

Programme

Wednesday, 18th March

14.15 – 19.30: Plenary Session (ICIQ auditorium)

- 12.30 Registration
- 14.15 Plenary 1 **Fahmi Himo:** *Quantum Chemical Modeling of Enzymatic and Homogeneous Catalysis*
- 15.15 Keynote 1 **Ronny Neuman:** *Polyoxometalate Mediated Oxidative Transformations*
- 15.45 Keynote 2 **Anna Trzeciak:** *Palladium complexes of the type $[IL]_2[PdCl_4]$ as catalysts of organic reactions*
- 16.15 *Coffee break*
- 16.45 Poster flash presentations
- 17.15 Poster presentations
- 20.00 *Dinner* (optional at Hotel Ciutat de Tarragona)

Thursday, 19th March

8.45 – 12.45: Working Group Meetings

Working Group 1 (URV-Foundation)

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| 08.45 | WG1-1 | Marta Valencia: <i>Iridium-carbene-mediated activation of alcohols and amines</i> |
| 09.15 | WG1-2 | Vincent Vreeken: <i>C–H Activation of Benzene by a Photoactivated Ni^{II}(azide)</i> |
| 09.45 | WG1-3 | George Murray: <i>Direct Amination of Alcohols: Comparative Activity of Ruthenium-Pincer Complexes</i> |
| 10.15 | WG1-4 | Eva Zolnhofer: <i>An Intermediate Cobalt(IV) Nitrido Complex and its N-Migratory Insertion Product</i> |
| 10.45 | | <i>coffee break</i> |
| 11.15 | WG1-5 | Kalman Szabo: <i>Preparation and application of allylboronic acids</i> |
| 11.45 | WG1-6 | Markus Kinauer: <i>Square-planar Iridium(II-IV) Amido, Imido, and Nitrido Complexes</i> |
| 12.15 | WG1-7 | Chloe Thieuleux: <i>Preparation and characterization of single-site Ru-NHC supported catalysts: Application to bio-ressources transformation and CO₂ reduction</i> |

Working Group 2 (ICIQ library)

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| 08.45 | WG2-1 | Victor Laserna: <i>Organic Carbonates as Versatile Intermediates in Organic Chemistry</i> |
| 09.08 | WG2-2 | Mathieu Sauthier: <i>Conversion of polyols through the hydroesterification reaction: One phase and two phase catalysis</i> |
| 09.31 | WG2-3 | Sigridur Suman: <i>Synthesis of a Cobalt(II) Glutathione Complex</i> |
| 09.54 | WG2-4 | Rianne Lord: <i>Pacman” macrocycles: versatile ligands for coordination chemistry and their abilities in small molecule activation</i> |
| 10.17 | WG2-5 | Marte S Holmsen: <i>Au(III) complexes and their reactivity towards alkenes and alkynes</i> |
| 10.45 | | <i>coffee break</i> |
| 11.15 | WG2-6 | Luca Gonsalvi: <i>Hydrogen storage and release by bicarbonate-formic acid hydrogenation-dehydrogenation cycle catalysed by novel Fe and Ru complexes</i> |
| 11.38 | WG2-7 | Guillaume Lefèvre: <i>Efficient disproportionation of formic acid to methanol using molecular Ruthenium catalysts. Application to the methylation of aromatic amines</i> |

- 12.01 WG2-8 **Carman Claver:** *Immobilized Pd catalysts for C-C bond formation*
- 12.24 WG2-9 **Sara Realista:** *New binuclear transition metal complexes for CO₂ reduction*

Working Group 3 (ICIQ auditorium)

- 08.45 WG3-1 **Georg Britovsek:** *Activation of H₂ and CO for the Conversion of Syngas with Ruthenium PNP Complexes*
- 09.15 WG3-2 **Alceo Macchioni:** *Homogeneous and Heterogenized Iridium WOCs* **Alberto Bucci:** *An Iridium Complex as Functional Mimic of Both OEC and FNR*
- 09.45 WG3-3 **Johannes Messinger:** *First Turnover Analysis of Water-Oxidation catalyzed by Co-oxide nano-particles*
- 10.15 WG3-4 **Andrea Genoni:** *A molecular approach to light driven artificial photosynthesis*
- 10.45 *coffee break*
- 11.15 WG3-5 **Valerie Conte:** *Ferrocenylporphyrins: from synthesis to photoelectrochemical dioxygen activation*
- 11.45 WG3-6 **Aidan R. McDonald:** *Characterization and Reactivity of a Terminal Nickel(III)-Oxygen Adduct*
- 12.15 WG3-7 **Feliu Maseras:** *DFT studies on the mechanism of the photoinduced dioxygen insertion in a Pt-Me bond*
- 12.45 *Lunch*

14.15 – 16.15: intra-Working Group Meetings

iWG Synthesis (ICIQ auditorium)

