Report on Cat1P: The Psi-k/CECAM research conference – Catalysis from 1st Principles

Place:

Magleås Conference Center, Denmark

Date:

May 22-26, 2011

Sponsors:

Psi-k, CECAM, CAMD – Technical University of Denmark

Scientific Organizers:

Thomas Bligaard, Technical University of Denmark
Karsten Reuter, Technical University Munich
Jürgen Hafner, University of Vienna
Matthias Scheffler, Fritz-Haber-Institute, Berlin
Jens K. Nørskov, Stanford University

Administrative Organizer:

Marianne Ærsøe, Head of Administration
Center for Atomic-scale Materials Design, Department of Physics, Technical University of Denmark

Web-page:

http://www.cecam.org/workshop-0-569.html

In brief:

The Psi-k and CECAM joint research conference: "Catalysis from 1st Principles" was held May 22-26, 2011 at the Magleås Conference Center in Northern Sjælland in Denmark. Thanks to the 53 participants the conference there was a lively discussion at the conference, which primarily focused on the topics relating to challenges for the design of catalytic materials by first principles simulations. The conference was the 7th in the "Cat1P - Catalysis from first Principles" series that have been arranged by Matthias Scheffler, Jürgen Hafner, Jens Nørskov and colleagues. The meeting thus followed workshops in Magleås, Denmark (1999 and 2004), CECAM Lyon (2000 and 2006), and Vienna (2002 and 2009). It was also inspired by the series of 1998, 2007, and 2009 Psi-k workshops entitled "Theory meets industry" which were organized by Jürgen Hafner and colleagues. This conference was held as a European Gordon-type conference in an isolated site with natural surroundings with exclusively posters and invited talks, afternoons off, and a relatively long time scheduled for discussions around each talk.

Motivation:

Quantum theoretical calculations of extended atomic- scale systems have reached a level of speed and accuracy that allows determining many interesting materials properties directly from simulations. This gives unprecedented possibilities for addressing materials design problems from a bottom-up approach, where theoretical simulations and concepts derived from such simulations are used directly to propose new materials for subsequent experimental synthesis and testing. Solid surfaces are used extensively as catalysts in the chemical and energy industry and the development of new approaches to discovering catalysts with high efficiency, activity, stability, and selectivity are essential.

Objectives and scientific report:

The aim of the meeting was be to bring together researchers who characterize and design technical catalysts in industry, with experimental catalysis researchers, researchers who carry out computer simulations on catalytic materials and reactions, theoreticians who develop methodology enabling larger and more accurate electronic structure calculations on more complex materials and molecules, method developers who are working on the development of methods for more accurate thermodynamic and kinetics sampling, and researchers working on more general aspects of atomic-scale materials design. In this forum the challenges for the design of novel catalytic materials were to be discussed.

The main objectives of the 2011 meeting were: (i) to review and discuss the current status of and future prospects for applying *ab initio* and statistical mechanics approaches to the study of chemical processes at solid surfaces; (ii) to discuss how calculational methods are now being used as a tool for the design of new materials in general and of heterogeneous and electrochemical catalysts in particular; (iii) to discuss

recent applications and future prospects of using such approaches to understand interfaces of electrochemical and environmental importance; (iv) to discuss the possibilities for improving the present state of the art towards better describing complex compounds such as oxides and van der Waals-bonded systems; (v) to identify and analyze main obstacles for the atomic-scale simulations to be utilized more broadly as a platform for developing new catalytic materials; (vi) to inspire leading experimental researchers towards identifying which types of future experiments that could be central for synergy with the computational community in order to extend the limited existing methods for computational catalyst screening into the regime of more complex materials and compounds. All these issues were carefully addressed. Especially the roles of the atomic-scale structure at interfacial boundaries and the realistic simulation treatment of reaction conditions and their influence of structure were discussed in detail.

