



89th International Bunsen Discussion Meeting "Chemical processes at oxide surfaces: from experiment to theory"  
June 15.-17.06.2005, Welcome-Hotel Hennesee in Meschede

The scientific program starts at 2 pm on June 15<sup>th</sup>

<b>Wednesday June 15<sup>th</sup>, 2005</b>	
14.00 – 14.15	<b>Welcoming</b>
14.15 – 15.00	<b>R. Catlow (London) (I)</b> Understanding nucleation and growth in inorganic materials
15.00 – 15.30	<b>B. Meyer (Bochum) (I)</b> Strong metal-support interaction in Cu/ZnO catalysts: Insights from first-principles calculations?
15.30 – 16.00	<b>F. Traeger (Bochum) (I)</b> Molecular adsorbates on inert and reactive metal oxides: He-atom scattering applied to MgO and ZnO
16.00 – 16.30	<b>Coffee break</b>
16.30 – 17.15	<b>G. Kresse (Wien) (I)</b> Structure and domain boundaries of the ultrathin aluminum oxide film on NiAl(110)
17.15 – 18.00	<b>B. Hammer (Aarhus) (I)</b> Reactivity of oxidized Pt surfaces
18.00 – 18.30	<b>O. Hinrichsen (München) (I)</b> New insights into the mechanism of methanol synthesis catalyzed by Cu/ZnO catalysts
18.30 – 19.00	<b>M. Muhler (Bochum) (I)</b> Strong-metal support interactions in Cu/ZnO catalysts probed by CO adsorption: the combined application of microcalorimetry, temperature-programmed desorption and FTIR spectroscopy
<b>19.00 – 20.30</b>	<b>Barbecue</b>
20.30 – 22.00	<b>Poster session with discussion</b>



**Thursday June 16<sup>th</sup>, 2005**

8.30 – 9.15	<b>G. Thornton (London) (I)</b> Nanostructuring titanium oxide surfaces
9.15 – 9.45	<b>Th. Bredow (Hannover)</b> ATR-FTIR and quantum chemical calculations at the TiO <sub>2</sub> surface
<b>9.45 – 10.15</b>	<b>F. Schüth (Mülheim) (I)</b> <b>Copper and gold based catalysts - from model systems to real catalysts</b>
10.15 – 10.45	<b>K. Merz (Bochum)</b> Molecular models of ZnO-carrier systems in methanol synthesis
<b>10.45 – 11.15</b>	<b>Coffee break</b>
11.15 – 12.00	<b>F. Boccuzzi (Turin) (I)</b> CO adsorption and reactivity with oxygen on supported gold: new insights
12.00 – 12.30	<b>K. M. Neyman (Barcelona)</b> Surface complexes of small transition metal particles on metal oxides: First-principles theoretical studies
12.30 – 13.00	<b>W. Grünert (Bochum) (I)</b> The reduction of copper in porous matrices
<b>13.00 – 14.30</b>	<b>Lunch</b>
14.30 – 15.15	<b>U. Diebold (Tulane) (I)</b> The adsorption of water on single-crystalline metal oxide surfaces
15.15 – 15.45	<b>K. Reuter (Berlin)</b> Relevance of oxide formation in oxidation catalysis: An emerging trend understanding from first-principles statistical mechanics?
15.45 – 16.15	<b>R. A. Fischer (Bochum) (I)</b> Open framework coordination polymers as novel host lattices for nanoparticles: New perspectives for the study of the metal/support-interaction in the Cu/ZnO-system
16.15 – 16.45	<b>S. Polarz (Berlin) (I)</b> Formation of particles under spatial confinement
16.45 – 17.15	<b>A. Birkner (Bochum) (I)</b> Investigation of ZnO and nano-sized ZnO particles with a combined SEM/STM instrument
17.30 – 18.45	<b>Boat trip with coffee and drinks</b>

19.00 – 20.30	<b>Dinner</b>
20.30 – 22.00	<b>Poster session with discussion</b>
<b>Friday June 17<sup>th</sup>, 2005</b>	
8.30 – 9.00	<b>V. Staemmler (Bochum) (I)</b> Ab initio calculation of X-ray spectra of ZnO, ZnO surfaces and adsorbates on ZnO
9.00 – 9.30	<b>K. Fink (Bochum) (I)</b> Ab initio calculations of F centers and magnetic impurities in ZnO
9.30 – 10.00	<b>W. Langel (Greifswald)</b> First principles and classical MD of surface processes on titanium dioxide
10.00 – 10.30	<b>Coffee break</b>
10.30 – 11.00	<b>Ch. Kolczewski (Berlin)</b> Ab initio DFT cluster studies for oxygen 1s NEXAFS spectra at V <sub>2</sub> O <sub>5</sub> and V <sub>2</sub> O <sub>3</sub> surfaces
11.00 – 11.45	<b>B. Clausen (Topsoe Denmark) (I)</b> Morphological and structural aspects of catalytic nanoparticles
11.45 – 12.15	<b>P. Bagus (University of North Texas) (I)</b> XPS binding energy shifts of metal nanoparticles: A rigorous theoretical analysis

