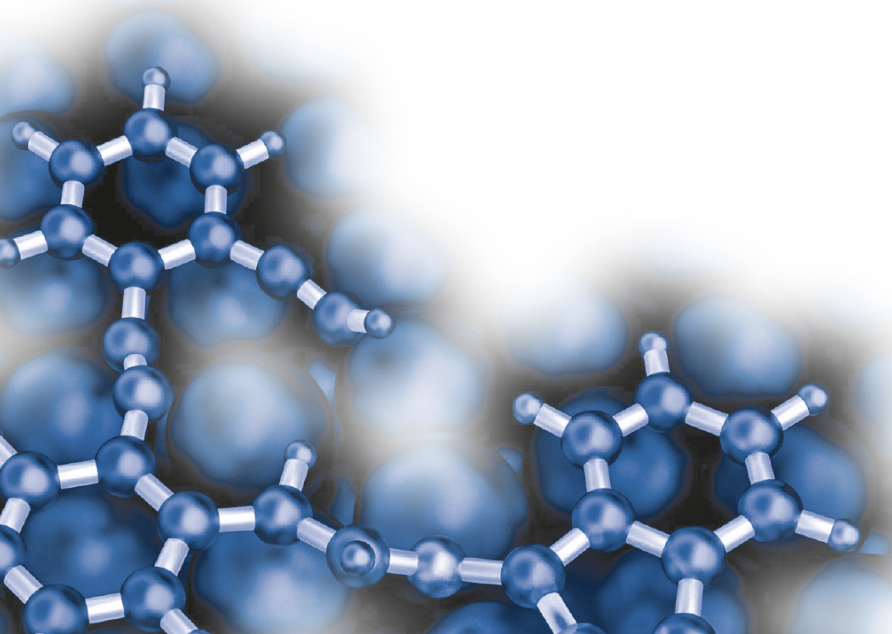


Workshop on

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