## Wednesday 8th-March

| 09h10 | WG sessions | |
|---|---|---|
| 09h10 | André Pontes da Costa<br>Sorbonne Universités Paris<br>Pd-containing Core-Shell Nanogels: Application to the MizorokiHeck Reaction | Greco Gonzales Miera<br>Stockholm University<br>Redox Transformations Mediated by Ir(III) Complexes with bifunctional N-Heterocyclic Carbene ligands |
| 09h30 | Sara Realista<br>Universidade de Lisboa<br>Capture and activation of CO2 using multifunctional metal-organic materials | Jordi Creus<br>Universitat Autònoma de Barcelona<br>Ru-based catalyst for energy related transformations |
| 09h50 | Mathieu Sauthier<br>Université Lille<br>Nickel catalyzed allylation reactions with allyl alcohol | Ignacio Funes<br>Inst. of Chemical Research of Catalonia (ICIQ)<br>The Single Electron Transfer Mechanism for Oxygen-Oxygen Bond Formation in Copper-Based Water Oxidation Catalysis |
| 10h10 | Anna Trzeciak<br>University of Wroclaw<br>In situ generated Pd(0) nanoparticles stabilized by bis(aryl)acenaphthenequinone diimines as catalysts for aminocarbonylation reactions in water | Blaz Likozar<br>National Institute of Chemistry<br>Noble Metal Catalysts' Activity, Selectivity and Stability for Lignin, Cellulose and Hemicellulose Compound Conversion |
| 10h30 | coffee break | |
| 11h00 | WG Session | |
| 11h00 | Mats Tilset<br>University of Oslo<br>Functionalization of Ethylene and Acetylene at Au(III) Complexes | Andrea Squarcina<br>Università degli studi di Padova<br>Merged Heme and non-Heme Manganese Co-factors for a Dual Anti-Oxidant Surveillance |
| 11h20 | Pher Andersson<br>Stockholm University<br>Regio- and enantioselective hydrogenation of 1,4-dienes | Nadia Zanetti<br>University of Graz<br>Mo and W complexes for the activation of $O_2$ and $C_2H_2$. Reactivity towards Lewis acids. |
| 11h40 | Zahra Mazloomi<br>Universitat Rovira i Virgili<br>Syntesis and catalytic application of heterodonor mesoionic carbene iridium complexes. | Lucia Fagiolari<br>University of Perugia<br>Gabriel Menendez<br>University of Perugia |
| 12h10 | Nikolaus Gorgas<br>University of Technology Viena<br>Synthesis, Characterisation and Catalytic Application of non-classical Iron Polyhydride Complexes supported by PNP-pincer ligands | Toni Llobet<br>Inst. of Chemical Research of Catalonia (ICIQ)<br>Rational Design of Efficient and Robust Molecular WOCs |

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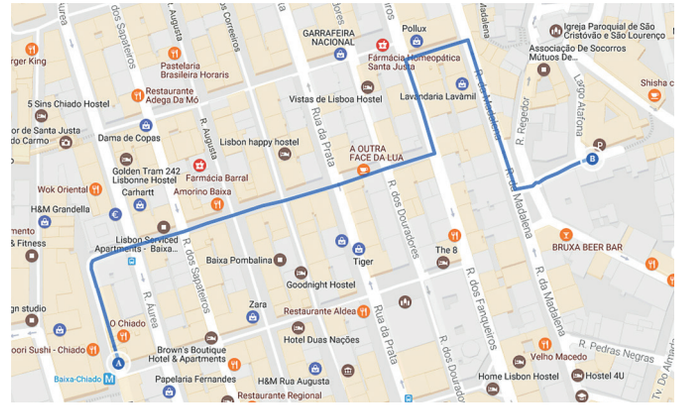
| 12h30 | LUNCH & NETWORKING |
| 14h00 | PLEANARY SPEAKER<br>Sebastien Bontemps<br>CNRS Toulouse<br>Controlled $CO_2$ Reduction:<br>a Path Toward Inorganic Calvin Cycle? |
| 14h50 | KL4 Karl Kirchner<br>Vienna University of Technology<br>Environmentally Benign Reactions Catalyzed by Well-Defined Manganese and Iron Complexes |
| 15h20 | coffee break |
| 15h50 | KL5 Luca Gonsalvi<br>CNR-ICCOM<br>Recent Advances on the Use of the Carbon Dioxide - Formic Acid Cycle as a Carbon-Neutral Approach to Hydrogen Storage and Delivery |
| 16h20 | Carmen Claver<br>University Rovira i Virgili<br>Catalysis for Sustainable Development<br>Homogeneous Catalysis and Nanocatalysis |
| 16h45 | Martin Albrecht (MC Chair) / Giulia Licini (Vice Chair)<br>CARISMA |
| 17h20 | Luca Gonsalvi<br>ICOMC 2018 Presentation |
| 20h30 | CONFERENCE DINNER |

