asparaginase (hASNase3)
19:30 h	OC13	**Pau Congost:** Deciphering the biomedical performance of antimonene in correlation with is chemical evolution under biological conditions
19:45 h	OC14	**Ricardo Torán:** Asymmetric organocatalytic arylation of isoxazolin-5-ones with ortho-benzoquinone diimides

20 th of May

Session 5 Chair: Mireia Pérez		
9:00 h	OC15	**Jaume Noguera:** Low-demanding in-situ crystallization method for tunable and stable perovskite nanoparticle thin-films.
9:15 h	OC16	**Javier Navarro:** Multivariate Metal-Organic Framework as a potential mimicker of active site of enzymes
9:30 h	OC17	**María Esteve:** Conductivity enhancement in a perylene-based MOF via iodine doping: A theoretical insight.
9:45 h	OC18	**Roberto Sáez:** A chemometric strategy to distinguish among roman pigments using colorimetric data
Session 6 Chair: Ricardo Torán		
10:00 h	OC19	**Carmen Fernández:** Incorporation of Gold Nanoparticles in Titanium-Organic Frameworks by dynamic methodologies
10:15 h	OC20	**Juliana Cuéllar:** Decomposition mechanism of the dioxetane derivate of the melanin DHICA-DO: A theoretical study
10:30 h	OC21	**Daniel Gaviña:** Development of the diastereoselective cross metathesis/cycloaromatization/Pictet-Spengler one pot reaction
10:45 h	OC22	**Pablo Navarro:** A superoxide dismutase mimetic nanozyme with outstanding antioxidant activity
11:00 h	**Coffee break & Poster session**	
Session 7 Chair: Roberto Sáez		
11:30 h	**L2**	**Elisa Fernández: Modificación de la Ley de Ciencia y aplicación de la Reforma Laboral en el sector de la investigación**
12:00 h	OC23	**Mireia Pérez:** Retention behavior and enantioresolution with polysaccharide-based chiral stationary phases and hydroorganic mobile phases of basic and neutral structurally unrelated chiral compounds
12:15 h	OC24	**Mireia Ruiz:** Coordination and removal of heavy metal ions by boehmite macrocyclic polyamines.
12:30 h	OC25	**Cristina Negro:** BioMOFs as Environmental Remediation: a Highly and Efficient Removal of Insecticides
12:45 h	OC26	**Raquel Rubert:** A Theoretical Insight on the Diradical Character of Dicyanomethylene π-Conjugated Compounds
Session 8 Chair: Raquel Rubert		
13:00 h	OC27	**M. Dolores Garrido:** Generalized “one-pot” preparative strategy to obtain highly functionalized silica-based mesoporous spherical particles
13:15 h	OC28	**Miriam Navarrete:** Theoretical study on the photoinduced repair mechanism of (6-4) photoproduct DNA lesions using oxetane models
13:30 h	OC29	**Jaume Rostoll:** Light-Driven Electrophilic Functionalization of Quinoxalin-2-ones
13:45 h	OC30	**Pablo F. Betancur:** Working mechanisms of photodetectors based on High a stable metal-halide perovskite nanocrystals composite with broad Frequency response.
14:00 h	**Lunch break**	
Session 9 Chairs: Azahara Doncel and Miriam Navarrete		
15:30 h	OC31	**Paola Zezza:** DNA-based Hydrogels for High-performance Microarray and Potential Optical Biosensing Application
15:45 h	OC32	**Rubén Turó:** Spin crossover modulation via guest interaction in 2D Hofmann-type coordination polymers
16:00 h	**L3**	**Round table: “Beyond the PhD”**
17:00 h	**Closure**	

