

It is our great pleasure to welcome you to the "Vuitena Edició de les Jornades Doctorals" that are 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. In this eighth edition, the "Jornades Doctorals-2018" includes an exciting series of conferences by 3rd-4th year UAB-Chemistry PhD students and three lectures by academic experts.

**Prof. Dr. Christoph Janiak**, Full Professor at the Institute for Inorganic Chemistry and Structural Chemistry, University of Düsseldorf

Christoph Janiak obtained his PhD at the Technische Universität Berlin in 1987, followed by postdoctoral stays at Cornell University with Prof. Roald Hoffmann and at BASF AG, Ludwigshafen in the polyolefin division. Since 2010 he is full professor for Bioinorganic Chemistry and Catalysis at the University of Düsseldorf. Dr. Janiak has received several awards and is serving or has served on several Editorial and Advisory Boards. His main research interests are porous coordination polymers/metal-organic frameworks, metal nanoparticles also in ionic liquids, catalysis and supramolecular structural chemistry. He is co-author of about 420 journal publications, book chapters, text books and patents.

+ information: <http://www.janiak.hhu.de/>

**Prof. Dr. Guillem Aromí**, Aggregate Professor, Department of Inorganic and Organic Chemistry and Director of the Institute of Nanoscience and Nanotechnology (IN2UB)

Guillem Aromí graduated in Chemistry and Chemical Engineering at the University of Barcelona (UB) and EHICS (Strasbourg, France), respectively. He earned his PhD in Chemistry at Indiana University (USA) in 1999 and completed postdoctoral stays at Leiden and at Manchester Universities. In 2003 he became a "Ramon y Cajal" Fellow at the UB where he is Aggregate Professor of Chemistry since 2007. Dr. Aromí has been awarded the UB/Generalitat de Catalunya distinction for "enhanced research profile" and an ICREA Academia twice. He is also recipient of an ERC Starting Grant. His research interests focus on the design, synthesis and study of molecular functional materials and is coauthor of about 180 papers.

+ information: [https://www.gmmf-ub.com/who\\_we\\_are](https://www.gmmf-ub.com/who_we_are)

**Dra. Sílvia Osuna Oliveras**, ICREA Researcher Professor, Universitat de Girona

Sílvia Osuna received her PhD in 2010 from the University of Girona (UdG). In 2010, she moved to the group of Prof. Houk at the University of California, Los Angeles. She currently holds an ICREA research position at the Institute of Computational Chemistry and Catalysis (IQCC) at the University of Girona. Sílvia has more than 60 research publications and has received several awards such as that of the Royal Spanish Society of Chemistry, the Fundación Princesa de Girona and the EuCheMS Organic Division. Her main interest is the computational design of enzymes with potential medical applications, and is funded by a ERC- Starting Grant.

+ information: <http://iqcc.udg.edu/wordpress/portfolio/silvia-osuna/>

We look forward to your participation in this event.

#### Organizing, Scientific and Prizes Committee:

- Prof. Mariona Sodupe, PhD Coordinator of the studies in Chemistry and President of the Chemistry PhD Committee (UAB)
- Prof. Félix Busqué, Master Coordinator of the studies in Chemistry and President of the Chemistry Master Committee (UAB)
- Prof. Xavier Sala, Secretary of PhD and Master Studies Committee (UAB)
- Prof. Rosa M<sup>a</sup> Sebastian, Vocal of PhD and Master Studies Committee (UAB)
- Prof. Clara Viñas, Vocal of PhD and Master Studies Committee (ICMAB)
- Prof. Daniel Maspoch, Vocal of PhD and Master Studies Committee (ICN2)
- Jordi Creus, PhD Student, Department of Chemistry, (UAB)
- Luis Carlos Garzón, PhD student Department of Chemistry, (UAB)

#### Further information:

The Lectures and Flash Presentations will take place at **Sala d'Actes**, Faculty of Sciences

The Poster Exhibition and coffee break will take place at the **1st floor hall**, in front of the Sala de Juntes (next to the Sala de Graus), Faculty of Sciences

#### Contact details

Prof. Mariona Sodupe  
PhD Coordinator of PhD studies in Chemistry

Elena Jiménez Navau  
Administrative Assistant PhD Studies in Chemistry

Tel.: 935811997

E-mail: [gestio.postgrau.quimica@uab.cat](mailto:gestio.postgrau.quimica@uab.cat)

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## Department of Chemistry

May 30 to June 1, 2018

Sala d'Actes  
Faculty of Sciences

Universitat  
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Barcelona



# May, 30

10:00 - 10:15 Opening Ceremony

10:15 - 11:15 Jornades Doctorals Lecture

*Chairman: Prof. Daniel Maspoch*

“MOFs for water sorption for cycling heat transformation processes”.

