

Symposium

Clusters, nanoparticles and nanostructures in catalysis and beyond

Computational Material Science Laboratory, Institute of Theoretical and Computational Chemistry (IQTCUB), Universitat de Barcelona, Room 400 (4th floor, Chemistry building), c/ Martí i Franquès 1, 08028 Barcelona

June 27th, 2014

9:20 *Welcome: Francesc Illas (Director of the IQTCUB), Konstantin Neyman*

9:30 **Sergey M. Kozlov, Konstantin M. Neyman**

Universitat de Barcelona / ICREA, Barcelona, Spain

Studies of Nanostructuring Effects on Model Catalysts

10:20 **Anastassia Alexandrova**

University of California, Los Angeles, USA

Surface-Deposited Clusters for Catalysis through the Prism of Chemical Bonding

11:10 *Refreshments*

11:40 **Alberto Córdoba, Pilar Ramírez de la Piscina, Narcís Homs**

Catalonia Institute for Energy Research (IREC), Dept. de Química Inorgànica and Institut de Nanociència i Nanotecnologia, University of Barcelona, Spain

Nanostructured Pt/TiO₂ Systems as Photocatalysts for H₂ Production

12:10 **Francesc Illas**

Universitat de Barcelona, Barcelona, Spain

Modelling Realistic Supported Catalysts

13:00 *Lunch break*

15:00 **Mark Saey**

University of Ghent, Belgium

Operando Computational Catalysis: Structure and Coverage of Co Catalysts during Fischer-Tropsch Synthesis

15:50 **Alexander I. Boldyrev**

Utah State University, USA

Deciphering Multicenter Bonding in Molecules, Clusters, 2D-Systems, and Solids

16:40 **Stefan T. Bromley**

Universitat de Barcelona / ICREA, Barcelona, Spain

From Supported Oxide Nanoclusters to Nanoporous Oxide Polymorphs

17:15 *Closure*