

It is our great pleasure to welcome to the "Novena 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 ninth edition, the "Jornades Doctorals-2019" includes an exciting series of conferences by 3rd-4th year UAB-Chemistry PhD students and three lectures by academic experts.

**Prof. Dr. Javier Vela**, Professor, Chemistry Department, Iowa State University.

Dr. Javier Vela, professor of chemistry, received his B.S. with Honors from the National Autonomous University of Mexico (UNAM) in 2001. He then obtained M.S. and Ph.D. degrees working with Prof. Patrick L. Holland at the University of Rochester in 2003 and 2005, respectively. Before coming to Iowa State University, he was a postdoctoral research associate with Prof. Richard F. Jordan at the University of Chicago from 2005 to 2006, and a Director's Postdoctoral Fellow in the team of Jennifer A. Hollingsworth and Victor I. Klimov at Los Alamos National Laboratory's Center for Integrated Nanotechnologies from 2007 to 2009. Dr. Vela's current research focuses on the development of new nanostructured and optical materials for energy, catalysis, and imaging applications. Dr. Vela joined Iowa State University in 2009, and was promoted to full professor of chemistry in 2019. He has also served as Equity Advisor for the ISU College of Liberal Arts and Sciences (LAS).  
+ information: [https://www.chem.iastate.edu/faculty/Javier\\_Vela](https://www.chem.iastate.edu/faculty/Javier_Vela)

**Prof. Dr. Edwin Constable**, Professor of Chemistry, University of Basel .

Edwin (Ed Constable) completed his D.Phil at Linacre College, U. Oxford, followed by a number of research fellowships at the U. Cambridge. In 1993 he was appointed Prof. of Inorganic Chemistry at the U. Basel. He publishes over 600 publications (20,800 citations, h-index 72). He is a member of the steering committee of the European Universities Association Council for Doctoral Education and Chairman of the Swiss Academies Expert Group on Research Integrity and the European Universities Association Task Group on Research Ethics and Integrity. He is or has been on the Editorial Boards of numerous journals, including Chem. Commun., Chem. Rev., Chem. Soc. Rev., Coord. Chem. Rev., New J. Chem., Polyhedron and Supramolecular Chem. He is currently one of the editors in chief for "Comprehensive Coordination Chemistry III" and is on the Management Board of the Open Access Publisher MDPI. He has recently been appointed Editor-in-Chief for a new open access journal "Chemistry – an International Journal".  
+ information: <https://www.chemie1.unibas.ch/~constable/index.html>

**Prof. Dr. Prashant V. Kamat**, Professor of Science, Department of Chemistry and Biochemistry and Radiation Laboratory at the University of Notre Dame.

He earned his doctoral degree (1979) in Physical Chemistry from the Bombay University, and postdoctoral research at Boston University (1979-1981) and University of Texas at Austin (1981-1983). He joined Notre Dame in 1983. Professor Kamat has for more than three decades worked to build bridges between physical chemistry and material science to develop advanced nanomaterials that promise cleaner and more efficient light energy conversion. He has published more than 450 scientific papers (64000 citations, h-index 129). He is currently serving as the Editor-in-Chief of ACS Energy Letters. He has also served as the deputy editor of the Journal of Physical Chemistry Letters. He is a member of the advisory board of several scientific journals. He was awarded Honda-Fujishima Lectureship award by the Japanese Photochemical Society in 2006, CRSI medal by the Chemical Research Society of India in 2011 and Langmuir lectureship award in 2013.  
+ information: <https://www3.nd.edu/~pkamat/>

#### Organizing, Scientific and Prizes Committee:

- Prof. Gregori Ujaque, 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)
- Anna Cebrian, PhD Student, Department of Chemistry, (UAB)
- Arpita Saha, 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

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# JORNADES DOCTORALS

## Department of Chemistry

**May 22 - 24, 2019**

**Sala d'Actes**

**Faculty of Sciences**

**UAB**  
Universitat Autònoma  
de Barcelona

May, 22

09:30 -10:00 Opening Ceremony

10:00 - 11:00 Jornades Doctorals Lecture

*Chairman: Prof. Gonzalo Guirado*

**“Chemistry of Materials for Sustainability: From Halide Perovskites to Binary Metal Phosphides”**  
**Prof. Dr. Javier Vela**

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

12:00 - 13:00 Flash Presentations I

*Chairman: Prof. Javier Vela*

12:00 - 12:15 Nanoparticle Reactivity Beyond the Slab Approach: The BCN\_model platform and application to IrO<sub>2</sub> nanoparticles for Oxygen Evolution Reaction. **Danilo González Forero**, (FP1.1)

12:15- 12:30 Development of New Nanocarriers Based on Catechol Compounds for Biomedical Applications. **Carolina Casagualda Clapés** (FP1.2)

12:30 - 12:45 Influence of a Biostimulant on Se-enriching Wheat Plants. **Tingting Xiao** (FP1.3)