Plenary lectures

Johannes Gierschner received his Ph.D. in Physical Chemistry at the University of Tübingen (UT), Germany, in 2000. After stays at UT, Univ. Mons (UMons), and at Georgia Tech, Atlanta, he joined the Madrid Institute for Advanced Studies - IMDEA Nanoscience - in 2008 as a Senior Research Professor (Ramón y Cajal fellow 2008-13). In 2014, he habilitated at UT and holds an Adjunct Professor position there since then. He is regular visiting researcher at University of Valencia (since 2014), and at Seoul National University (SNU) since 2008, and held an Adjunct Professor position at SNU and at UMons in 2014/15. His 140 papers (h = 49) integrate optical spectroscopy and computational chemistry to elucidate structure-property relationships in conjugated organic materials for optoelectronics and energy conversion. Besides his research, he is dedicated to consolidate the community knowledge through regular insightful, educative reviews, and is further committed to 'good scientific practice' student courses. Further information: www.uv.es/jogiers



Elisa Fernández Núñez. Responsable de comunicación y juventud de la Sección Sindical Estatal de CCOO en el CSIC. Licenciada en Biología con la doble especialidad de Genética y Biotecnología por la Universidad Complutense de Madrid y doctora en Biociencias Moleculares por la Universidad Autónoma de Madrid. Desde el año 2013, Técnica Superior Especializada del Consejo Superior de Investigaciones Científicas (CSIC) en el Instituto de Investigaciones Biomédicas “Alberto Sols”.

Scientific Misconduct in Current Chemistry Research: Aspects and Conditions

Johannes Gierschner[1*]

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In the past two decades, awareness of 'good scientific practice' has grown in universities and research institutions, in particular with the increasing cases of fraud and plagiarism, as well as with conflict of interest and authorship. Along with this, also more ethical questions were raised concerning human genetics, animal welfare and data protection, the abuse of confidence or funding, or diversity and gender issues. For these broader ethical concerns, commissions were established[1] and ombudswoman & -men are now frequently appointed,[2] while for scientific misconduct, safeguarding guidelines are readily available.[3,4,5] In any case, such rules usually focus on most obvious violations (like plagiarism and fraud)[6,7] while their increasing, and systematic occurrence provide evidence for a much deeper, inherent crisis in scientific research and publication.

The seminar intends to shed light on these less obvious, but more fundamental aspects of scientific misconduct, being the fertile soil on which the more apparent violations proliferate. Diving deeper below the 'tip of the iceberg', we will discuss examples from current chemical research, having direct practical implications for researchers in the early stage of their career.

In a broader sense, the current crisis in good scientific practice touches the self-conception of science, it's distinction from (in particular applied) research, and its significance in times of a rapidly changing society with grand challenges ahead. Hence, we will then turn to the underlying reasons for the increase of scientific misconduct in research, addressing societal conditions and the implications for science politics, which (partly inadvertently) foster the crisis.[8]

With this in mind, we finally draft fundamental elements of good scientific practice as guidelines for daily work of (young) researchers in (chemical) research.

References

[1] Universidad Valencia: Comité de Ética, https://www.uv.es/hrs4r/es/areas/aspectos-eticos/comite-etica-uv.html
[2] Universidad Valencia Vice-Rectora de Igualdad, Diversidad y Políticas Inclusivas, https://www.uv.es/uvweb/unidad-igualdad/es/unidad-igualdad-1285869753878.html
[3] German Science Foundation (DFG): Code of Conduct "Guidelines for Safeguarding Good Research Practice", see https://wissenschaftliche-integritaet.de/en/
[4] Universidad Valencia: "Código de Buenas Prácticas", https://www.uv.es/hrs4r/es/areas/aspectos-eticos/codigo-buenas-practicas.html.
[5] COPE - Committee on Publication Ethics: https://publicationethics.org
[6] *Teaching Scientific Ethics Using the Example of Hendrik Schön*, B. J. Feldman, US-China Education Review A **2012**, 4, 418.
[7] *Correcting the Scientific Record: Retraction Practices in Chemistry and Materials Science*, F.-X. Coudert, Chem. Mater. **2019**, 31, 10, 3593.
[8] **For further reading on some relevant aspects**, see e.g.
(a) *Blocking the Hype-Hypocrisy-Falsification-Fakery Pathway is Needed to Safeguard Science*, H. Hopf, S. A. Matlin, G. Mehta, A. Krief, Angew. Chem. Int. Ed. **2020**, 59, 2150.;
(b) *A Role for Funders in Fostering China's Research Integrity*, L. Tang, Science **2022**, 375, 979.;
(c) *To Err is Human; To Reproduce Takes Time*, S. L. Scott, T. B. Gunnoe, P. Fornasiero, C. M. Crudden, ACS Catal. **2022**, 12, 6, 3644.;
(d) *How the Scientific Method Invalidates "Fake News"*, M. Carlton, L. Leininger, in: *Teaching About Fake News: Lessons Plans for Different Disciplines and Audiences*, (Ed.: C. Benjes-Small, C. Wittig, M. K. Oberlies). ACRL **2021**.

