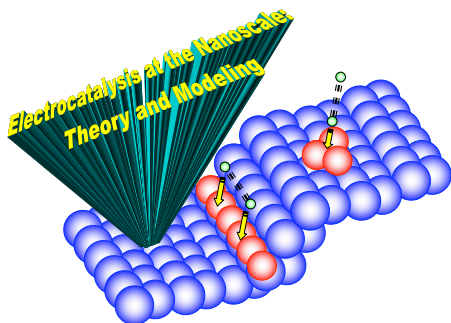


ANNEX VII. 2nd TRAINING SCHOOL – REGENSBURG CASTLE, near ULM

The 30 participants received a CD that includes:

- A folder with fundamental papers
- A folder with the lectures given
- A folder with tutorials
- A folder with a collection of pictures taken during the School

The program is presented in the following pages



U Ulmer
UG Universitäts-
Gesellschaft

Electrocatalysis at the Nanoscale: Theory and Modeling

Oct. 4 till Oct. 8, 2009, Reisenburg Castle near Ulm, Germany

Programme

Sunday, Oct. 4, 16:00 - 19:00: Registration

Monday, Oct. 5

Fundamentals of Electrocatalysis at Surfaces

chairman A. Colina

9:00 Opening Remarks

9:10 Prof. Renat Nazmutdinov

Theory of electrochemical outer sphere electron transfer

10:00 Prof. Elizabeth Santos

Anderson-Newns theory applied to electrocatalysis

10:50 Coffee break

chairman D. Fermin

11:20 Dr. Karsten Reuter

First principles modelling of surface physics and catalysis

12:10 Dr. Francesc Vines

Modeling of Supported Metal Nanoparticles to Study Surface Processes by Density Functional Methods

13:00 lunch

15:00 Round Table discussion: A. Colina, D. Fermin, and this mornings speakers.

16:30 tutorials and group discussions Concepts for electronic structure: bands in solids, projected densities of states, d-band model, Wannier orbitals

Tuesday, Oct. 6
Reactions of Special Interest

chairman V. Ruiz

9:00 Prof. Axel Groß

Electrochemical methanol oxidation

9:50 Dr. Paola Quaino

Hydrogen oxidation and evolution on platinum.

10:40 Coffee break

chairman R. Dryfe

11:10 Prof. Wolfgang Schmickler

Hydrogen evolution on nanostructures

12:00 Dr. Itai Panas

Modelling electrocatalysis on oxides

13:00 lunch

15:00 Round Table discussion: Virginia Ruiz, Robert Dryfe, and this mornings speakers.

16:30 tutorials and group discussions tutorials and group discussions

concepts for using quantum-chemical packages; selection criteria, basis sets, energy cut-off, k points

Wednesday, Oct. 7
Heterogeneous Catalysis

chairman E. Santos

9:00 Dr. Frederik Tielens

Characterization of transition-metal doped silica materials using experiment and theory

9:40 Dr. Guido Mul

The quest for artificial photosynthesis using photo- and electrocatalysis

10:20 Dr. Monica Calatayud given by Dr. Frederick Tielens

Surface hydroxyle groups: structure and reactivity from periodic DFT.

11:00 Coffee break

chairman W. Schmickler

11:30 Dr. Anna Maria Venezia

Supported Bimetallic catalysts: electronic and geometric effects.

12:10 Dr. Miguel Bañares

Raman spectroscopy during reaction, an insight on the working catalyst, modeling and reality

13:00 lunch

15:00 Round table discussion on relation between heterogeneous and electrocatalysis

16:30 tutorials and group discussions tutorials and group discussions

Introduction to imulations techniques and programming.

Thursday, Oct. 8
Simulation and Modelling

chairman P. Unwin

9:00 Dr. Cecilia Gimenez

Kinetic Monte Carlo Simulations of electrochemical surface processes

9:50 Prof. Eckhard Spohr

Classical Molecular Dynamics of electrochemical reactions

10:40 Coffee break

chairman J. Macpherson

11:10 Dr. Timo Jakob

Ab initio molecular dynamics

12:00 Prof. Marc Koper

Closing lecture: Opportunities for theory in electrocatalysis.

13:00 lunch

Tutorials will be given by the Department of Theoretical Chemistry, University of Ulm, and its guests. Provisional list of tutors: Dr. Noelia Luque, German Soldano, Dr. Paola Quaino, Dr. Angelika Lundin, and the organizers.