**PATHWAY FROM CHIADO** SUBWAY TO **ZAMBEZE** RESTAURANT

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# 5th COST CARISMA meeting 2017

## 6-8 mar · lisbon

## Catalytic Routines for Small Molecule Activation

cost EUROPEAN COOPERATION IN SCIENCE AND TECHNOLOGY

COST is supported by EU framework initiative Horizon 2020

CARISMA

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# MONDAY 6th March

**12h00** — **MC MEETING**

**12h45** — **REGISTRATION & LUNCH**

**14h00** — **WELCOME**

**PLENARY SPEAKER**
Tim Storr
Simon Fraser University
Electronic Structure and Reactivity of Oxidized Metal Phenoxides

**15h00** — KL1: Thibault Cantat
CNRS, Université Paris-Saclay
Catalytic Strategies for the Reductive Functionalization of $CO_2$

**15h30** — coffee break

**16h00** — **STSM PRESENTATIONS**
Carla Casadevall
Cristiano Glessi
Claudia Miceli
Zahra Mazloomi
Angela Vivancos
Nikolaus Gorgas

**17h00** — KL2: Marten Ahlquist
KTH Royal Institute of Technology Stockholm
Interaction of Water with Ru Water Oxidation Catalysts

**17h30** — KL3: Karsten Meyer
University Erlangen-Nürnberg
From high-valent metal nitrides to a pentad of low-valent iron nitrosyls $[Fe\text{-}NO]^{6-10}$

# TUESDAY 7th March

**09h00** — **WELCOME** by Barbara Milani | **WELCOME** by Toni Llobet

| | WG2 sessions | WG3sessions |
|---|---|---|
| 09h10 | Polly Arnold<br>University of Edinburgh<br>f-block complexes for multiple electron reductive activation;two metals are better than one | Jernej Iskra<br>University of Ljubljana<br>Multiple Catalysis for the Aerobic Oxidation of Alcohols – Nitric Acid, Iron(III) and Fluorinated Alcohol |
| 09h30 | Erwan Le Roux<br>University of Bergen<br>Tridentate N-Heterocyclic Carbene Complexes of Group 4: Structures, Reactivity and Activity in the Copolymerization of Epoxides with $CO_2$ | Giulia Licini<br>University of Padova, Italy<br>Vanadium Catalyzed Aerobic Oxidative Processes for Lignin Depolymerization |
| 09h50 | Claudio Cometto<br>Université Paris Diderot<br>Selective Photochemical and Electrochemical CO2 to CO conversion by [Fe (2,2':6',2'':6'',2'''-quaterpyridine)$(OH_2)_2$]$^{2+}$ | Konstantin Kottrup<br>Leiden University<br>Iron-based complexes as electrocatalysts for water oxidation |
| 10h10 | Martin Prechtl<br>Universität zu Köln, Cologne<br>Future Perspectives for Formaldehyde: Pathways for reductive synthesis and energy storage | George Britovsek<br>Imperial College London<br>Ethylene Oligomerisation Beyond Schulz-Flory Distributions |
| 10h30 | coffee break | |
| 11h00 | Vera Rosar<br>University of Trieste<br>Pd-catalyzed CO/vinyl arene copolymerization: when the comonomer controls the stereochemistry | Bert Klein Gebbink<br>Utrecht University<br>Proton and electron responsive ß-diiminates: studies of redox activities in transition metal complexes |
| 11h20 | Lindsey Monger<br>University of Iceland<br>Reactivity of a novel Pd(II) complex with alkene carbon monoxide | Chloe Thieuleux<br>Université de Lyon<br>From organometallic complexes to metallic nanoparticles: Application to the preparation of heterogeneous catalysts |
| 11h40 | Blanca Martin-Vaca<br>Université Paul Sabatier<br>Efficient conversion of $CO_2$ to oxazolidinones with Indenediide Palladium Pincer Complexes | Bastian Schlusschass<br>Universität Göttingen<br>Dinitrogen Splitting Triggered by Protonation |
| 12h00 | Claudia Miceli<br>Università degli Studi di Padova<br>Vanadium(V) aminotriphenolate complexes as effective catalysts for epoxide activation | Urs Gellrich<br>Weizman Institute of Science Rehovot<br>Reversible aromaticity transfer in a bora-cycle: Boron-ligand cooperation |
| 12h20 | Sergio Sopena<br>Institute of Chemical Research of Catalonia (ICIQ)<br>Regioselective Organocatalytic Formation of Carbamates from Substituted Cyclic Carbonates | Colin Diner<br>Stockholm University<br>Catalytic asymmetric allylboration of cyclic imines for the stereodivergent synthesis of prenylated indolines and tetrahydroisoquinoline |