- 14.15 iWG-1 **Beatriz Royo:** *Cyclopentadienyl Functionalized N-Heterocyclic Carbene Ligands: Synthesis and Coordination Chemistry*
- 14.45 iWG-2 **Julio Lloret-Fillol:** *Intermediates in Homogeneous Iron-Catalysed Water Oxidation*
- 15.15 iWG-3 **K. Kirchner:** *Chemistry based on non-precious metal PNP and PCP pincer complexes*
- 15.45 iWG-4 **Didier Bourissou:** *Ligand Design and Gold Reactivity: New Opportunities in Catalysis*

iWG Mechanism (ICIQ library)

- 14.15 iWG-5 **Carolina Gimbert -Surinach** : *Solar-driven water splitting: from molecular catalysis to functional devices*
- 14.45 iWG-6 **Koen van der Ham**: *In situ characterization of iron and copper based water oxidation catalysts*
- 15.15 iWG-7 **Martin Albrecht**: *What factors drive water oxidation at iridium carbene centers?*
- 15.45 iWG-8 **Giovanni Poli**: *Mastering Intramolecular Pd(II)-Catalyzed Aminations*

iWG Computational (URV-Foundation)

- 14.15 iWG-9 **Marten Ahlquist**: *Using theory to interpret experimental data on Ru and Ir intermediates*
- 14.45 iWG-10 **Emmanuel Nicolas**: *Frustrated Lewis Pairs as Ligands and in Catalysis: From Experiment Modelization to Catalyst Design*
- 15.15 iWG-11 **Claire Mc Mullin**: *Kinetics and Mechanisms of C-I Activation by Ru(II)-PPh₃ Complexes*
- 15.45 iWG-12 **Eric Clot**: *Experimental and Computational Studies of C-H and N-H Bond Activation in Amido-Zircononium Complexes*

16.15 *Coffee Break*

16.45 – 18.45: Plenary Session (ICIQ auditorium)

- 16.45 Keynote 3 **Pher Andersson**: *Development and Application of Iridium Catalysts for Asymmetric Hydrogenation of "Non-traditional" Substrates*
- 17.15 Keynote 4 **Bert Klein Gebbink**: *Oxidative cleavage of alkenes to carbonyl compounds using non-heme iron catalysts*
- 17.45 Plenary 2 **Deryn Fogg**: *The Paradoxically Inhibiting Effect of Strong NHC Donation in Catalysis: A Showcase Study in Olefin Metathesis*
- 20.00 *Conference dinner*

Friday, 20th March

9.15 – 10.45: Working Group Meetings

Working Group 1 (URV-Foundation)

- 09.15 WG1-8 **Augusti Lledos:** *Gold-catalyzed Hydroamination of C-C Multiple Bonds with Small Nucleophiles: Substrate and Ligand Effects*
- 09.45 WG1-9 **Nikolas Gorgas:** *Highly efficient and selective hydrogenation of aldehydes by a well-defined Fe(II) PNP pincer complex*
- 10.15 Networking

Working Group 2 (ICIQ library)

- 09.05 WG2-10 **M. D. Segarra-Maset:** *A Combined Approach to the Catalytic Formation of Acrylate from Carbon Dioxide and Ethene*
- 09.25 WG2-11 **Simona Mazza:** *Iron Catalysts for Hydrogenation of Aldehydes: an Alternative to Precious Noble Metals*
- 09.45 WG2-12 **Iban Azcarate:** *Optimization of the catalytic electrochemical reduction of CO₂ with electrogenerated iron(0) porphyrins*
- 10.05 WG2-13 **Labrini Sygellou:** *XPS characterization of the catalyst before and after the carbonylative Suzuki cross-coupling reaction*
- 10.25 WG2-14 **Barbara Milani:** *Unprecedented stereocontrol in Pd-catalyzed CO/vinyl arene polyketone synthesis*

Working Group 3 (ICIQ auditorium)

- 09.15 WG3-8 **Giulia Licini:** *Vanadium catalytic aerobic oxidative C-C bond cleavage/*
Cristiano Zonta: *Oxygen addition to double bonds. Can a carbonyl double bond become a nucleophile?*
- 09.45 WG3-9 **Gabor Speier:** *Oxidation/Oxygenation of Thiols and PPh₃ by ³O₂ Catalyzed by a Bioinspired Organocatalyst*
- 10.15 WG3-10 **Jernej Iskra:** *Template Catalysis in Fluorinated Alcohols for Activation of Oxidation*
- 10.45 *Coffee Break & Networking*

11.15 – 12.45: Plenary Session (ICIQ auditorium)

- 11.15 Keynote 5 **J.I. van der Vlugt:** *Redox-Active and Reactive Ligands – Attractive & Versatile Concepts for Small Molecule Activation and Much More*
- 11.45 Keynote 6 **Peter Fristrup:** *Molybdenum-Catalyzed Deoxydehydration of Polyols*
- 12.15 *concluding remarks*
- 12.45 *Lunch & departure*