

The CAMD Summer School

Electronic Structure Theory and Materials Design 2016

Program:

Saturday, August 13: Arrival and registration

Sunday, August 14:

- 11:30-13:15 Registration and lunch
- 13:15-13:30 Welcome
- 13:30-14:30 Density Functional Theory and its Extensions - *tutorial* (Hardy Gross)
- 14:30-15:00 Coffee break
- 15:00-16:00 Projector augmented wave method and the GPAW code (Jens Jørgen Mortensen)
- 16:00-18:00 Setting up for computer exercises

Monday, August 15:

- 09:30-10:30 Materials Design and Catalysis (Jens K. Nørskov)
- 10:30-11:00 Coffee break
- 11:00-12:00 Catalysis informatics (Thomas Bligaard)
- 12:00-13:30 Lunch
- 13:30-14:30 Materials Design with Databases (Christopher Wolverton)
- 14:30-15:00 Coffee break
- 15:00-16:00 Multiscale Modeling of Catalytic Processes (Karsten Reuter)
- 16:00-18:00 Computer exercises
- 18:00-20:00 Poster session

Tuesday, August 16:

- 09:30-10:30 Many-Body Perturbation Theory - *tutorial* (Patrick Rinke)
- 10:30-11:00 Coffee break
- 11:00-12:00 Ultrafast electronic processes (Andrea Marini)
- 12:00-13:30 Lunch
- 13:30-14:30 2D materials and heterostructures (Kristian S. Thygesen)
- 14:30-15:00 Coffee break
- 15:00-16:00 Correlation energies beyond the Random Phase Approximation (Thomas Olsen)
- 16:00-18:00 Computer exercises

Wednesday, August 17:

- 09:00-10:00 Berry Phase Physics from First Principles - *tutorial* (Ingrid Mertig)
- 10:00-10:30 Coffee break
- 10:30-11:30 Non-collinear Magnetism and Spin-Orbit coupling in DFT - *tutorial* (Stefan Blügel)
- 11:30-12:30 Lunch
- 12:30-13:30 Graphene nanoelectronics (Mads Brandbyge)
- 13:30-14:30 Large-scale GW calculations (Giulia Galli)
- Rest of the day: Excursion and social dinner

Thursday, August 18:

09:30-10:30	Machine learning and density functionals - <i>tutorial</i> (Karsten W. Jacobsen)
10:30-11:00	Coffee break
11:00-12:00	Simulating nanoparticles at the atomic and electronic scale (Jakob Schiøtz)
12:00-13:30	Lunch
13:30-14:30	Orbital-density-dependent functionals (Nicola Marzari)
14:30-15:00	Coffee break
15:00-16:00	Electronic Structure Theory on the World Market (Kurt Stokbro)
16:00-18:00	Computer exercises

Friday, August 19:

09:30-10:30	Electrochemistry (Jan Rossmeisl)
10:30-11:00	Coffee break
11:00-12:00	Electrochemical energy conversion and storage (Tejs Vegge)
12:00-13:30	Lunch
13:30-14:30	Computational Materials Science and the Future (Matthias Scheffler)
14:30-15:00	Closing remarks