12:45 - 13:00 Photoactive Platinum(II) Complexes as Oxygen-Regulated Light-Triggered Photocages. **Kevin Morales Fernandez** (FP1.4)

13:00 - 15:30 Break

15:30 - 17:00 Flash Presentations II

*Chairwoman: Prof. Clara Viñas*

15:30 - 15:45 Synthesis and Catalytic Applications of Soluble Metal Nanoparticles. **Guillem Fernandez Freixes** (FP2.1)

15:45 - 16:00 Syntheses, Structures, and Properties of Carborane-based Cooper Metal Organic Frameworks. **Lei Gan** (FP2.2)

16:00 - 16:15 Water Determination in Parenteral Drug Products. **Laia Garcia Uceda** (FP2.3)

16:15 - 16:30 Synthesis of conformationally restricted cyclohexanyl nucleoside analogues as Antiviral Agents. **Sergio Jurado Moreno** (FP2.4)

16:30 - 16:45 Integrated Instrumental/Computational approach to study metal species binding to proteins. **Giuseppe Sciortino** (FP2.5)

16:45 - 17:00 Study of the Calcium Oxalate Hydrates Transformation and the role of the organic matter on their development by Synchrotron-based  $\mu$ -FTIR spectroscopy. **Iris Henríquez Valido** (FP2.6)

May, 23

10:00– 11:00 Jornades Doctorals Lecture

*Chairman: Prof. Xavier Sala*

**“Sustainable Materials Chemistry –Light-emitting electrochemical cells”**  
**Prof. Edwin Constable**

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

12:00 - 13:00 Flash Presentations III

*Chairman: Prof. Xavier Sala*

12:00 - 12:15 In vitro dental remineralization assisted by amelogenin. **Sandra Diez Garcia** (FP3.1)

12:15 - 12:30 Ru-Based Nanomaterials as Co-Catalyst with Carbon Nitride for Light-Driven Proton Reduction. **Luis Ignacio Álvarez Prada** (P3.2)

12:30 - 12:45 Simultaneous Voltammetric determination of Ascorbic Acid, Uric Acid and Acetaminophen by Use of modified screen-printed Electrodes and Chemometrics tools. **Dionisia Ortiz Aguayo** (FP3.3)

12:45 - 13:00 Implementing one-shot multiple-FID acquisition into homonuclear and heteronuclear NMR experiments. **Kumar Motiram Corral** (FP3.4)

13:00 - 15:30 Break

15:30 - 17:00 Flash Presentations IV

*Chairman: Prof. Felix Busqué*

15:30 - 15:45 Fluorinated Polyurethanes. **Miriam Laiz Treceño** (FP4.1)

15:45 - 16:00 New chiral schiff bases for asymmetric catalysis. **Jose Antonio Perez Mejias** (FP4.2)

16:00 - 16:15 Computational study of the transglycosylation reaction catalyzed by Glycoside Hydrolases and Glycosyltransferase. **Sonia Romero Tellez** (FP4.3)

16:15- 16:30 Obtention of value-added products from olive oil and wine production wastes through thermochemical treatments. **Cristina del Pozo Carvajal** (FP4.4)

16:30- 16:45 Towards novel electroinduced healing of polybenzoxazines. **Carolina Gascó Catalán** (FP4.5)

16:45 - 17:00 Functionalized mesoporous silica nanoparticles for catalytic and biomedical applications. **Hao Li** (FP4.6)

May 24

09:30 – 10:30 Jornades Doctorals Lecture

*Chairman: Prof. Gregori Ujaque*

**“Perovskite Photovoltaics. Research Opportunities and Challenges”**  
**Prof. Prashant V. Kamat**

10:30 - 11:15 Flash Presentations V

*Chairman: Prof. Gregori Ujaque*

10:30 - 10:45 Process development for the synthesis at industrial scale of a New Chemical Entity (NCE) drug for clinical trials. **Javier Santos Ramos** (FP5.1)

10:45 - 11:00 DFT mechanistic analysis of Alkene Cyclohydroamination of Primary amines catalysed by a Co(II) Complex. **PabloGómez-Orellana Seguí** (FP5.2)

11:00 - 11:15 Multistimuli-Responsive Fluorescent Switches Based on Spirocyclic Meisenheimer Compounds: Smart Molecules for Optical Probes and Electrochromic Materials. **Marc Villabona Pedemonte** (FP5.3)

11:15 - 12:00 Coffee Break

12:00 - 13:00 Jornades Doctorals Lecture

*Chairman: Prof. Gregori Ujaque*

**“The Art of Scientific Publication  
(How to Make Your Next Paper Scientifically Effective?)”**  
**Prof. Prashant V. Kamat**

**13:00 - 13:15 Award and closing ceremony.** Jornades Doctorals 2019 distinguished Diploma, along with a gift, will be given to the three best Poster -Flash Presentations (Gifts: E-book).