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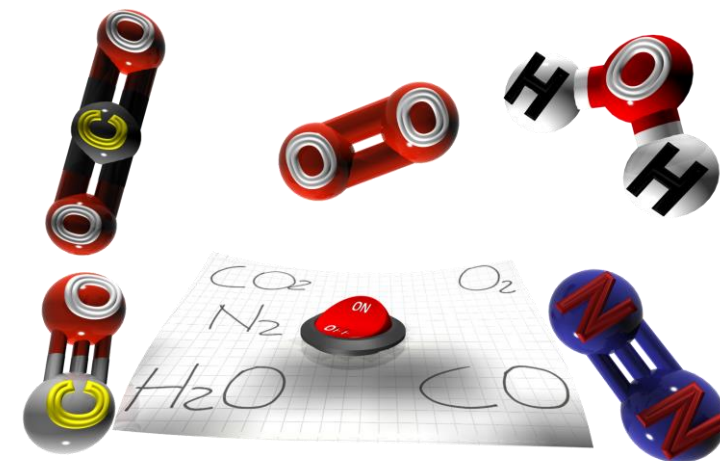
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Small Molecules Activation

*Workshop of the Joint Doctoral
Programme in Chemistry*



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Invited speakers

Prof. Matthias Beller
Leibniz-Institut für Katalyse, Rostock

Prof. Alessandro Fortunelli
CNR-ICCOM, Pisa and Caltech, Mat. & Proc. Simulat. Ctr, Pasadena,
CA, USA

Prof. Arjan Kleij
ICIQ-Tarragona, Spain

Prof. Thibault Cantat
Institut Rayonnement-Matière de Saclay (IRAMIS)

February 15th and 16th 2018

**Aula Magna Ca' Dolfin
Università Ca' Foscari Venezia**

Small Molecules Activation

Humankind heavily depends on fossil fuel resources which however, will become severely limited in the near future. Sustainability is one of the pillars for the current and the upcoming development of our society. In this context, a great deal of attention from the scientific community is addressed to the discovery of new alternative, environmentally friendly, strategies to tackle the sustainable synthesis of chemicals and the energy production.

One of the main tools to achieve this ambitious target is based on the activation of small molecules including H₂, O₂, H₂O, CO₂, CO, N₂, and NH₃, which may act as sources of H, O, C, and N, respectively, to build up useful compounds and intermediates.

Due to their intrinsic stability, small molecules require highly efficient activation approaches which pose a fascinating, though challenging, issue that gains interest from both the academic and the industrial standpoints. The integration of inter-sectorial expertise within chemical and physical-chemical areas is pivotal to address this topic.

The Organizing Committee

Thursday February 15th 2018

11:00 **Welcome opening**

11.15 - 13.00 **Conference**

Prof. Matthias Beller

Leibniz-Institut für Katalyse, Rostock

Small Molecules Activation: Teaching Non-Noble Metals to Replace Precious Catalysts

13.00 **Lunch**

14.30 - 16.15 **Conference**

Prof. Alessandro Fortunelli

CNR-ICCOM, Pisa and Caltech, Mat. & Proc. Simulat. Ctr, Pasadena, CA, USA

Computational Modeling of Small Molecule Activation: Oxygen Reduction Reaction and Haber-Bosch

16.15 - 16.45 **Coffee break**

16.45 - 18.30 **Conference**

Prof. Arjan Kleij

ICIQ-Tarragona, Spain

Catalytic Valorization of Carbon Dioxide and Beyond in Organic Chemistry Space

Dinner

Friday February 16th 2018

9.00 - 10.45 **Conference**

Prof. Thibault Cantat

Institut Rayonnement-Matière de Saclay (IRAMIS)

Catalytic Strategies for the Reduction of C–O Bonds in CO₂ and Lignin

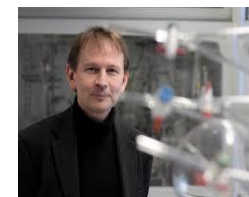
10.45 - 11.15 **Coffee break**

11.15 - 12.45 **Meeting groups**

12.45 **Concluding remarks**

13:00 **Lunch**

Matthias Beller works in Rostock as Director of the Leibniz-Institut für Katalyse. The work of his group has been published in >800 original publications, reviews and >90 patent applications. He has received several awards including the Leibniz-Price of the DFG, the Paul-Rylander Award of the Organic Reaction Catalysis Society of the USA. In 2006 he received the German Federal Cross of Merit. Besides he received the first "European price for Sustainable Chemistry". He was awarded honorary doctoral degrees from the University of Antwerp and the University of Rennes.



Alessandro Fortunelli is Senior Researcher at CNR-ICCOM, Pisa and Visiting Associate at Caltech, CA, USA. Research interests: Theoretical description and predictive simulation of chemical and physical systems and processes of interest in (photo- and electro-)catalysis, optics, magneto-optics, and materials science; Development of global optimization (GO) algorithms for exploring multi-dimensional phase spaces with rugged potential energy surfaces; Development of the Reactive Global Optimization (RGO) approach for structural dynamics of activated kinetics-driven stochastic processes; Nanostructured metal systems and 2D oxide materials.



Arjan Kleij worked as Group Leader at ICIQ since 2016 and joined ICREA as a junior fellow, where he was promoted to ICREA professor in 2011. He has (co)authored around 160 international journal publications and 2 patent applications. He is an advisory board member for Current Organic Chemistry (since 2014), ChemSusChem (since 2016), and member of the editorial board for the Journal of CO₂ Utilization (since 2017), and Molecules (since 2017), and he is also associate editor for Frontiers in Chemistry (2017). He was invited guest-editor for Catalysis Science & Technology in 2014 and ChemSusChem in 2017 arranging special issues on CO₂ catalysis.



Thibault Cantat started a research group focused on the activation and recycling of CO₂, at CEA Saclay, after he held a joint Director's Postdoctoral position at Los Alamos National Laboratory (USA) in the groups of Dr. J. Kiplinger and Dr. P.J. Hay. He was awarded with the Grand Prix Scientifique of the Louis D. Foundation by the Institut de France (2013) and was granted a Starting Grant by the ERC in 2013. The general topic of his research is the development of novel catalytic reactions for the efficient reduction of CO₂ and biomass. His research interests therefore span organometallic chemistry of the transition metals and the f-elements to homogenous catalysis and computational.

