

# Catalysis from First Principles

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# 1 Workshop Details

## Timing

Number of days : 4

Start : 2006-09-11

end : 2006-09-14

## Location of the activity

CECAM

46 allé e d'Italie

69007 Lyon

France

# 2 Proposal

## 2.1 Scientific Background

The properties of surfaces and the processes that occur on them are relevant to many aspects of daily life and scientific endeavor. The efficiency of numerous heterogeneous catalysts and electrochemical devices depends directly, for example, on reactions that occur at precious metal surfaces. The key to future advances in these areas is to understand surface processes at the atomic level. One way to reach this understanding is through first-principles simulations and indeed such simulations have now reached a state of maturity such that they can contribute toward the development of new catalysts [1] or make faithful predictions about any number of surface properties [2-3]. Increasingly such first-principles electronic structure approaches are being combined with techniques from statistical mechanics and thermodynamics in order to understand the statistical mechanical interplay of the (typically) many elementary reaction steps that take place “in concert” on the surface of a working (heterogeneous) catalyst [4]. The power of this combined, multiscale modeling, approach is also increasingly being exploited to make predictions about the properties of catalytic substrates at the high pressures and temperatures at which the majority of catalytic processes operate. Successfully combining these techniques and in so doing “bridging” the often-discussed pressure and materials gaps that separate the atomic zero-temperature zero-pressure regime of electronic structure calculations from the more realistic conditions of industrial catalysis remains one of the grand challenges of catalysis research. It is an aim of this workshop to bring together leading experts and practitioners from the electronic structure theory and statistical mechanics communities to discuss the prospects and potential for further coupling of these approaches leading to future “first principles catalytic design”. Further, since there is an often symbiotic relationship between experiment and theory in this area, with many sophisticated experimental surface probes relying on theoretical modeling for their quantitative interpretation, experimental surface science and catalysis practitioners will also be invited.

## 2.2 Motivations and Objectives

The main objectives of this meeting are: (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 heterogeneous and electrochemical catalysts; (iii) to discuss recent applications and future prospects of using such approaches to understand interfaces of electrochemical and environmental (atmospheric) importance; and (iv) to bring together researchers from the electronic structure, the molecular-dynamics and the statistical physics communities, as well as experimental surface-science and catalysis researchers from academia and industry. This meeting will be the fifth in the “Catalysis from first Principles” series, and will follow successful workshops in Magleas, Denmark (1999 and 2004), CECAM Lyon (2000) and Vienna (2002).

## 2.3 Format

A small meeting with about 40 participants, in the approximate ratio theory:experiment:industry 2:1:1, is envisaged. The meeting will take place in September 2006 and will run for three and a half days. We plan to arrange about 20-25 thirty-five minute review talks by invited experts, about 10 twenty minute contributed talks and one introductory presentation by a highly distinguished experimental colleague. In accordance with the character of the event as a workshop, ample time will be reserved for discussion, including a wrap-up discussion at the end of the event and a poster session for a small number of graduate students (in the final phase of their doctoral studies) and other next-generation young scientists.

## 2.4 Budget

The budget that can be requested from CECAM depends on the total number of days of the activity. For the present activity, the requested budget will be 10000 €

### Comments on the budget

The projected local cost per participant, which includes accommodation for three nights in Lyon and meals, is 250 EUR. This comes to a total of 10,000 EUR for which we request support from CECAM. In addition we plan to support the travel expenses of some speakers, particularly the younger speakers and those from China, for this we will request 9,000 EUR from Psi-k.

## 3 Participant List

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## 4 Requested Support

CECAM

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Psi-k



## 5 Key references

[1] F. Besenbacher, I. Chorkendorff, B.S. Clausen, B. Hammer, A.M. Molenbroek, J.K. Norskov, and I. Stensgaard, *Design of a Surface Alloy Catalyst for Steam Reforming*, *Science* **279** 1913 (1998)

[2] K. Reuter, C. Stampfl, and M. Scheffler, *Ab initio atomistic thermodynamics and statistical*

*mechanics of surface properties and functions*, Handbook of Materials Modeling. ((Ed.) Sidney Yip. Springer, The Netherlands) **1** 149 (2005)

[3] J. Greeley, J. K. Nørskov, and M. Mavrikakis, *Electronic Structure and Catalysis on Metal Surfaces*, Annual Reviews of Physical Chemistry **53** 319 (2002)

[4] K. Reuter, D. Frenkel, and M. Scheffler, *The steady state of heterogeneous catalysis*, Phys. Rev. Lett. **93** 116105 (2004)