Modificación de la Ley de Ciencia y aplicación de la Reforma Laboral en el sector de la investigación

Elisa Fernández Núñez[1*]

[1]Instituto de Investigaciones Biomédicas "Alberto Sols" CSIC-UAM, Madrid, Spain.
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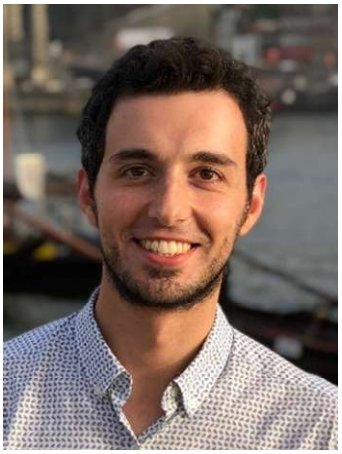
El año 2022 esta siendo un año de cambios normativos importantes relacionados con cuestiones laborales generales con la Reforma Laboral y, de manera específica en el ámbito la investigación, con la modificación de la Ley 14/2011 de la Ciencia, Tecnología e Innovación.

La modificación del Estatuto de los Trabajadores limitando la contratación temporal, junto a la derogación de la disposición adicional 23ª de la Ley 14/2011 de la Ciencia, Tecnología e Innovación, que mantenía al sector de investigación en una situación de estado de excepción laboral, ha generado la necesidad imperiosa de buscar una nueva fórmula de contratación en el Sistema Español de Ciencia y Tecnología (SECTI), que se ha hecho realidad con la reciente aprobación del Real Decreto-ley 8/2022, de 5 de abril, por el que se adoptan medidas urgentes en el ámbito de la contratación laboral del SECTI.

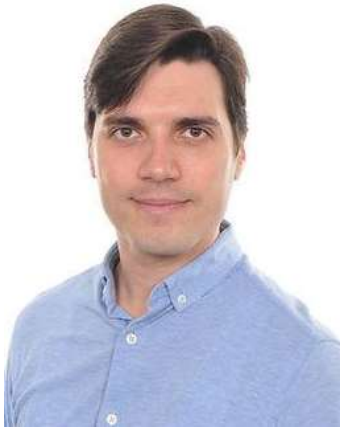
Por otro lado, la necesaria modificación de la Ley de la Ciencia, que el sector de la investigación lleva reclamando durante años, introduce cambios muy importantes en las condiciones laborales específicas del personal de investigación. Reconocimiento de derechos históricamente reclamados, sobre todo en el personal más precario, un nuevo modelo de contratación indefinida y una modificación en el diseño de carrera investigadora son recogidos en un texto aún pendiente de aprobar en las Cortes Generales. ¿Cuáles son estos cambios tan importantes? ¿Realmente va a cambiar tanto la vida del conjunto del personal de investigación? ¿Cómo afectan estos cambios a los estudiantes de doctorado? ¿Qué es lo que falta para tener la Ley de Ciencia que el sector de la investigación se merece?

