

The CAMD Summer School
Electronic Structure Theory and Materials Design 2018

TENTATIVE 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 Setting up for computer exercises

Monday, August 13:

- 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:

- 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

Wednesday, August 15:

- 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 Materials Informatics (Thomas Bligaard)
- Rest of the day: Excursion and social dinner

Thursday, August 16:

09:30-10:30	Spin-orbit physics (Thomas Olsen)
10:30-11:00	Coffee break
11:00-12:00	Topological States of Matter (Claudia Felser)
12:00-13:30	Lunch
13:30-14:30	TBD (TBA)
14:30-15:00	Coffee break
15:00-16:00	Discovery of Novel Electronic Materials (Stefano Curtarolo)
16:00-18:00	Computer exercises

Friday, August 17:

09:30-10:30	Solar Cells (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