



Catalysis From First Principles – Wien, May 25-28, 2009

MONDAY, MAY 25, 2009

Agenda

Registration

Afternoon Chair: **Jens Nørskov** (Technical University of Denmark)

13:00 Opening:
Jürgen Hafner (University of Vienna)

(A) Recent progress in density functional theory of solids – and beyond

- 13:15 – 13:45 **John Perdew** (Tulane University)
- A semilocal “workhorse” density functional for atoms, molecules, and solids
- 13:45 – 14:25 **Bengt Lundqvist** (Göteborg University)
- vdW-DF – A density functional applied to strong and weak bonds
- 14:25 – 15:05 **Stefan Grimme** (Westfälische Wilhelms-Universität Münster)
- Status and perspectives of double-hybrid density functionals in electronic structure theory

Coffee break

15:05 – 15:30

15:30 – 16:10 **Georg Kresse** (University of Vienna)

- The CO adsorption puzzle: Is there a final solution?

16:10 – 16:50 **Angelos Michaelides** (University College London)

- Towards a first principles understanding of water-solid interfaces

(B) Ab initio calculations of free-energy barriers and reaction rates

16:50 – 17:30 **Christoph Dellago** (University of Vienna)

- Pressure induced phase transformations of nanocrystals studied with transition path sampling simulations

17:30 - 18:10 **Karsten Reuter** (Fritz-Haber-Institut der MPG)

- From UHV to in situ: Multiscale modelling across the pressure gap



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TUESDAY; MAY 26, 2009

Agenda

Morning Chair: **Matthias Scheffler** (FHI Berlin)

- 9:00 - 9:40 **Davide Branduardi** (Italian Institute of Technology)
- Free energy calculations with path collective variables
- 9:40 - 10:20 **Horia Metiu** (University of California)
- Catalyst activation by molecular sized centers
- 10:20 – 11:00 **Tomáš Bučko** (University of Vienna)
- Role of the thermal and entropy effect in alkane conversion reactions catalyzed by acidic zeolites

11:00 – 11:30 **Coffe break**

- 11:30 – 12:10 **Thomas Bligaard** (TU Lyngby)
- Free energy trends from linear adsorption energy relations

(C) Materials design

- 12:10 – 12:50 **Dane Morgan** (University of Wisconsin-Madison)
- Ab-initio modeling of solid oxide fuel cell cathodes

12:50 – 14:30 **Lunch break**

Afternoon Chair: **Horia Metiu** (University of California)

- 14:30 – 15:10 **Felix Studt** (Technical University of Denmark)
- Rational catalyst design applied to the selective hydrogenation of acetylene

(D) Catalysis by metals and metal-support interactions

- 15:10 – 15:50 **Gianfranco Pacchioni** (Università di Milano-Bicocca)
- Modifying the adsorption properties of oxide ultrathin films via work function control
- Simone Piccinin** (National Simulation Center, Trieste)
- 15:50 – 16:30
- The system chemistry of an alloy catalyst insight from DFT calculations
- 16:30 – 17:00 **Coffee break**
- 17:00 – 17:40 **Robert Grybos** (Polish Academy of Science)
- Selective catalytic reduction of NO by CH₄ on Pd-exchanged mordenite periodic DFT simulations
- 17:40 – 18:30 **Pascal Raybaud** (Institut Français du Pétrole)
- Effect of γ -alumina acidity on the stability of metallic nanoparticles
- 18:30 **Poster Session (with refreshments)**



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WEDNESDAY, MAY 27, 2009

Agenda

Morning Chair: **Thomas Bligaard** (Technical University of Denmark)

9:00 - 9:40 **Martin Fuchs** (Fritz-Haber-Institut der MPG)
• Towards an exact treatment of exchange correlation in materials

9:40 - 10:20 **Axel Gross** (Ulm University)
• Reaction steps in C1 chemistry on metal surfaces studied from first principles

(E) Electrocatalysis

10:20 – 11:00 **Marc Koper** (Leiden University)
• Theory and experiment of the electrochemical CO oxidation

11:00 – 11:40 **Coffee break**

11:40 – 12:20 **Jan Rossmeisl** (Technical University of Denmark)
• Searching for Electro-Catalyst Materials for Oxygen Reduction Reaction

12:20 – 14:00 **Lunch break**

Afternoon Chair: **Karsten Reuter** (Fritz-Haber-Institut der MPG)

14:00 – 14:40 **Osamu Sugino** (University of Tokyo)
• A combined dynamical and static approach to electrocatalysis

(F) Acid-based catalysis in zeolites and related materials

14:40 – 15:20 **Joachim Sauer** (Humboldt University)
• Adsorption and reaction steps in nano-porous systems – accurate prediction by quantum chemistry and molecular statistics

15:20 – 16:00 **Lubomir Benco** (University of Vienna)
• Activity and reactivity of Fe²⁺ cations in the zeolite. Ab initio free-energy MD simulation

16:00 – 16:30 **Coffee break**

16:30 – 17:10 **Silvia Bordiga** (Università di Torino)
• Vibrational spectroscopies to describe acid based reactivity in microporous materials

(G) Catalysis by oxides

17:10 – 17:50 **Robert Schlögl** (Fritz-Haber-Institut der Max-Planck-Gesellschaft)
• Simple and complex oxides in selective oxidation reactions

17:50 – 18:10 **Cesare Franchini** (University of Vienna)
• Halogen-induced corrosion platinum



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THURSDAY, MAY 28, 2009

Agenda

- Morning Chair: **Jürgen Hafner** (University of Vienna)
- 9:00 - 9:40 **Richard Catlow** (University College London)
- Computer Modelling of Active Sites in Microporous Materials
- 9:40 - 10:20 **Florian Mittendorfer** (University of Vienna)
- Low dimensional surface oxides in the oxidation of Rh
- 10:20 – 11:00 **Claudine Noguera** (Institut des Nanosciences de Paris)
- Electrostatic forces and polarity: From semi-infinite oxide surfaces to ultrathin films
- 11:00 – 11:30 **Coffee break**
- 11:30 – 12:10 **Jeroen van Bokhoven** (ETH Zurich)
- Inside a reactor: Time- and space-resolved structure of a heterogeneous catalyst
- 12:10 **Conference summary** (Matthias Scheffler)