Round table

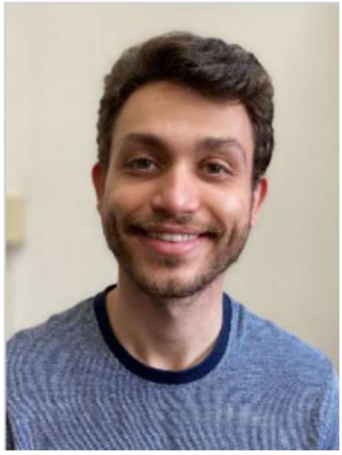
Beyond the PhD



Jose Alberto Carrasco obtained his degree in Chemistry from the University of Valencia in 2012. Afterwards, he achieved his master's degree in Nanoscience and Nanotechnology in 2014. From 2014 to 2018 he obtained a PhD in the group of Prof. Eugenio Coronado at the Institute of Molecular Science (ICMol), focused on the magnetic and catalytic properties of inorganic two-dimensional materials. After finishing his PhD, he achieved a master's degree in Secondary Education Teaching in 2019 and worked as a postdoctoral fellow both in the ICMol (2019-2020) and the Institue of Chemical Technology (ITQ, 2021). Now he is working in his true passion as a teacher of physics and chemistry, sharing his love for science to the younger generations.

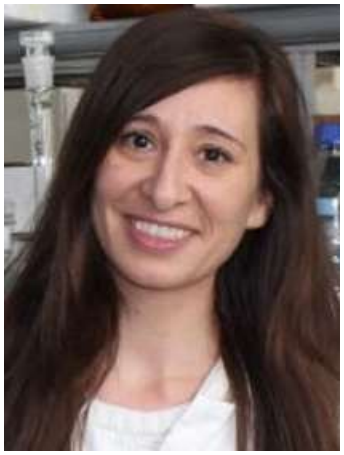


Javier Segarra-Martí obtained his PhD in theoretical chemistry and computational modelling at Instituto de Ciencia Molecular (ICMol) under the supervision of Prof. Manuela Merchán and Dr. Daniel Roca-Sanjuán in 2014. From 2014 to 2018 he worked in the group of Prof. Marco Gavarelli, first at the Università di Bologna and later on at the École Normale Supèrieure (ENS) de Lyon. In 2018 he joined Imperial College London as a Marie Curie Fellow, where he worked with Profs. Mike Bearpark and Mike Robb FRS. Since 2020 he has been back at ICMol initially as a Generació de Talent (GenT) Fellow, and currently as a La Caixa MSCA Postdoctoral Junior Leader Fellow, where he works in the broad topics of theoretical photochemistry and spectroscopy.



Javier Torres studied chemistry at the University of Valencia (UV) and obtained his B.Sc. degree in 2015. He studied the Master of Organic Chemistry at the UV in 2017. Since then, he has been the recipient of a predoctoral Fellowship from the Valencian ministry "Generalitat Valenciana" and has been carrying out PhD studies on the synthesis of natural products and the evaluation of biological activities of new frameworks in the Department of Organic Chemistry at the UV, under the supervision of Prof. Carlos del Pozo. Now, he is a professor in the private university "Universidad Europea de Valencia", in the dentistry and biotechnology degrees, in several subjects like "anatomy and physiology of the human body" or "Instrumental techniques laboratory".

Víctor Ignacio Costa Vayá. Since 2018, he is Director of the UBE Performance Chemicals Business Unit in the Atlantic area. He is responsible for the business strategy of various products produced in Europe and Asia by group companies and industrial partners, for sectors such as special materials in Automotive, Mining, Oil & Gas or intermediates in Flavours and Fragrances, Agrochemicals and Pharmaceuticals. He holds a degree in Chemistry (Extraordinary Career Award 1997) and a PhD in Chemistry, both degrees obtained at the Universitat de València. He also holds a Master's Degree in Business Administration and Management (ESIC, 2005).



