The scientific program starts at 2 pm on June 15th

<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
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<tr>
<td>14.00 – 14.15</td>
<td>Welcoming</td>
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</table>
| 14.15 – 15.00 | R. Catlow (London) (I)  
Understanding nucleation and growth in inorganic materials |
| 15.00 – 15.30 | B. Meyer (Bochum) (I)  
Strong metal-support interaction in Cu/ZnO catalysts: Insights from first-principles calculations? |
| 15.30 – 16.00 | F. Traeger (Bochum) (I)  
Molecular adsorbates on inert and reactive metal oxides: He-atom scattering applied to MgO and ZnO |
| 16.00 – 16.30 | Coffee break                               |
| 16.30 – 17.15 | G. Kresse (Wien) (I)  
Structure and domain boundaries of the ultrathin aluminum oxide film on NiAl(110) |
| 17.15 – 18.00 | B. Hammer (Aarhus) (I)  
Reactivity of oxidized Pt surfaces |
| 18.00 – 18.30 | O. Hinrichsen (München) (I)  
New insights into the mechanism of methanol synthesis catalyzed by Cu/ZnO catalysts |
| 18.30 – 19.00 | M. Muhler (Bochum) (I)  
Strong-metal support interactions in Cu/ZnO catalysts probed by CO adsorption: the combined application of microcalorimetry, temperature-programmed desorption and FTIR spectroscopy |
<p>| 19.00 – 20.30 | Barbecue                                  |
| 20.30 – 22.00 | Poster session with discussion             |</p>
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<tr>
<th>Time</th>
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<th>Topic</th>
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<tr>
<td>8.30 – 9.15</td>
<td>G. Thornton (London)</td>
<td>Nanostructuring titanium oxide surfaces</td>
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<tr>
<td>9.15 – 9.45</td>
<td>Th. Bredow (Hannover)</td>
<td>ATR-FTIR and quantum chemical calculations at the TiO₂ surface</td>
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<tr>
<td>9.45 – 10.15</td>
<td>F. Schüth (Mülheim)</td>
<td>Copper and gold based catalysts - from model systems to real catalysts</td>
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<tr>
<td>10.15 – 10.45</td>
<td>K. Merz (Bochum)</td>
<td>Molecular models of ZnO-carrier systems in methanol synthesis</td>
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<tr>
<td>10.45 – 11.15</td>
<td></td>
<td>Coffee break</td>
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<tr>
<td>11.15 – 12.00</td>
<td>F. Boccuzzi (Turin)</td>
<td>CO adsorption and reactivity with oxygen on supported gold: new insights</td>
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<tr>
<td>12.00 – 12.30</td>
<td>K. M. Neyman (Barcelona)</td>
<td>Surface complexes of small transition metal particles on metal oxides: First-principles theoretical studies</td>
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<tr>
<td>12.30 – 13.00</td>
<td>W. Grünert (Bochum)</td>
<td>The reduction of copper in porous matrices</td>
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<td>13.00 – 14.30</td>
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<td>Lunch</td>
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<tr>
<td>15.15 – 15.45</td>
<td>K. Reuter (Berlin)</td>
<td>Relevance of oxide formation in oxidation catalysis: An emerging trend understanding from first-principles statistical mechanics?</td>
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<td>15.45 – 16.15</td>
<td>R. A. Fischer (Bochum)</td>
<td>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</td>
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<td>16.15 – 16.45</td>
<td>S. Polarz (Berlin)</td>
<td>Formation of particles under spatial confinement</td>
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<td>16.45 – 17.15</td>
<td>A. Birkner (Bochum)</td>
<td>Investigation of ZnO and nano-sized ZnO particles with a combined SEM/STM instrument</td>
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<tr>
<td>17.30 – 18.45</td>
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<td>Boat trip with coffee and drinks</td>
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<td>Time</td>
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<tr>
<td>19.00 – 20.30</td>
<td>Dinner</td>
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<tr>
<td>20.30 – 22.00</td>
<td>Poster session with discussion</td>
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**Friday June 17th, 2005**

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<tr>
<th>Time</th>
<th>Speaker</th>
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<tr>
<td>8.30 – 9.00</td>
<td>V. Staemmler (Bochum) (I)</td>
<td>Ab initio calculation of X-ray spectra of ZnO, ZnO surfaces and adsorbates on ZnO</td>
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<tr>
<td>9.00 – 9.30</td>
<td>K. Fink (Bochum)</td>
<td>Ab initio calculations of F centers and magnetic impurities in ZnO</td>
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<tr>
<td>9.30 – 10.00</td>
<td>W. Langel (Greifswald)</td>
<td>First principles and classical MD of surface processes on titanium dioxide</td>
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<td>10.00 – 10.30</td>
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<td>Coffee break</td>
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<tr>
<td>10.30 – 11.00</td>
<td>Ch. Kolczewski (Berlin)</td>
<td>Ab initio DFT cluster studies for oxygen 1s NEXAFS spectra at V₂O₅ and V₂O₃ surfaces</td>
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<tr>
<td>11.00 – 11.45</td>
<td>B. Clausen (Topsoe Denmark) (I)</td>
<td>Morphological and structural aspects of catalytic nanoparticles</td>
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<tr>
<td>11.45 – 12.15</td>
<td>P. Bagus (University of North Texas) (I)</td>
<td>XPS binding energy shifts of metal nanoparticles: A rigorous theoretical analysis</td>
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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 Mühlheim)  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/Al2O3 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 CO2 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 TiO2 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