

Winter School in Theoretical Chemistry 2008

Reactions on Surfaces - Towards Realistic
Computational Modelling of Surface Reactions

December 10th-12th, 2008

Department of Chemistry, University of Helsinki,
A.I. Virtasen aukio 1, Helsinki, Finland

Lecturers are:

Karoliina Honkala, University of Jyväskylä
Ari Seitsonen, University of Pierre and Marie Curie, Paris
Thomas Bligaard, Danish Technical University, Copenhagen

More information about it can be found on the web page:

<http://www.chem.helsinki.fi/Info/WinterSchool/ws2008.html>

Preliminary program:

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Date Time Lecture & content

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Wed 10/12

09:15	Welcome
09:30	DFT intro (Seitsonen) Why Density Functional Theory ? Short introduction to DFT How to calculate exchange energy
10:15	DFT intro continues: practical issues (Seitsonen) K-points, pseudo potentials, different methods to calculate reaction barriers, modeling a surface with a slab
11:00	Break
11:30	Adsorption and activation energies (Seitsonen) Atomic, molecular, dissociative adsorption LH and ER reaction mechanisms
12:15	Lunch
13:15	More about adsorption and reactions (Seitsonen/Honkala) Flat and stepped surfaces, clusters, thin films, alloys, Sabatier's principle
14:00	Towards realistic systems: part I (Honkala) Special adsorption sites (geometric versus electronic effects) pressure and temperature gaps, the role of the adsorbate coverage

14:45 Break

15:15 Towards realistic systems: part II (Honkala)
d-band model, Bronsted-Evans-Polanyi relation,
compensation effect

16:00 Towards realistic systems: part III (Honkala)
comparison of theoretical results to experimental findings
reactions: beyond CO oxidation

16.45 Poster session

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Thu 11/12

09:00 Atomistic thermodynamics part I (Seitsonen/Honkala)
What is it ?
Introduction to atomistic thermodynamics

09:45 Atomistic thermodynamics part II (Honkala)
More details

10:30 Break

11:00 Microkinetics (Honkala)
Introduction to the microkinetics, harmonic transition
state theory, apparent reaction barriers, reaction orders

11:45 Lunch

13:00 Combining DFT with other methods (Honkala)
What does this mean ?
Combining DFT to Monte Carlo
Case story: Ammonia synthesis

13:45 Ammonia synthesis from first principles (Honkala)
directly from DFT calculations to the activity
of real nanoparticle catalyst under industrial conditions

14:30 Break

15:00 Case stories (Seitsonen)

15:45 Case stories (Seitsonen)

16:30 Poster session

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Fri 12/12

10:15 Conceptualizing the electronic structure of transition metal
surfaces (Bligaard)

11:00 Linear energy relations & microkinetics (Bligaard)
Universality in Volcano curves

Scaling relations for various systems

11:45 Lunch

12:45 Case stories (Bligaard)
Methanation reaction, selective acetylene hydrogenation

13:30 The future in Computational Materials design (Bligaard)

14:15 Departure

Cordially,
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