Inmaculada Conejos Sánchez obtained her PhD in Organic Chemistry in the Chemical & Pharmaceutical Industry in 2013 at Centro de Investigación Príncipe Felipe. In July 2015, she was awarded with a Val i+d postdoctoral grant between her PhD lab and the Department of Clinical Neuroscience in the University of Cambridge (UK). Her project focused on the design, development and biological evaluation of novel non-viral gene delivery vectors for treatment of progressive forms of multiple sclerosis using siRNA as the bioactive molecule. In 2021 she was awarded the AECC Investigador grant for developing novel combination therapies for the treatment of pediatric solid tumors at the Hospital Sant Joan de Deu in Barcelona (Spain).

Oral contributions

OC1. Alejandro Orellana-Silla. An Excellent MOF Precursor of New Series of Spin-Crossover Clathrates via Single Crystal to Single Crystal Transformation

OC2. Javier Carmona García. Photochemical reactivity of atmospheric sulfur compounds of interest in solar geoengineering.

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OC32. Rubén Turó-Cortés. Spin crossover modulation via guest interaction in 2D Hofmann-type coordination polymers.

Poster contributions

P1. Cristian Martínez Hernández. Anilato-based heterometallic networks showing ferrimagnetic ordering and proton transfer.

P2. Francisco José Sierra Molero. Photo-Catalyzed Aerobic Oxidative Functionalization of 3,4-Dihydroquinoxalin-2-ones with Pyrazolones as Nucleophiles.

P3. Jordi Torró. Catalytic enantioselective addition of isoxazol-5-ones to aurone-derived 1-azadienes.

P4. Joan Vicent Estornell Martínez. Oxidative functionalization of 1,2,4,5-tetrahydro-1,4-benzodiazepine-3-ones.

P5. Cristina Pintado Zaldo. The impact of ethylene glycol versatility on magnetic properties and structure in anilato-based Single Ion Magnets.

P6. Víctor García García. Organophotoredox 1,6-addition of dihydroquinoxalin-2-ones to p-quinone methides using visible-light.

P7. Pablo García Aznar. Computational investigations on the reactivity of inverse electron-demand Diels-Alder reactions of fused-norbornenes with 3,6-dipyridin-2-yl-1,2,4,5-tetrazine.

P8. Laura Carceller Ferrer. Organocatalytic enantio- and diastereoselective cyclopropanation of alkylidenepyrazolones with bromomalonates.

P9. Marcos Escolano. Novel organocatalytic protocol to access chiral fluorinated indolizidines.

P10. Aitor Cubells Gómez. Holographic Surface Diffraction Gratings Made of Protein Hydrogels for Label-Free Biosensing.

P11. Murta Capella-Argente. From ladder to dimer, the size matters and from paramagnetic to single-ion magnets, lanthanoids make the difference.

P12. Lidia Prieto. Development of new anticancer agents: synthesis of combretastatin A4 analogues.

P13. Birgit Felderer. Quantification of THP-1 cells in medium measured in FT-IR Transflection.

P14. Kevin U. Antela. Development of a colorimetric device by using Arduino.

P15. Patricia García. Assessment of the inhalation uptake of MDMB-4en-PINACA using a smoking simulation chamber.

P16. Jaume Béjar Grimalt. Diagnosis of Prostate Cancer using IR spectroscopy and Machine Learning.

P17. Francisco López Moreno. Organocatalytic Enantioselective Double Michael Addition of Isoxazol-5-ones to Symmetric Dibenzalacetones.

P18. Jeanne Charollais. Theoretical study of the optical properties of a peroxynitrite generator activatable with red light.

P19. Belén Monforte Gómez. Improvement of Griess reaction for nitrite and nitrate determination in water samples with PDMS membranes and ZnNPs as reductor.

P20. Jose Luis Moreno Casillas. Miniaturized liquid chromatography of paracetamol.

P21. Alberto Llopis Lacruz. Chiral Functionalization of Polymer-Based Nanoparticles for Catalysis and Photocatalysis.

P22. Christian Rodríguez Boscà. Polymer Coatings with Nanoencapsulation of Organic Phase Change Materials for Thermal Energy Storage.

P23. Miguel Muñoz Bartual. Laser pointer activation for polimerization of paper-based devices.

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