

**International Summer School on Basic Concepts
and First-Principles Computations for Surface Science:
Applications in Chemical Energy Conversion and Storage**

Norderney, Germany; July 21-26, 2013

Program

Sunday, July 21, 2013

- 15:00 – 16:30 Registration
16:30 – 19:00 Session: *Basics*
Electronic Structure Theory (M. Scheffler)
Treating surfaces: Clusters vs. supercells (L. Ghiringhelli)
19:00 – 20:30 Dinner
20:45 – 22:00 Session: *Surface Spectroscopy*
Surface science approach, experimental techniques (M. Weinelt)

Monday, July 22, 2013

- 9:00 – 13:00 Session: *Molecular Nanoscience*
Organics at surfaces, self-assembly (Ch. Wöll)
Bonding at surfaces (A. Tkatchenko)
11:00 – 11:30 Coffee break
Hot topic 1: DFT self-interaction failures (N. Marzari)
13:00 – 15:00 Discussions & Break
15:00 – 19:00 Session: *Materials for Energy*
High throughput, materials genome (N. Marzari)
16:00 – 16:30 Coffee break
Scaling relations (A. Vojvodic)
Hot Topic 2: Bulk doping effects in hybrid organic/inorganic systems from quantum mechanical first principles (P. Rinke)
Hot Topic 3: Femtomagnetism: The transient band structure of Gadolinium (M. Weinelt)
19:00 – 20:30 Dinner
20:30 – 22:30 Poster Session I (even numbered posters)

Tuesday, July 23, 2013

- 9:00 – 13:00 Session: *From Energy to Kinetics*
Reactions at surfaces (C. Friend)
Barrier calculations (G. Henkelman)
11:00 – 11:30 Coffee break
Hot topic 4: First-principles based catalytic reaction engineering (M. Maestri)
13:00 – 15:00 Discussions & Break
15:00 – 19:00 Session: *Heterogeneous Catalysis*
Microkinetic modeling (K. Reuter)
16:00 – 16:30 Coffee break
Heat and mass transport (M. Maestri)
Hot topic 5: Chemistry and Catalysis on Alloy surfaces (C. Friend)
Hot topic 6: Why (100) terraces make and break bonds (M. Koper)

- 19:00 – 20:30 Dinner
20:45 – 22:00 Session: *Excited States*
Electronic excitations, computational spectroscopy (P. Rinke)

Wednesday, July 24, 2013

- 9:00 – 13:00 Session: *Light harvesting*
Molecular levels at surfaces, optical properties (A. Selloni)
Photocatalysis at surfaces (M. Nest)
- 11:00 – 11:30 Coffee break
Hot topic 7: Space charge transfer at metal-oxide surfaces (M. Scheffler)
- 13:00 – 15:00 Discussions & Break
- 15:00 – 19:00 Session: *Photovoltaics*
Solar cells (C. Persson)
- 16:00 – 16:30 Coffee break
Charge transfer (H. Oberhofer)
Hot topic 8: Intriguing physics of on Cu-based solar cell materials (C. Persson)
Hot topic 9: Advances in electron dynamics with real-time time-dependent density-functional theory (M. Nest)
- 19:00 – 20:30 Dinner
20:30 – 22:30 Poster Session II (odd numbered posters)

Thursday, July 25, 2013

- 9:00 – 14:00 Session: *Electrochemistry*
Solid-liquid interfaces and external bias (A. Groß)
Electrocatalysis (M. Koper)
- 11:00 – 11:30 Coffee break
Hot topic 10: Hybrid organic/inorganic systems:
Blurring borders between chemisorption and physisorption
(A. Tkatchenko)
Hot topic 11: Lowering reaction barriers at surfaces through concerted
reaction mechanisms (A. Groß)
- 14:00 – 17:00 Discussions & Break
- 17:30 – 19:30 Conference Outing: Mudflat Hiking at the Wadden Sea
- 20:30 – 22:30 Conference Dinner

Friday, July 26, 2013

- 9:30 – 12:30 Session: *Modeling: Quo vadis?*
Theory and experiment in heterogeneous catalysis (J. Nørskov)
- 11:00 – 11:30 Coffee break
Perspective on battery research (A. Luntz)
Thermoelectrics (M. Verstraete)
- 13:00 Departure