cecam Centre Européen de Calcul Atomique et Moléculaire 2019

Thinking outside the box - beyond machine learning for quantum chemistry

Bremen Center for BCCMS Computational Materials Science

Tuesday, October 08th 2019
(House of Science Bremen/Downtown)

08:00 - 08:50 Registration

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

Session — **Machine Learning for Complex Quantum Systems**
Chair: Sheng Meng

09:00 - 09:40 Anatole von Lilienfeld, University of Basel (Switzerland)
Quantum machine learning

09:40 - 10:20 Tristan Bereau, Max Planck Institute for Polymer Research, Mainz (Germany)
Modeling intermolecular interactions with physics and ML

10:20 - 10:50 Coffee Break

10:50 - 11:30 Karsten Reuter, Munich University of Technology (Germany)
Knowledge-based approaches in catalysis and energy modelling

11:30 - 12:10 Hiromi Nakai, Waseda University, Shinjuku (Japan)
Semi-local machine-learned kinetic energy density functional with third-order gradients of electron density

12:10 - 12:15 Group Photo

12:15 - 13:50 Lunch Break (Restaurant Q1) and Coffee

13:50 - 14:30 Guanhua Chen, University of Hong Kong (China)
Deep learnt exchange-correlation potential

Session — **Machine Learning for Structure Prediction**
Chair: Thomas A. Niehaus

14:30 - 15:10 Bjørk Hammer, Aarhus University (Denmark)
Speeding up atomistic structure search with machine learning

15:10 - 15:50 Rickard Armiento, Linköping University (Sweden)
Machine learning for materials stability

15:50 - 16:20 Coffee Break

16:20 - 17:00 Stefano Leoni, University of Cardiff (UK)
ML in multiple timescale molecular dynamics simulations

17:00 - 17:40 Jacek Jakowski, Oak Ridge National Laboratory, Tennessee (USA)
Directed transformations of nanomaterials and beam-matter interactions

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

Wednesday, October 09th 2019
(House of Science Bremen/Downtown)

Session — **Machine Learning for DFTB repulsive interactions (I)**
Chair: Malte Schüler

08:30 - 09:10 Maxime Van den Bossche, Sorbonne University, Paris (France)
Accelerating global optimization searches with an adaptive DFTB parametrization scheme

09:10 - 09:50 David J. Yaron, Carnegie Mellon University, Pittsburgh, Pennsylvania (USA)
A DFTB layer for deep learning of electronic hamiltonians

09:50 - 10:30 Nir Goldman, Lawrence Livermore National Laboratory, California (USA)
Combining ML approaches with DFTB for simulations of reactive materials

10:30 - 11:00 Coffee Break

11:00 - 11:40 Benjamin Hourahine, University of Strathclyde, Glasgow (UK)
Learning around the DFTB model

12:20 - 12:20 Stefan Grimme, University of Bonn (Germany)
New tight-binding quantum chemistry methods

12:20 - 14:00 Lunch Break (Restaurant Q1) and Coffee

Session — **Machine Learning and MD**
Chair: Adam McSloy

14:00 - 14:40 Kipton Barros, Los Alamos National Laboratory, New Mexico (USA)
Advances in machine learned potentials for molecular dynamics simulation

14:40 - 15:20 Weitao Yang, Duke University, Durham, North Carolina (USA)
Machine learning in simulations and force fields with quantum mechanics/molecular mechanics and in DFT

15:20 - 16:00 Stephan Irle, Oak Ridge National Laboratory, Tennessee (USA)
Neural network corrected DFTB/MD simulations of long-timescale self-assembly and transport processes

16:00 - 16:30 Coffee Break

16:30 - 17:10 Roland Mitric, University of Wuerzburg (Germany)
Simulation of light-induced nonadiabatic dynamics in molecular aggregates