Programme

Sunday 22nd
Check-in possible from 16:00
18:00-19:30 Dinner
Evening session, Chair: T. Bligaard
19:30-20:20 J.K. Nørskov
20:20-21:10 A. Michaelides

Monday 23rd
7:40-8:40 Breakfast
Morning session, Chair: A. Michaelides
8:40-9:30 A. Schäfer
9:30-10:20 P. Sautet
10:20-10:50 Coffee
10:50-11:40 M. Amft
11:40-12:30 T. Ziegler
12:30-13:30 Lunch
13:30-16:00 Free time
16:00-18:00 Poster Session
18:00-19:30 Dinner
Evening session, Chair: P. Sautet
19:30-20:20 S. Piccinin
20:20-21:10 J. Rossmeisl

Tuesday 24th
7:40-8:40 Breakfast
Morning session, Chair: J. Rossmeisl
8:40-9:30 P. Raybaud
9:30-10:20 F. Mittendorfer
10:20-10:50 Coffee
10:50-11:40 N. Lopez
11:40-12:30 K.W. Jacobsen
12:30-13:30 Lunch
13:30-16:20 Free time
Afternoon session, Chair: A. Schäfer
16:20-17:10 R. Schomäcker
17:10-18:00 V. Ganduglia-Pirovano
18:00-19:30 Dinner
Evening session, Chair: P. Sautet
19:30-20:20 G. Pacchioni
20:20-21:10 M. Salmeron

Wednesday 25th

7:40-8:40 Breakfast
Morning session, Chair: F. Mittendorfer
8:40-9:30 K. Reuter
9:30-10:20 S. Dahl
10:20-10:50 Coffee
10:50-11:40 T. Bucko
11:40-12:30 M. Maestri
12:30-13:30 Lunch
13:30-16:20 Free time
Afternoon session, Chair: V. Ganduglia-Pirovano
16:20-17:10 S. Levchenko
17:10-18:00 B. Temel
18:00-19:30 Dinner
Evening session, Chair: N. Lopez
19:30-20:20 R. Horn
20:20-21:10 C. Dellago

Thursday 26th

Before 9:00 Check-out of rooms before 9:00
7:40-8:40 Breakfast
Early morning session, Chair: K. Reuter
8:40-9:30 E. Beret
9:30-10:20 B. Hammer
10:20-10:50 Coffee
Late morning session, Chair: T. Bucko
10:50-11:40 G. Jones
11:40-12:30 F. Abild-Pedersen
12:30-13:30 Lunch

List of Participants

J.K. Nørskov	Stanford
A. Michaelides	UCL
M. Salmeron	LBNL
P. Sautet	ENS-Lyon
C. Dellago	U. Vienna
T. Ziegler	U. Calgary
S. Piccinin	CNR-IOM Democritos
J. Rossmeisl	DTU
P. Raybaud	IFP
F. Mittendorfer	TU Wien
N. Lopez	ICIQ
K.W. Jacobsen	DTU
R. Horn	FHI
R. Schomäcker	TU Berlin
G. Pacchioni	U. Milano-Bicocca
F. Abild-Pedersen	SLAC
K. Reuter	TU München
S. Dahl	CASE/DTU
T. Bucko	Comenius University
M. Maestri	Politecnico di Milani
S. Levchenko	FHI
B. Temel	Haldor Topsøe A/S
V. Ganduglia-Pirovano	I. Catal. & Petrochem., Madrid
A. Schäfer	BASF
E. Beret	FHI
B. Hammer	U. Aarhus
G. Jones	Johnson Matthey
M. Amft	U. Uppsala
T. Bligaard	SLAC
J. Wellendorff	DTU
K. Lundgård	DTU
H. Falsig	DTU
A. Toftelund	DTU
T. Khan	DTU
J. Howalt	DTU
V. Tripkovic	Comp. Mat. Design ApS
ZhenHua Z.	DTU
M. Karamad	DTU
S. Siahrostami	DTU
N. Ammitzbøll	DTU
I. Man	DTU
L. Vilhelmsen	U. Aarhus
A. Rasmussen	U. Aarhus
H. Gao	U. Aarhus
Seung-Cheul Lee	Korea Institute of Science & Technology
C. Mangold	FHI
F. Göltl	U. Vienna
C. Ebensperger	U. Erlangen
D. Karhanek	ICIQ
K. Kwapien	Humboldt-U. Berlin
M. Petersen	Sasol
K. Andersen	DTU
M. Björketun	DTU