## Poster presentations

- P1**  
**K. Al Shamery (Oldenburg)** Water at clean and silver modified H(1x1)-O-ZnO(000-1)
- P2**  
**A. Berlich (Leipzig)** Characterization of Ni/NiO heterogeneous systems by metastable induced electron spectroscopy (MIES) as a case study for metal supported catalysts
- P3**  
**A. Birkner (Bochum)** Investigation of ZnO and nano-sized ZnO particles with a combined SEM/STM instrument
- P4**  
**M. Comotti (MPI Mülheim)** CO oxidation with gold based catalysts: influence of the preparation method and metal-support interaction
- P5/P6**  
**K. Fink (Bochum)** Ab initio calculations of F centers and magnetic impurities in ZnO
- P7**  
**H. Gies (Bochum)** Preparation of metal-support model catalysts by deposition of nano-confined metals and metal oxides in mesoporous matrices
- P8**  
**Y. Guo (Essen)** Preparation of ZnO nanoparticles by controlled thermolysis of a zinc cyanide complex
- P9**  
**Ch. Hagendorf (Halle)** Adsorbate phases and thin films of NiO and MnO on Pt(111) studied by in-situ STM experiments
- P10**  
**I. Hegemann (Bochum)** Methanol synthesis on Cu/ZnO – Ab initio calculations on model systems
- P11**  
**W. Hergert (Halle)** Electronic structure of thin transition metal oxide films on Ag(001)
- P12**  
**T. Hikov (Bochum)** New approaches to nanostructured heterogeneous catalysts
- P13**  
**L. Khodeir (Bochum)** New approaches to Cu/ZnO/Al<sub>2</sub>O<sub>3</sub> catalysts for the synthesis of methanol
- P14**  
**K. Kotsis (Bochum)** Ab initio calculation of O1s XPS and XES spectra of bulk ZnO and ZnO surfaces
- P15**  
**R. Kovacik (Bochum)** Low-energy defects on ZnO surfaces and their characterization by STM image calculations
- P16**  
**D. Langenberg (Bochum)** Adsorption of CO<sub>2</sub> on the oxygen-terminated ZnO(0001) surface
- P17**  
**E. Löffler (Bochum)** IR spectroscopic and theoretical studies on molecular models of ZnO systems for methanol synthesis

- P18**  
**B. Meyer (Bochum)** From UHV to reaction conditions: ZnO surface and adsorbate structures in realistic experimental environments
- P19**  
**R. Naumann d'Alnoncourt (Bochum)** Strong-metal support interactions in Cu/ZnO catalysts probed by CO adsorption: the combined application of microcalorimetry, temperature-programmed desorption and FTIR spectroscopy
- P20**  
**A. Neubauer (HMI Berlin)** Spacer controlled ultrafast electron transfer dynamics from a perylene chromophore to different TiO<sub>2</sub> surfaces
- P21**  
**A. Patrakov (Würzburg)** Quantum chemical investigations about the behaviour of adsorbates on CdTe(001) surfaces
- P22**  
**Ch. Pettenkofer (HMI Berlin)** Morphology and electronic structure of MOMBE grown ZnO surfaces
- P23**  
**D. Rosenthal (Berlin)** Growth of titanium oxides on metals – Rutile(011) on Rhenium(10-10)
- P24**  
**K.-M. Schindler (Halle)** A tensor LEED structure determination of a CoO ultrathin film on Ag(100)
- P25**  
**R. Schönen (Bochum)** Molecular models for the ZnO-carriersystem
- P26**  
**F. Schröder (Bochum)** Preparation of highly Zn-loaded [ZnO@MCM-48](#) Nanocomposites by Nonaqueous Organometallic Impregnation with Diethylzinc
- P27**  
**J. Strunk (Bochum)** The adsorption of CO on copper catalysts:  
A microkinetic study based on calorimetric results
- P28**  
**S. Vucojevic (Mülheim)** Copper colloids – a model catalyst system for methanol synthesis
- P29**  
**G. Walther (Bochum)** STM investigation of ZnO(0001)-Zn, ZnO(10-10) single crystal surfaces and copper deposition on polycrystalline ZnO layers
- P30**  
**Y. Wang (Bochum)** Interaction of CO, hydrogen and water with ZnO(10-10):  
HREELS and TDS studies
- P31**  
**R. Weiß (Essen)** Coordination compounds based on cyanide - precursors for a methanol catalyst