cecam Centre Européen de Calcul Atomique et Moléculaire 2017

Charge carrier dynamics in nanostructures: optoelectronic and photo-stimulated processes

Bremen Center for BCCMS Computational Materials Science

Tuesday, October 10th 2017
(House of Science Bremen/Downtown)

08:00 - 08:50 **Registration**

08:50 - 09:00 **Opening and welcome, Thomas Frauenheim**

Session: **Energy and charge transfer I**
Chair:

09:00 - 09:40 Gregory D. Scholes, Princeton University, New Jersey (US)
Is there a functional role for coherence in charge transfer reactions?

09:40 - 10:20 Yosuke Kanai, University of North Carolina at Chapel Hill (US)
First-principles modeling of excited electron dynamics at heterogene-ous interface

10:20 - 10:50 **Coffee Break**

10:50 - 11:30 Oleg V. Prezhdo, University of Southern California, Los Angeles(US)
Excited state dynamics in nanoscale materi-als for solar energy harvesting

Session: **Energy and charge transfer II**

11:30 - 12:10 Thomas A. Niehaus, University of Lyon (France)
Light absorption of contacted molecules

12:10 - 12:50 Jochen Blumberger, University College London (UK)
Fragment orbital-based surface hopping for simulation of charge transport in organic and biological molecules and materials

12:50 - 13:00 **Group photo**

13:00 - 14:30 **Lunch Break (Restaurant Stadtwirt) and Coffee**

Session: **Photo-induced processes**
Chair:

14:30 - 15:10 Ignacio Franco, University of Rochester, New York (US)
Stark control of electrons

15:10 - 15:50 Elisa Molinari, University of Modena and Reg-gio Emilia (Italy)
Bridging atomistic and coarse-grained simula-tions for unraveling long-time scale membra-ne protein dynamics

15:50 - 16:20 **Coffee Break**

16:20 - 17:00 Sheng Meng, Chinese Academy of Sciences, Beijing (China)
Excited state quantum dynamics in con-densed matter from real time TDDFT

17:00 - 17:40 Sergei Tretiak, Los Alamos National Labora-tory, New Mexico (US)
Modeling of photophysics and energy transfer in organic molecules

19:00 - 21:30 **Welcome Reception (Bremen Town Hall)**

Wednesday, October 11th 2017
(House of Science Bremen/Downtown)

Session: **Optoelectronic processes and devices**
Chair:

09:00 - 09:40 Steven Cundiff, University of Michigan, Ann Arbor (US)
Optical multi-dimensional coherent spectro-scopy of semiconductor nanostructures

09:40 - 10:20 Guanhua Chen, University of Hongkong (China)
Quantum mechanical simulation of organic optoelectronic devices

10:20 - 10:50 **Coffee Break**

10:50 - 11:30 Heiko Appel, Max Planck Institute, Hamburg (Germany)
Ab-initio description of the quantum nature of light for photo-stimulated processes

11:30 - 12:10 Enrico Perfetto, University of Rome Tor Vergata (Italy)
Nonequilibrium Green's function approach to time-resolved spectroscopies from first principle

12:10 - 12:50 Jascha Repp, University of Regensburg (Germany)
Tracking ultrafast processes in a single molecule by lightwave scanning tunneling microscopy

12:50 - 14:30 **Lunch Break (Restaurant Stadtwirt) and Coffee**

Sesson: **Time-resolved spectroscopy**
Chair:

14:30 - 15:10 Christoph Lienau, University of Oldenburg (Germany)
Multi-dimensional electronic spectroscopy of organic semiconductor materials

15:10 - 15:50 Tenio Popmintschev, University of California, San Diego, JILA and University of Colorado at Boulder (US)
Quantum design of coherent X-rays for 5D imaging at the space-time resolution extre-me

15:50 - 16:20 **Coffee Break**

16:20 - 17:00 Alfred Leitenstorfer, University of Konstanz (Germany)
Time-domain quantum physics of electrons and photons

17:00 - 17:40 Sascha Schaefer, University of Goettingen (Germany)
Ultrafast nanoscale dynamics mapped by time-resolved TEM

18:40 **Bus Pickup to Conference Dinner**
(Pickup Venue: RAMADA Ueberseehotel Bremen, Wachtstraße 27-29)

19:00 - 22:30 **Conference Dinner (Juergenshof)**

Thursday, October 12th 2017
(House of Science Bremen/Downtown)

Session: **Excitonic processes**
Chair:

08:30 - 09:10 Akshay Rao, Cavendish Laboratory, Cambridge (UK)
From strongly bound excitons to free charges without energy loss: the the role of vibronic dynamics and entropy

