mpsd

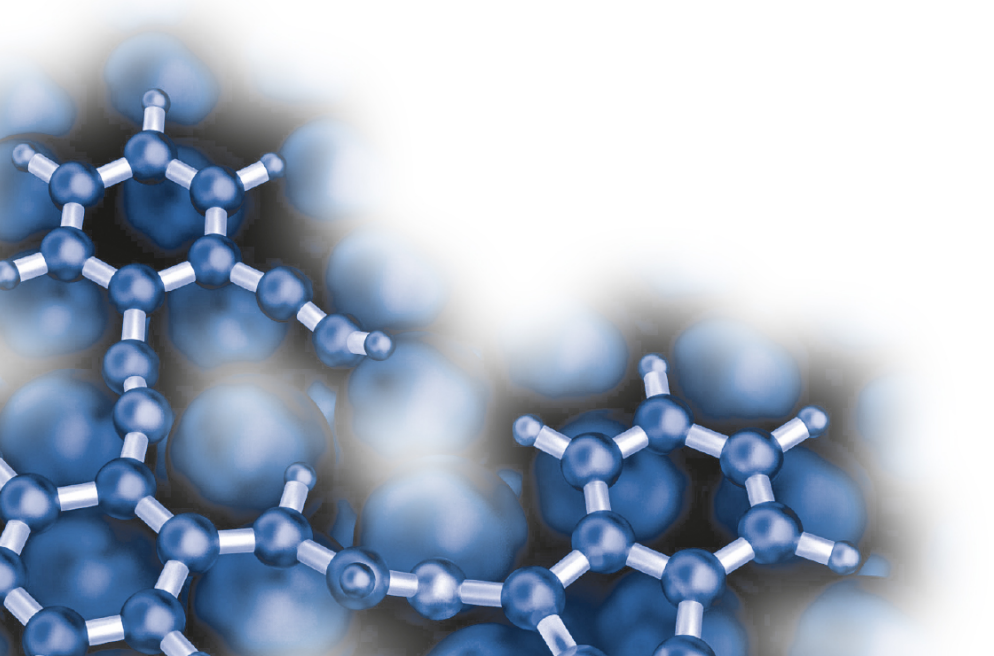
Max-Planck-Institut für
Struktur und Dynamik der Materie

Workshop on

Theoretical challenges: simulating materials out of equilibrium

CFEL, Hamburg, June 1–3, 2016

Workshop Program



Wednesday, June 1, 2016

17.00 Welcome and introduction: Andrea Cavalleri

17.10 Grußworte ("greetings"):

- Eberhard Bodenschatz, Chairperson of the Chemistry, Physics, and Technology Section of the Max Planck Society
- Jan Louis, Head of the Physics Department of the University of Hamburg
- Dr. Hermann Franz, Deputy Director in charge of Photon Science, DESY

17.40 Scientific Introduction: Angel Rubio

18.00 Reception

Thursday, June 2, 2016

8.50-9.00	Matthias Scheffler (Fritz Haber Institute of the Max Planck Society) *In Memoriam of Walter Kohn*
9.00-9.40	Andrea Cavalleri (MPSD) *Optical control of collective phenomena in solids*
9.40-10.20	Matthias Scheffler (Fritz Haber Institute of the Max Planck Society) *Patterns, Correlations, and Causality in Big Data of Materials: Analytics for Novel Materials Discovery*
10.20-11.00	Massimo Altarelli (European XFEL) *Some Theoretical Challenges from X-ray Free-Electron Lasers*
11.00-11.30	*Coffee break*
11.30-12.10	Ignacio Franco (University of Rochester) *Stark control of electrons along nanojunctions*
12.10-12.35	Michael Sentef (MPSD) *Light-induced new states of matter in solids: Prospects, concepts, and challenges*
12.35-13.00	Hannes Hübener (University of the Basque Country) *Creating stable Floquet-Weyl semimetals by laser-driving of 3D Dirac materials*
13.00-13.30	*Lunch break*
13:30-14:30	Discussion Session
14.30-15.10	Eberhard Gross (Max Planck Institute of Microstructure Physics) *Ultrafast laser-induced demagnetisation of solids: Understanding the mechanism with real-time TDDFT simulations*
15.10-15.50	Walter Thiel (Max-Planck-Institut für Kohlenforschung) *Surface-hopping excited-state dynamics*
15.50-16.15	Guillermo Albareda (University of Barcelona) *Towards ab-initio Molecular Dynamics without Born-Oppenheimer Potential-Energy Surfaces*
16.15-16.45	*Coffee break*
16.45-17.25	Erio Tosatti (SISSA / ICTP / DEMOCRITOS) *Mechanical Non-equilibrium — Nanofriction*
17.25-17.50	Michael Ruggenthaler (MPSD) *Light-matter coupling in density-functional theory for quantum electrodynamics (I)*
17.50-18.15	Heiko Appel (MPSD) *Light-matter coupling in density-functional theory for quantum electrodynamics (II)*

Friday, June 3, 2016

9.40-10.20	Raffaele Resta (Università di Trieste / DEMOCRITOS) *Orbital Magnetization*
10.20-11.00	Ignacio Cirac (Max Planck Institute of Quantum Optics) *Tensor Network Techniques and systems out of equilibrium*
11.00-11.30	*Coffee break*
11.30-11.55	Umberto De Giovannini (University of the Basque Country) *Time-resolved ARPES from first principles and applications*
11.55-12.20	Alberto Castro (ARAID Foundation / Universidad de Zaragoza) *Optimal control of electron dynamics*
12.20-13.00	Lucia Reining (École Polytechnique / ETSF) *Fingerprints of electron correlation in materials:* *understanding and predictions from electronic structure theory*
13.00-14.00	*Lunch break*
14:00-15:30	Hamburg Photon Science Colloquium: Roberto Car (Princeton University) *Water: from ab-initio simulations to coarse grained models*