

## Scientific Report

Chemistry and Molecular Sciences and Technologies

### COST Action CM1104

*Reducible Oxide Chemistry, Structure and Functions*

*Working Groups 1-Fundamentals and 3-Reactivity Meeting*

*April 18-19, 2013*



*Vienna University of Technology, Vienna, Austria*

#### **Organizers:**

- **Günther Rupprechter – local organizer**  
**Vienna University of Technology, Vienna**
- **M. Verónica Ganduglia-Pirovano – WG1 coordinator**  
**Institute of Catalysis and Petrochemistry-CSIC, Madrid**
- **Jörg Libuda – WG3 coordinator**  
**University of Erlangen-Nuremberg**

The aims and activities of Working Groups 1 and 3 are closely interrelated. The objective of Working Group 1 is to have a fundamental atomic scale understanding of the structure, electronic, magnetic and chemical properties of reducible oxide systems, as well as to elucidate the origin of their reducibility changes (doping, film thickness, particle size, nature of the support, surface exposed, density of defects, etc.) in connection to their functionalities, with a strong focus on establishing close cooperations between experimental and theoretical studies. Working Group 3, on the other hand, aims at an atomic level understanding of surface chemistry on reducible oxides. Similarly as in Working Group 1, this includes both experimental and theoretical studies, specifically focussing on the elucidation of surface reaction mechanisms and microkinetics. In particular, mastering complexity in multi-component oxide materials is the primary challenge here. Several joint activities and cooperations have already been established within the working groups. In order to promote synergies between the two working groups, the 2013 workgroup meeting of the two groups has been organized as a joint event.

The meeting was locally organized by Günther Rupprechter (member of Working Group 3) in close connection with the respective Workgroup Coordinators (M. Verónica Ganduglia-Pirovano for Working Group 1, Jörg Libuda for Working

Group 3). It was held on April 18<sup>th</sup> and 19<sup>th</sup> at the Vienna University of Technology (Prechtlsaal). Due to its joint character the meeting was comparably large with approximately 60 participants. As an invited expert, Edvin Lundgren (Lund, Sweden) presented an overview over novel in-situ methods in model catalysis. A total of 26 talks were given by members of the two working groups, again a relatively large number that resulted from the idea of giving all participating research groups the opportunity to present their work and hence possibly increase connections between the COST Action members. In addition a total of 24 posters were presented (see Book of Abstracts).

As documented by the oral and poster contributions, there was a clear and strong connection between several experimental and theoretical participant groups, applying state-of-the-art approaches toward a microscopic-level understanding of the chemical and physical processes at oxide surfaces. Furthermore, the specific properties of reducible-oxide-supported metal clusters and nanoparticles and in situ studies at ambient pressure received considerable attention. Already at the present stage, several contributions were reporting on joint activities between several COST partners, illustrating the level of cooperation activities which have been achieved already. Concerning the materials, a strong focus was on the reducible oxides ceria and titania, however, new ideas and concepts were presented on alternative reducible oxide materials such as cobalt oxides. The latter research line is of particular interest toward the aims of the action, as it represents a strategy to replace critical materials, e.g., in catalytic applications.

In spite of the intense program, a lively atmosphere could be created fostering new interactions and intense and vivid discussions, e.g., during poster sessions, joint lunch on both days, and a joint conference dinner. The response of the participants to the meeting was very positive, making it a successful start for further workgroups or annual meetings during the course of the Action.



