Final Report for Catalysis Meeting "Catalysis from First Principles"

Magleås Conference Center, Høsterkøb, Denmark

June 7-9, 2004

International Organization Committee: Jurgen Hafner, Matthias Scheffler, and Jens Norskov
Local Organization Committee: Jens Norskov, Karoliina Honkala, and Helle Wellejus

The Catalysis from First Principles meeting provided a broad cross-section to resent theoretical work done on catalysis by different groups in Europe and the USA, spiced with talks given by experimentalists and people working in industry. This concept worked very well and the atmosphere of the meeting was very positive and inspiring. The interaction between experimentalists and theorists as well as between younger scientists and the more senior researchers was open and spontaneous, thus hopefully creating new projects and collaboration.

The meeting consisted of 32 invited talks selected by the international committee and approximately 15 poster presentations. The total number of participants was 54, from which 34 persons do theoretical work and 11 do experimental work in heterogeneous catalysis and 8 work in industry. The speakers from industry gave an important practical aspect to the meeting. Discussion after talks was vivid and continued on coffee and lunch breaks and in the evenings. The talks were distributed into different sessions according to the topic as well as speakers' background, but the main theme behind all the theory talks were density-functional –theory (DFT) calculations. Some of the talks concentrated on more basic questions, such as understanding the interaction between a molecule and a surface - in itself an essential topic in catalysis - while some were very applied talks where DFT calculations had been addressed to study, for example, fuel cell catalysis.

For theorists, fuel cell catalysis opens lots of new possibilities to study the topic computationally, but it became obvious during the meeting that it is not always a straightforward task to perform electronic structure calculations for electrocatalysis problems or interpret the obtained results. Talks given about experimental and industrial fuel cell catalysis research put the theoretical work done so far in perspective and pointed out the problems and questions relevant to industrial research.

The following topics were also presented in the sessions: hydrocarbon reactions, ammonia synthesis, CO oxidation, water gas shift reaction, zeolites in catalysis, metal-nanoparticles on oxides etc. This large variety of different topics gave an overview of the problems DFT can be used to resolve in heterogeneous catalysis. The common denominator of these topics is complexity: Either the catalytic material or the reaction is complex, or both. This is a challenge for theorists and at the moment we are only beginning to look into it in more detail! Each topic includes important subtopics. For example:

The session devoted to hydrocarbon reactions on transition metal surfaces showed that hydrocarbon reactions are suitable for theoretical investigations of selectivity in heterogeneous catalysis. Understanding selectivity is a real challenge to the catalysis community since it is a key to a more rational catalysts design, based on insight and not guessing. The utilization of parallel computational and experimental screening for design catalysts was demonstrated in a couple of talks. It is an efficient way to scan properties of the catalysts and can be expected to become more popular in the near future.

The meeting showed how enormous the progress in atomistic theory in heterogeneous catalysis is at present: Interpretation of experimental results in surface science greatly benefits from calculations. On the other hand, first time ever, DFT calculations can be used as building blocks to construct models, which describe details of catalytic processes under realistic conditions. Such realistic models were presented in the meeting for reactions like CO oxidation and NH_3 formation. These models provide a link between model experiments and real catalysts.
The meeting also pointed out a need for new theory developments; Questions of how to include the van der Waals interaction to DFT or how to describe the interaction between O_2 and a simple metal surface correctly need to be answered soon. At the moment, DFT fails to find the experimentally observed O_2 dissociation barrier on Al.

Summary

Catalysis Meeting: " Catalysis from First Principles" took place in June 7-9 2004 in Magleås Conference Center near Copenhagen in Denmark. In addition to The European Science Foundation the meeting was sponsored by Fritz-Haber-Institut, Berlin, Germany, University of Vienna, Austria, Haldor Topsöe A/S Lyngby, Denmark and Center for Atomic-scale Materials Physics (CAMP) Technical University of Denmark, Lyngby, Denmark. CAMP took care of all the practical organizing of this meeting. The meeting consisted of 32 invited talks and two poster sessions. Most of the speakers were European, but some came from USA. The background of the speakers was mostly in theory although couple speakers work in industry or do experiments in heterogeneous catalysis.
Topics covered in the talks:

(i) Hydrocarbon reactions on transition metal surfaces
(ii) Water gas shift reaction
(iii) Water-metal interaction
(iv) Metal-oxide interaction
(v) Fuel cell catalysis
(vi) Utilization of STM to study catalytic reactions
(vii) Design of new catalysts
(viii) Models working under realistic conditions

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PROGRAMME

The meeting is sponsored by:

The European Science Foundation (ESF)

Fritz-Haber-Institut, Berlin, Germany

University of Vienna, Austria

Haldor Topsøe A/S, Lyngby, Denmark

Center for Atomic-scale Materials Physics (CAMP)
Technical University of Denmark, Lyngby, Denmark

Monday, June 7, 2004

10:00 - 12:30 Arrival / Coffee

12:30 - 13:20 Lunch

13:20 - 13:30 **Jens K. Nørskov**: Welcome
13:30 - 14:00 **Jürgen Hafner:** Selective hydrogenation of C=O and C=H double bonds on bimetallic catalysts
14:00 - 14:30 **Suljo Linic**: Selectivity in heterogeneous ethylene epoxidation on Ag: From fundamental studies to rational catalyst design
14:30 - 15:00 **Ioannis Remediakis**: DFT study of CO hydrogenation on Ni(111)
15:00 - 15:30 **Tone Kokalj**: Dehydrogenation of methane catalyzed by transition metal surfaces