09:10 - 09:50 Chiyung Yam, Beijing Computational Science Research Center (China)
Multiscale modelling of optoelectronic devices

09:50 - 10:30 Francesca Calegari, University of Hamburg, DESY (Germany)
Tracking electron dynamics in bio-relevant molecules

10:30 - 11:00 **Coffee Break**

11:00 - 11:40 Ravishankar Sundaraman, Rensselaer Poly-technic Institute, Troy, New York (US)
Designing nano-materials for plasmonic hot carrier applications using ab initio multiphysics

11:40 - 12:20 Irene Burghardt, University of Frankfurt, Frankfurt (Main) (Germany)
Quantum dynamics of ultrafast exciton and charge migration in pi-conjugated materials: coherence, confinement, and localization

12:20 - 13:00 Steven G. Louie, University of California at Berkeley (US)
Excited-state phenomena and photophysics of atomically thin two-dimensional material

13:00 - 14:30 **Lunch Break (Restaurant Stadtwirt) and Coffee**

Session: **Charge and spin dynamics**
Chair:

14:30 - Eberhard K.U. Gross, Max Planck Institute, Halle (Saale) (Germany)
Charge carrier dynamics in nanostructu-res: optoelectronic and photo-stimulated processe

15:10 - 15:50 Johannes Lischner, Imperial College London (UK)
Hot electron processes in plasmonic nanos-tructures

15:50 - 16:30 Gulio Cerullo, Politechnico di Milano (Italy)
Ultrafast carrier and spin dynamics in 2-dimensional semiconductors

17:55 **Poster Mounting**

18:00 - 21:00 **Poster Session and Catering Buffet**

Friday, October 13th 2017
(House of Science Bremen/Downtown)

Session: **Multi-dimensional spectroscopy**
Chair:

09:00 - 09:40 Shaul Mukhamel, University of California, Irvine (Ireland)
Microscopic understanding of the biomo-lecular corona

09:40 - 10:20 Carlo Andrea Rozzi, CNR S3, Institute of Nanoscience, Modena (Italy)
On the role of ultrafast lattice dynamics in photo-induced charge separation

10:20 - 11:00 Tobias Brixner, University of Wuerzburg (Germany)
Multidimensional spectroscopy with spatial and temporal resolution

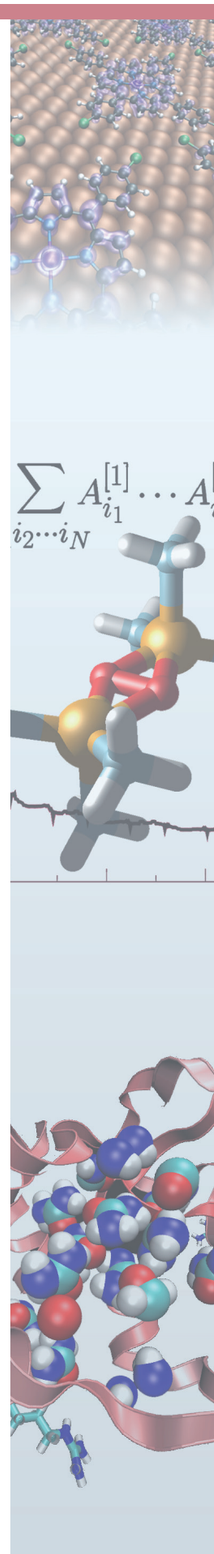
11:00 - 11:30 **Coffee Break**

11:30 - 12:10 Cristián G. Sánchez, National University of Cordoba (Argentina)
Dynamics of excited electrons in nano-structures from real-time time-depen-dent DFTB

12:10 - 12:50 Ivano Tavernelli, IBM Research-Zurich (Switzerland)
Excited states electronic and nuclear dynamics using TD-DFT

12:50 - 13:30 Andrew P. Horsefield, Imperial College London (Uk)
Simulation of response of organic mole-cules to ultrafast laser pulses

13:30 - 13:40 **Closing remarks: Thomas Frauenheim**



Conference Organisers

Thomas Frauenheim — University of Bremen, BCCMS, www.bccms.uni-bremen.de

Christoph Lienau — University of Oldenburg, Institute of Physics, https://www.uni-oldenburg.de/en/uno/

Oleg V. Prezhdo — University of Southern California, Deparment of Chemistry, http://chem.usc.edu/faculty/Prezhdo.html

Angel Rubio — Max Planck Institute Hamburg, https://www.mpsd.mpg.de/employees/39745/113438

Chiyung Yam — Beijing Computational Science Research Center, http://www.csrc.ac.cn/~yamcy/

http:/www.bccms.uni-bremen.de/evens/2017/cecam-ccdyn

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DFG Deutsche Forschungsgemeinschaft

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