

The CAMD Summer School

Electronic Structure Theory and Materials Design 2018

Program:

Sunday, August 12:

11:30-13:15 Registration and lunch
13:15-13:30 Welcome
13:30-14:30 Fundamentals of DFT and TDDFT - *tutorial* (Hardy Gross)
14:30-15:00 Coffee break
15:00-16:00 Electronic structure tools: ASE and GPAW - *tutorial* (Jakob Schiøtz)
16:00-18:00 Computer exercises
19:00 Dinner

Monday, August 13:

06:30-09:30 Breakfast
09:30-10:30 Rate Theory (Hannes Jonsson)
10:30-11:00 Coffee break
11:00-12:00 Computational Design in Catalysis (Jens Nørskov)
12:00-13:30 Lunch
13:30-14:30 Structures and Reactions at Surfaces (Bjørk Hammer)
14:30-15:00 Coffee break
15:00-16:00 Electrochemistry - *tutorial* (Jan Rossmeisl)
16:00-18:00 Computer exercises
18:00-20:00 Poster session

Tuesday, August 14:

06:30-09:30 Breakfast
09:30-10:30 Many-Body Perturbation Theory - *tutorial* (Georg Kresse)
10:30-11:00 Coffee break
11:00-12:00 Theoretical Spectroscopy (Claudia Draxl)
12:00-13:30 Lunch
13:30-14:30 2D materials (Nicola Marzari)
14:30-15:00 Coffee break
15:00-16:00 Excitations in 2D materials (Kristian S. Thygesen)
16:00-18:00 Computer exercises
19:00 Dinner

Wednesday, August 15:

06:30-09:00 Breakfast
09:00-10:00 Machine Learning Basics (Karsten W. Jacobsen)
10:00-10:30 Coffee break
10:30-11:30 Machine Learning and Materials Science (Christopher Wolverton)
11:30-12:30 Lunch
12:30-13:30 Machine Learning and Chemistry (Anatole von Lilienfeld)
13:30-14:30 Machine Learning and Structural Search (Bjørk Hammer)
Rest of the day: Excursion and social dinner

Thursday, August 16:

06:30-09:30 Breakfast
09:30-10:30 Spin-orbit physics (Thomas Olsen)
10:30-11:00 Coffee break
11:00-12:00 Topological States of Matter (Yan Sun)
12:00-13:30 Lunch
13:30-14:30 Materials Informatics (Thomas Bligaard)
14:30-15:00 Coffee break
15:00-16:00 Discovery of Novel Electronic Materials (Stefano Curtarolo)
16:00-18:00 Computer exercises
19:00 Dinner

Friday, August 17:

06:30-09:30 Breakfast
09:30-10:30 Materials Modelling for Solar Cells: Perovskites and Beyond (Aron Walsh)
10:30-11:00 Coffee break
11:00-12:00 Batteries (Tejs Vegge)
12:00-13:30 Lunch
13:30-14:30 The Future of DFT (Kieron Burke)
14:30-15:00 Closing remarks