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COST Action CM 1104

 **cost**
EUROPEAN COOPERATION
IN SCIENCE AND TECHNOLOGY

Modena 21-22 March, 2013
Complesso San Geminiano
Via San Geminiano 3

**First
WG2 meeting**

Reducible oxide chemistry, structure and functions

The meeting will bring together scientists active in research on reducible oxides for applications in chemical catalysis, sustainable energy conversion, novel electronic devices and more. The meeting will foster discussion on experimental and theoretical research devoted to exploring novel routes for the growth and synthesis of nanostructured reducible oxide systems, aimed at exploiting and tailoring reducibility to yield specific functionalities.

Thursday, March 21st

14:00-14:15 Opening (Sergio Valeri, Michael Reichling)

Chairperson: Geoff Thornton

14:15-14:40 Svetlozar Surnev "Ternary oxide nanolayers: a novel 2-D Cu-tungstate phase on Cu(110)2x1-O surface oxide"

14:40-15:05 David Grinter "Ultrathin CeO₂(111) films to investigate water gas shift catalysis"

15:05-15:30 Jan Ingo Flege "Surfactant-mediated growth of rare-earth oxides on silicon"

15:30-15:55 Stefano Prada "Charging of gold atoms on doped MgO and CaO: identifying the key parameters by DFT calculations"

15:55 -16:35 Coffee break and poster session

Chairperson: Zbigniew Sojka

16:35-17:00 Reinhard Olbrich "Surface properties of thick ceria films grown on Si(111)"

17:00-17:25 Joachim Paier "Stability and migration barriers of small vanadium oxide clusters on the CeO₂(111) surface: A DFT+U study"

17:25-17:50 Marco Fanciulli "Atomic Layer Deposition"

17:50-18:15 Suzana Petrović "Laser-induced surface oxidation of bimetallic multilayer thin films"

20:00 Social dinner

Friday, March 22nd

Chairperson: Paola Luches

09:00-09:45 INVITED P. Fornasiero "Advancing the Frontiers in Ceria Based Catalysis"

09:45-10:10 Elio Giamello "Charge carriers in bare and modified Titanium dioxide for photochemical applications : the role of EPR in understanding a complex problem"

10:10- 11:35 Sergio Tosoni "Prediction of Optical Excitation Energies of Oxides with DFT and Quasi Particle Calculations"

10:35-11:15 Coffee break and poster session

Chairperson: Michael Reichling

11:15-11:40 Stefan Bromley "Structure and growth of nano-oxides: insights from computer modeling"

11:40-12:05 Witold Piskorz "Adsorption of large organic molecules on TiO₂ surfaces: DFT Modeling of the STM images beyond the Tersoff-Hamman approximation"

12:05-12:30 Martin Ferus, Svatopluk Civiš "Reduced TiO₂ Anatase: room temperature self-operating convertor of CO₂ and OCS"

12:30-13:00 Discussion: the meeting, the oxides, WG2, ... & conclusions

13:00-14:00 Lunch



con il patrocinio di



con il contributo di



FONDAZIONE
Cassa di Risparmio di Modena