## List of Participants

Aleksandrov	Hristiyan A.	University of Sofia	Bulgaria
Broqvist	Peter	Ångström Laboratory, Uppsala University	Sweden
Bruix	Albert	Universitat de Barcelona, Barcelona, Spain	Spain
Carrasco	Javier	Instituto de Catalis y Petroleoquimica, CSIC	Spain
Chandramathy S.	Praveen	CNR-IOM DEMOCRITOS Simulation Center and SISSA	Italy
Conesa	Jose Carlos	Inst. de Catálisis y Petroleoquímica, CSIC	Spain
Cormack	Alastair N.	New York State College of Ceramics at Alfred University	USA
Fabris	Stefano	CNR-IOM DEMOCRITOS Simulation Center and SISSA	Italy
Ferstl	Pascal	Physics Department, University Erlangen-Nuremberg	Germany
Fornasiero	Paolo	Department of Chemical and Pharmaceutical Sciences, University of Trieste	Italy
Ganduglia-Pirovano	M. Veronica	Instituto de Catalis y Petroleoquimica, CSIC	Spain
Grönbeck	Henrik	Competence Centre for Catalysis and Department of Applied Physics, Chalmers University of Technology	Sweden
Haque	Francia	UPMC- CNRS, Institut des Nanosciences de Paris, UMR7588	France
Hellström	Matti	Ångström Laboratory, Uppsala University	Sweden
Henry	Claude R.	CINAM-CNRS, Marseille	France
Hermansson	Kersti	Ångström Laboratory, Uppsala University	Sweden
Holzappel	Harald	Institute of materials chemistry, Vienna University of Technolog	Austria
Hu	Shunglin	Ångström Laboratory, Uppsala University	Sweden
Jensen	Thomas N.	Interdisciplinary Nanoscience Center, Aarhus University	Denmark
Kosak	Rukan	Institute of materials chemistry, Vienna University of Technolog	Austria
Kozlov	Sergey	ICREA and Universitat de Barcelona, Barcelona, Spain	Spain
Kristoffersen	Henrik H.	iNANO, Aarhus University	Denmark
Kullgren	Jolla	Ångström Laboratory, Uppsala University	Sweden
Lauritsen	Jeppe V.	Aarhus University, Interdisciplinary Nanoscience Center	Denmark
Li	Hao	Institute of materials chemistry, Vienna University of Technolog	Austria
Libuda	Jörg	Dept. Chemistry and Pharmacy, University Erlangen-Nuremberg	Germany
Lopez Duran	David	Instituto de Catalis y Petroleoquimica, CSIC	Spain
Lundgren	Edvin	Lund University, Division of Synchrotron Radiation Research	Sweden
Lykhach	Yaroslava	Dept. Chemistry and Pharmacy, University Erlangen-Nuremberg	Germany
Martinez-Arias	Arturo	Instituto de Catalis y Petroleoquimica, CSIC	Spain
Matolin	Vladimir	Charles University in Prague	Czech Republic
Mehl	Sascha	Dept. Chemistry and Pharmacy, University Erlangen-Nuremberg	Germany
Montini	Tiziano	Department of Chemical and Pharmaceutical Sciences, University of Triest	Italy
Neitzel	Armin	Dept. Chemistry and Pharmacy, University Erlangen-Nuremberg	Germany
Neyman	Konstantin	ICREA and Universitat de Barcelona, Barcelona, Spain	Spain

Nilius	Niklas	Fritz-Haber-Institut, Max-Planck-Society, Berlin	Germany
Nolan	Michael	Tyndall National Institute, Cork	Ireland
Nowak	Izabela	Adam Mickiewicz University	Poland
Olbrich	Reinhard	Fachbereich Physik, Universität Osnabrück	Germany
Pacchioni	Gianfranco	Dipartimento di Scienza dei Materiali, Università Milano Bicocca	Italy
Perez	Ruben	Universidad Autonoma de Madrid	Spain
Petkov	Petko St.	University of Sofia	Bulgaria
Reichling	Michael	Fachbereich Physik, Universität Osnabrück	Germany
Rieboldt	Felix	Interdisciplinary Nanoscience Center (iNANO), Aarhus University	Denmark
Rupprechter	Günther	Institute of Materials Chemistry, Vienna University of Technology	Austria
Schneider	M.Alexander	Physics Department, University Erlangen-Nuremberg	Germany
Shaikhutdinov	Shamil	Fritz-Haber-Institut, Max-Planck-Society, Berlin	Germany
Sljivancanin	Zeljko	Vinca Institute of Nuclear Sciences (020), Belgrade, Serbia	Serbia
Stankic	Slavica	UPMC- CNRS, Institut des Nanosciences de Paris, UMR7588	France
Tiseanu	Carmen	National Institute for Laser, Plasma and Radiation Physics, Bucharest- Magurele	Romania
Todorovic	Milica	Universidad Autonoma de Madrid	Spain
Ven Den Bossche	Maxime	Competence Centre for Catalysis and Department of Applied Physics, Chalmers University of Technology	Sweden
Vilhelmsen	Lasse B.	iNANO, Aarhus University	Denmark
Yang	Jingxia	Institute of materials chemistry, Vienna University of Technology	Austria