

Tuesday, February 28th 2017
(BCCMS, TAB Building, Entrance F, Ground Floor)

- 08:30 - 09:30 **Registration**
- 09:30 - 09:50 **Opening and welcome, Thomas Frauenheim**
- Session:** **Electronic structure theory**
Chair:
- 09:50 - 10:35 *Johannes Lischner, Imperial College London, UK*
Density Functional and Many-Body Perturbation Theory
- 10:35 - 11:20 *Weitao Yang, Duke University, US*
Exchange correlation functionals and computational approaches
- 11:20 - 11:50 **Coffee Break**
- 11:50 - 12:35 *Frank Lechermann, University of Hamburg, Germany*
Introduction to strongly correlated electron systems / Model Hamiltonians
- 12:35 - 13:20 *Dominika Zgid, University of Michigan, US*
Quantum chemistry, wave function methods and correlated electrons
- 13:20 - 14:40 **Lunch Break and Coffee (Restaurant Café Unique)**
- Session:** **Metal oxides**
- 14:40 - 15:25 *Katharina Al-Shamery, University of Oldenburg, Germany*
Surface photochemistry and photovoltaics
- 15:25 - 16:10 *Louis F. J. Piper, Binghamton University, US*
Electronic structure of transition metal oxides
- 16:10 - 16:40 **Coffee Break**
- 16:40 - 17:00 *Vladimir Bacic, Jacobs University Bremen, Germany*
Introduction to the DFT calculation of phonon dispersions with application to 2d materials
- 17:00 - 17:20 *Gunnar Schönhoff, University of Bremen, Germany*
Description of charge order, superconductivity and magnetism in 2d materials
- 18:30 - 22:00 **Dinner (Restaurant StadtWIRT)**

Wednesday, March 1st 2017
(BCCMS, TAB Building, Entrance F, Ground Floor)

- Session:** **2d Materials**
Chair:
- 09:00 - 09:45 *Thomas Heine, University of Leipzig, Germany*
Introduction to 2d materials
- 09:45 - 10:30 *Miguel Moreno Ugeda, University of the Basque Country, Spain*
Interaction effects in 2d materials
- 10:30 - 11:00 **Coffee Break**
- 11:00 - 11:45 *Ursula Wurstbauer, Technical University of Munich, Germany*
Optics and light matter interaction in 2d materials
- Session:** **Non-equilibrium and time-dependent physics**
Chair:
- 11:45 - 12:30 *Heiko Appel, Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany*
Introduction to time-dependent density functional theory
- 12:30 - 13:15 *Michael Lorke, University of Bremen, Germany*
Introduction to Keldysh Green functions
- 13:15 - 14:30 **Lunch Break and Coffee (Restaurant Café Unique)**
- 14:30 - 15:15 *Dmitry Ryndyk, University of Bremen, Germany*
Introduction to theoretical and computational quantum transport
- 15:15 - 15:45 **Coffee Break**
- 15:45 - 16:30 *Ulrich Kleinekathöfer, Jacobs University Bremen, Germany*
Exciton dynamics using mixed quantum-classical simulations
- 16:30 - 16:50 *Alexander Steinhoff, University of Bremen, Germany*
Influence of Excited Carriers on the Optical and Electronic Properties of Transition Metal Dichalcogenides
- 17:00 - 19:30 **Poster Session, Fingerfood Buffet**

Thursday, March 2nd 2017
(BCCMS, TAB Building, Entrance F, Ground Floor)

- Session:** **Structural Complexity and Environmental Effects**
Chair:
- 09:00 - 09:45 *Bálint Aradi, University of Bremen, Germany*
Introduction to the density functional tight binding method
- 09:45 - 10:30 *Lucio Colombi Ciacchi, University of Bremen, Germany*
Introduction to Force Field Methods
- 10:30 - 11:00 **Coffee Break**
- 11:00 - 11:20 *Thomas Teusch, University of Oldenburg, Germany*
Adsorption studies of ground and excited states of SO2 on the rutile(110) surface
- 11:20 - 11:40 *Meisam Farzalipour Tabriz, University of Bremen, Germany*
The challenges of calculating charge-transfer reactions across the interface
- 11:40 - 12:00 **Closing words: Thomas Frauenheim**
- 12:00 - 14:00 **Internal Meeting: 1st Year Planning**

