



COST ACTION D-41

INORGANIC OXIDES: SURFACES AND INTERFACES

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2010 Annual Meeting of the COST Action

Torino, October 7-9, 2010

*Museo Regionale di Scienze Naturali
Via Giolitti 36*

PROGRAM

Thursday, October 7	
12:00-13:55	Registration
14:00-14:10	G. Pacchioni (Milano) E. Giamello (Torino): Welcome
Section 1. Discussion leader: Francesc Illas, Barcelona	
14:10-14:50	Invited Talk. Hajo Freund , <i>Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany</i> Thin oxide films, supported oxide nanoparticles and their reactivity
14:50-15:00	Oliver Diwald (Erlangen) Report on WG1 activities
15:00-15:30	J. Goniakowski <i>CNRS, Institut des Nanosciences de Paris, Paris, France</i> Polarity of ultra-thin MgO(111) films deposited on a metal substrate
15.30-16:00	S. Surnev <i>Institute of Physics, Surface and Interface Physics, Karl-Franzens University Graz Graz, Austria</i> Fabrication of a NiO _x nanodot superlattice
16:00-16:30	<i>Coffee break</i>
Section 2. Discussion leader: Walter Langel, Greifswald	
16:30-17:00	G. Thornton <i>London Centre for Nanotechnology, University College London, London UK</i> Bonding of methyl phosphonate to TiO ₂ (110)
17:00-17:30	M. Chiesa <i>Dipartimento Chimica IFM and NIS. Università di Torino, Torino IT</i> Local environment of Ti ³⁺ ions in reduced TiO ₂ through spin density studies.
17:30-18:00	O. Diwald <i>Institute of Particle Technology, University of Erlangen-Nuremberg, Germany</i> Solar light and dopant induced recombination effects: photoactive nitrogen in TiO ₂ as a case study.
Friday, October 8	
Section 3. Discussion leader: Sergio Valeri, Modena	
09:00-09:40	Invited Talk. Adriano Zecchina , <i>Dipartimento Chimica IFM and NIS. Università di Torino, Torino IT</i> The surface structures of anatase and rutile microcrystals :a concise review
09:40-09:50	Elio Giamello (Torino) Report on WG2 activities
09:50-10:20	A. Adamski <i>Jagiellonian University, Faculty of Chemistry, Krakow, Poland</i> Design and spectroscopic investigations of nanoxide catalysts functionalized with tailored vanadia.
10:20-10:50	J. C. Conesa <i>Instituto de Catálisis y Petroleoquímica, CSIC, Madrid, Spain</i> On the relevance of dispersion interactions for the energetics of titania polymorphs
10:50-11:20	<i>Coffee break</i>
Section 4. Discussion leader: Greg Metha, Adelaide	
11:20-11:50	S. Stankic <i>CNRS, Institut des Nanosciences de Paris, Paris, France</i> Gold nanoparticles supported on smoke MgO
11:50-12:20	P. Sushko <i>Department of Physics and Astronomy and London Centre for Nanotechnology, University College London, UK</i> SO ₃ and SO ₄ species at the low coordinated sites of MgO nanocubes

12:20-12:50	H.-P. Steirück <i>Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Erlangen, Germany</i> Interaction of small molecules with thin NiO layers on Cu(111)
12:50-14:30	Lunch break
	Section 5. Discussion leader: Falko Netzer, Graz
14:30-15:10	Invited Talk. Piero Ugliengo , <i>Dipartimento Chimica IFM and NIS. Università di Torino, Torino IT</i> Computational simulation of prebiotic processes
15:10-15:20	Joerg Libuda (Erlangen) Report on WG3 activities
15:20-15:50	J. Libuda- K. Neymann <i>Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Erlangen, Germany and Departament de Química Física and IQTCUB, Universitat de Barcelona, Barcelona, Spain</i> Chemistry on pure and and Pt-loaded ceria surfaces: experiment and theory
15:50-16:20	A. Kartuzian <i>Chair of Physical Chemistry, Chemistry Department, Technische Universität München, Germany.</i> Linear and nonlinear optical properties of supported metal clusters and adsorbed molecules
16:20-16:50	H. Helmann <i>Applied Physics and Competence Centre of Catalysis, Chalmers University of technology, Göteborg, Sweden</i> Methane activation on palladium (-oxide)
16:50-18:50	Poster Session & MC Meeting
Saturday. October 9	
	Section 6. Discussion leader: Gianfranco Pacchioni, Milano Bicocca
09:00-09:40	Invited Talk. Scott Chambers , <i>Fundamental and Computational Sciences Directorate, Pacific Northwest National Laboratory, Richland, WA 99352 -- USA</i> Properties of MBE-grown Fe-doped and (Fe, N) co-doped TiO ₂ Rutile Epitaxial Films
09:40-09:50	Alex Shlugher (London) Report on WG4 activities
09:50-10:20	M. Reichling <i>Fachbereich Physik, Universität Osnabrück, BarbarasträÙe 7, 49076 Osnabrück, Germany</i> Characterizing TiO ₂ (110) surface states by their work function
10:20-10:50	M. Castell <i>Department of Materials, University of Oxford, Parks Road, Oxford OX1 3PH, UK</i> Surface structures of ultra-thin TiO _x and BaO films on Au (111)
10:50-11:20	Coffee break
	Section 7. Discussion leader: Friedrich Esch, München
11:20-11:50	G. Granozzi <i>Department of Chemical Sciences, , University of Padova, Italy</i> Probing transformation of relevance in catalysis on a single oxide layer: Fe on TiO _x /Pt(111)
11:50-12:20	A. Shluger . <i>Department of Physics and Astronomy, University College London, Gower Street, London WC1E 6BT, UK</i> Electronic and optical properties of polycrystalline metal oxides
12:20-12:30	G. Pacchioni (Milano Bicocca) E. Giamello (Torino) : Closing