**Prof. Dr. Christoph Janiak**

11:15 - 12:00 Coffee Break and Poster Session

12:00 - 13:00 Flash Presentations I

*Chairman: Prof. Daniel Maspoch*

12:00 - 12:15 Alternative Materials for Bio-sensing: Silk fibroin from *Bombyx mori*. **Augusto Márquez Maqueda** (FP1.1)

12:15 - 12:30 Synthesis of Metal-Organic Frameworks in Supercritical CO<sub>2</sub>. **Núria Portolés Gil** (FP1.2)

12:30 - 12:45 Novel Carborane-based Linkers for MOFs: Introduction of Flexibility and Reversible Single-Crystal Phase Transitions. **Fangchang Tan** (FP1.3)

12:45 - 13:00 Study of the regioselectivity of Prostaglandin G2 from Arachidonic Acid catalyzed by Cyclooxygenase-2: A Molecular Dynamics/QM/MM approach. **Anna Cebrián Prats** (FP1.4)

13:00 - 16:00 Break

16:00 - 17:30 Flash Presentations II

*Chairwoman: Prof. Rosa M<sup>a</sup> Sebastian*

16:00 - 16:15 Biomimetic core-canopy quantum dots: ions trapped in voids induce kinetic fluorescence switching. **Arpita Saha** (FP2.1)

16:15 - 16:30 INP@MOF Nanocomposites as NIR-Activated Drug Delivery Systems. **Gerard Boix i Soler** (FP2.2)

16:30 - 16:45 Metallacarboranes, a new electron acceptor generation. **Ana Begoña Buades Martín** (FP2.3)

16:45 - 17:00 Single-Crystal-to-Single-Crystal Solid-Gas Phase Postsynthetic Modification of Metal-Organic Frameworks via Ozonolysis. **Jorge Albalad Alcalá** (FP2.4)

17:00 - 17:15 HspX protein tuberculosis biomarker evaluated in sputum samples by plasmonic biosensing. **Enelia Cristina Peláez Gutiérrez** (FP2.5)

17:15 - 17:30 Development and optimization of a novel tooth whitening treatment. **Clara Babot Marquillas** (FP2.6)

# May, 31

10:00 - 11:00 Jornades Doctorals Lecture

*Chairwoman: Prof. Mariona Sodupe*

“Conformational heterogeneity in the evolution of enzyme function”.

**Dra. Silvia Osuna Oliveras**

11:00 - 11:45 Coffee Break and Poster Session

11:45 - 13:00 Flash Presentations III

*Chairwoman: Prof. Mariona Sodupe*

11:45 - 12:00 Rapid method for the detection of exosomes as a novel biomarker for cancer diagnosis. **Silio Lima de Moura** (FP3.1)

12:00 - 12:15 Sulfonated, trifluoromethylated and carboxylated triarylphosphines. Application in biphasic hydroformylation. **María de las Mercedes Cordón Acedo** (FP3.2)

12:15 - 12:30 NIRS and Chemometrics applied to challenging conditions in pharmaceuticals, forensics and biotechnology. **Aira Yira Miró Vera** (FP3.3)

12:30 - 12:45 Optimised azobenzene photoswitches for reliable two-photon neuronal excitation. **Gisela Cabré Segura** (FP3.4)

12:45 - 13:00 Designing water-soluble sulfonate and arginine-rich bioconjugated Cu(II) complexes with anticancer properties. A redox-active metallic core. **Joaquim Peña Aparicio** (FP3.5)

13:00 - 16:00 Break

16:00 - 17:30 Flash Presentations IV

*Chairwoman: Prof. Clara Viñas*

16:00 - 16:15 From Surface to Nanoparticles: Ruthenium Oxide (RuO<sub>2</sub>) Systems and Their Interaction with Water. **Javier Heras Domingo** (FP4.1)

16:15 - 16:30 Potential radiopharmaceuticals: “from synthesis to pre-clinical trials”. **Jordi Borrás Amoraga** (FP4.2)

16:30 - 16:45 Amperometric rGO-Nanocomposites Electrochemical Sensors Functionalized With Metal Nanoparticles. **Jordi Rodríguez Rodríguez** (FP4.3)

16:45 - 17:00 Optimisation Studies of Hard Carbon Negative Electrodes for Sodium Ion Batteries. **Enrique Irisarri Jiménez** (FP4.4)

17:00 - 17:15 Applications of the cyclobutane scaffold in new cell penetrating agents for drug delivery. **Jose Antonio Olivares Montia** (FP4.5)

17:15 - 17:30 Chemoselective polymerization using difunctional monomers: Towards polyacrylates with pendant cyanoacrylate moieties. **Cristina Monfort Fraga** (FP4.6)

# June, 1

10:00 - 11:00 Flash Presentations V

*Chairman: Prof. Xavier Sala*

10:00 - 10:15 The mechanism and adsorption study of Pine biomass and pyrolyzed Pine loaded with TiO<sub>2</sub> in aqueous solution. **Jingjing Zhao** (FP5.1)

10:15 - 10:30 A novel potentiometric microsensor for real-time detection of Irgarol using the ion-pair complex [Irgarol-H]<sup>+</sup>[Co(C<sub>2</sub>B<sub>9</sub>H<sub>11</sub>)<sub>2</sub>]. **Abhishek Saini** (FP5.2)

10:30 - 10:45 Printing technologies for biotechnological and environmental sensing applications. **Roberto Pol Arcas** (FP5.3)

10:45 - 11:00 Glycine polymerization catalyzed by the TiO<sub>2</sub> (101) anatase surface. **Stefano Pantaleone** (FP5.4)

11:00 - 11:45 Coffee Break

11:45 - 12:45 Jornades Doctorals Lecture

*Chairman: Prof. Xavier Sala*

“Solid State Transformations: A Gate to Polymorphism or Multi-stability in SCO Coordination Complexes”

**Prof. Guillem Aromi**

12:45 - 13:15 Award and closing ceremony

Jornades Doctorals 2018 distinguished Diploma, along with a gift, will be given to the three best Poster-Flash Presentations (Gifts: iPad for the 1st place, Bluetooth speaker for the second place and Wireless Headphones for the 3rd place). **Prizes awarded by HNA Group**