**12h40** — **LUNCH & NETWORKING**

**14h00** — **POSTER FLASH PRESENTATIONS & POSTER SESSION**

**16h00** — coffee break

| 16h30 | iWG syn | iWG compu | iWG Mech (6x20 mins) |
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| 16h30 | Kalman Szabo<br>Stockholm University<br>Asymmetric Allylation with Allylboronic Acids | Yavuz Dede<br>Gazi University<br>Proton Transfer without the Secondary Sphere Base: A Theoretical Study Towards a Functional Model of Homoprotocatechuate Dioxygenase Enzyme Active Site | Carla Casdevall<br>Institute of Chemical Research of Catalonia (ICIQ)<br>A new N-pentadentate iron (II) complex as an active homogeneous catalyst for water oxidation |
| 17h00 | Pedro Perez<br>Universidad de Huelva<br>Coinage metal based catalysts for C-C and C-N formation | Rositha Kunyil<br>Institute of Chemical Research of Catalonia (ICIQ)<br>Salient Role of Counterion in the Carboxylation of DSiloxysilanes via Brook Rearrangement – A DFT Study | Andrea Prevedello<br>University of Padova<br>Heterogeneous and homogeneous routes in copper based water oxidation catalysis |
| 17h30 | Chris Slootweg<br>University of Amsterdam<br>Circular Chemistry | Feliu Maseras<br>Institute of Chemical Research of Catalonia (ICIQ)<br>Computational characterization of a photoinduced dioxygen insertion | Pablo Garrido Barros<br>Institute of Chemical Research of Catalonia (ICIQ)<br>Improving the Activity Toward Water Oxidation with Heterogenized Molecular Copper Catalyst |
| 18h00 | Xile Hu<br>Ecole Polytechnique Fédérale de Lausanne<br>Nickel pincer complexes as hydrosilylation catalysts and enzyme mimics | Vidar Jensen<br>University of Bergen<br>Automated Design of Functional Organometallic Complexes | Marta Valencia<br>Universität Bern<br>Triazolylidene Iridium Complexes for Amine Recognition and Acceptorless Dehydrogenation |
| | | | Samuel Martinez-Erro<br>Stockholm University<br>From Allylic Alcohols to Halogenated Carbonyls: Metal- and Organocatalyzed Approaches |
| | | | Soosan Hosseinmardi<br>Friedrich-Alexander University<br>Synthesis and Characterization of Cubanoid Manganese, Cobalt and Nickel Complexes and Their Application for Water Oxidation Catalysis |