15:30 - 16:00 Coffee

16:00 - 16:30 **Karsten Reuter**: The steady state of heterogeneous catalysis, studied with first-principles statistical mechanics
16:30 - 17:00 **Karoliina Honkala**: Ab initio kinetics for ammonia synthesis
17:00 - 17:30 **Alex Bogicevic**: Energetics and kinetics of metal-support interactions in catalytic applications
17:30 - 18:00 **Stig Helveg**: *In situ* TEM

18:00 Dinner

20:00 **Poster session -** refreshments are sponsored by Haldor Topsøe A/S

Tuesday, June 8, 2004

08:00 - 09:00 Breakfast

09:00 - 09:30 **Manos Mavrikakis**: On the mechanism of the low temperature water gas shift reaction
09:30 - 10:00 **Flemming Besenbacher**: Dynamic STM studies on model systems relevant for catalysis
10:00 - 10:30 **Joost Frenken**: Experiments on working model catalysts: STM and SXRD at elevated temperatures and pressures

10:30 - 11:00 Coffee

11:00 - 11:30 **Lubomir Benco**: Active centers and reaction channels in zeolites
11:30 - 12:00 **Johannes Lercher**: Alkane activation and conversion in zeolites and anion modified oxides
12:00 - 12:30 **Herve Toulhoat**: Kinetic Monte Carlo simulations of reactions at MoS_2 Mo-edge surfaces

12:30 - 13:30 Lunch

13:30 - 14:00 **Joachim Sauer**: Understanding supported vanadium oxide catalysts - dft calculations on gas phase clusters, supported oxids and crystalline surfaces
14:00 - 14:30 **Rob Meier**: The challenge for first principles calculations in catalysis: where academic and industrial research meet
14:30 - 15:00 **Thomas Bligaard**: Implications of underlying BEP-relations on the choice of optimal catalysts
15:00 - 15:30 **Søren Dahl**: Otimal ammonia decomposition catalyst from knowledge of ammonia synthesis kinetics

15:30 - 16:00 Coffee

16:00 - 16:30 **Anders Nilsson**: Experiments on water
16:30 - 17:00 **Lars Pettersson**: Water bonding to metal surfaces
17:00 - 17:30 **Peter Strasser**: Parallel screening and fuel cell catalysis
17:30 - 18:00 **Jan Rossmeisl**: The origin of the overpotential for oxygen reduction at a fuel cell cathode

18:00 Dinner

20:00 **Poster session -** refreshments are sponsored by Haldor Topsøe A/S

Wednesday, June 9, 2004

08:00 - 09:00 Breakfast

09:00 - 09:30 **Bengt Lundqvist**: Aspects of molecule-surface interactions
09:30 - 10:00 **Jörg Behler**: Non-adiabatic spin effects in oxygen dissociation at Al(111)
10:00 - 10:30 **Geert-Jan Kroes**: Quantum dynamics of H_2 dissociation on metal surfaces: success stories and problems

10:30 - 11:00 Coffee

11:00 - 11:30 **Brian Hayden**: Electro-catalysis at alloy surfaces
11:30 - 12:00 **Axel Gross**: Problems in electrocatalysis addressed by electronic structure calculations
12:00 - 12:30 **Dave Thompsett**: Fuel cell catalysis

12:30 - 13:30 Lunch

13:30 - 14:00 **Hannes Jónsson**: Structure and dynamics of small Pd clusters on MgO(100)
14:00 - 14:30 **Bjørk Hammer**: Special reaction sites at oxide supported metal clusters
14:30 - 15:00 **Mathieu Digne**: Acidic and basic properties of g-alumina surfaces: a DFT study
15:00 - 15:30 **Ebbe Kruse Vestergaard:** High pressure STM studies of metal and alloy surfaces: Adsorption induced phase separation

15:30 Coffee / Departure

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- Carbon nanofibre growth: A DFT study
  (Frank Abild-Pedersen)

- On the ease of surface reduction of vanadia based systems
  (Veronica Ganduglia-Pirovano)

- Competitive Paths for Methanol Decomposition on Pt(111)
  (Jeffrey P. Greeley)

- Adiabatic and diabatic accounts of adsorption, part II
  (Anders Hellman)

- Activity differences between Type I and Type II MoS_2 based structures in hydrotreating catalysis - A density functional study
  (Berit Hinnemann)

- CO adsorption on Cu(111) surface
  (Qing Miao Hu)

- Walking on potential energy surfaces
  (Geert-Jan Kroes)

- Reactivity of oxidized Pt(111) and Pt(110)
  (Wei-Xue Li)

- H_2 dissociation on Pd(111) at high coverages
  (Nuria Lopez)

- Unexpected NO oxidation properties of Pt(111)
  (Bengt Lundqvist)

- Insight into water adsorption on metal surfaces from first principles simulations
  (Angelos Michaelides)

- Adsorption of O_2 and oxidation of CO at Au nanoparticles supported by TiO_2(110)
  (Luis Molina)

- Composition of the surface oxide on Pd(100) in an O2 and CO environment
  (Jutta Rogal)

- Dissociative Chemisorption of Hydrogen on Pt(111) and Ru(0001)
  (Jonathan Vincent)

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Center for Atomic-scale Materials Physics (CAMP)
Technical University of Denmark, Lyngby, Denmark

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