Modern developments in the ab initio description of charged systems for semiconductors and electrochemistry

Schedule

Sunday, 23. 10.

16.00–18.30 *Registration*
18.30 *Dinner*
20.00–21.30 **Chris Van de Walle**: First-principles calculations for defects and impurities: hydrogen in oxides and nitrides

Monday, 24.10.

09.00–10.30 **Wolfgang Schmickler**: Modelling electrochemical charge-transfer reactions
10.30–10.45 *Coffee*
10.45–12.00 **Dominik Marx**: H^+(aq) and OH^-(aq)
12.30 *Lunch*
14.00–15.15 **Kersti Hermansson**:
15.15 *Coffee*
15.30–16.45 **Richard Hennig**: Quantum Monte Carlo for defects in solids and solvation of molecules and surfaces
16.45–18.00 **Georg Kresse**: Hybrid functionals applied to extended systems
18.30 *Dinner*
20.00–21.30 Poster

Tuesday, 25.10.

09.00–10.15 **Mira Todorova**: Extending the concept of semiconductor defect chemistry to electro-chemistry: constructing electro-chemical E/pH diagrams based on ab-initio calculations
10.15–10.30 *Coffee*
10.30–11.45 **Axel Groß**: First principles description of structures and processes at electrode-electrolyte interfaces
12.30 *Lunch*
13.30–15.45 *Excursion*
15.45 *Coffee*
16.00–17.15 **Paolo Umari**: Large scale GW calculations with optimal polarizability basis sets and Lanczos chains
17.15–17.45 **Shengbai Zhang**: Charged dopants in semiconductor nanowire under partially periodic boundary conditions
17.45–18.15 **Hannu-Pekka Komsa**: Comparison of various finite-size supercell correction schemes for charged defect calculations
18.30 *Conference Dinner*

Wednesday, 26.10.

09.00–10.15 **Christoph Freysoldt**: Charge corrections in supercells
10.15–10.30 *Coffee*
10.30–11.45 **Eckhard Spohr**: Atomistic modeling of electrochemical reactions at the liquid/solid interface
12.30 *Lunch*