17:10 - 17:50 Franco P. Bonafé, Max Planck Institute for the Structure and Dynamics of Matter, Hamburg (Germany)
Simulations of impulsive vibrational spectra using Ehrenfest real-time TDDFTB

18:40 Bus Pickup to Conference Dinner
(Venue: Radisson Blu Hotel, Wachtstraße)

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

Thursday, October 10th 2019
(House of Science Bremen/Downtown)

Session — **Machine Learning for Quantum Chemistry & Electronic Structure**
Chair: Alessandro Pecchia

08:30 - 09:10 Benjamin T. Nebgen, Los Alamos National Laboratory, New Mexico (USA)
Hückel theory resurrected: dynamic parameterization of effective hamiltonians using deep learning

09:10 - 09:50 Volker W. Blum, Duke University, Durham, North Carolina (USA)
The ELSI infrastructure

09:50 - 10:30 Ursula Röthlisberger, Swiss Federal Institute of Technology, Lausanne (Switzerland)
Computational chemistry meets artificial intelligence

10:30 - 11:00 Coffee Break

11:00 - 11:40 Julian Gebhardt, Fraunhofer Institute for Mechanics of Materials, Freiburg (Germany)
Big data approach for next level hybrid perovskite solar cells

11:40 - 12:20 Alexandre Tkatchenko, University of Luxembourg (Luxembourg)
Towards exact molecular dynamics simulations with quantum chemistry and machine learning

12:20 - 14:00 Lunch Break (Restaurant Q1) and Coffee

Session — **Machine Learning for DFTB repulsive interactions (II)**
Chair: Cristopher Camacho

14:00 - 14:40 ChiYung Yam, Beijing Computational Science Research Center (China)
Theoretical investigation of current-induced light emission in scanning tunneling microscopy molecular junctions

14:40 - 15:20 Qiang Cui, Boston University, Massachusetts (USA)
Improvement of DFTB model for condensed phase simulations

15:20 - 16:00 Jolla Kullgren, University of Uppsala (Sweden)
Physically constrained splines - a step towards transferable repulsive potentials for SCC-DFTB

17:20 Poster Mounting

17:30 - 21:00 Poster Session + Catering Buffet
(House of Science)

Friday, October 11th 2019
(House of Science Bremen/Downtown)

Session — **ML for electronic and spectroscopic properties**
Chair: Balint Aradi

08:30 - 09:10 Patrick Rinke, Aalto University, Helsinki (Finland)
ARTIST: artificial intelligence for spectroscopy

09:10 - 09:50 Olexandre Isayev, University of North Carolina, Chapel Hill (USA)
GW+T-Matrix approach to the excitonic Mott transition

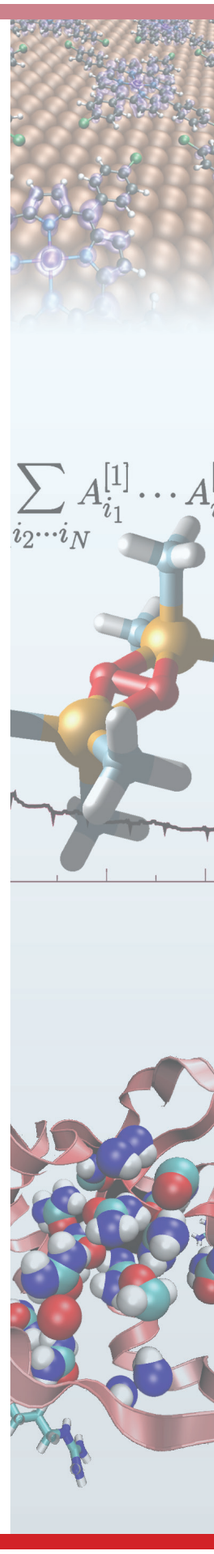
09:50 - 10:30 Anders M. N. Niklasson, Los Alamos National Laboratory, New Mexico (USA)
Graph-based linear scaling electronic structure theory

10:30 - 11:00 Coffee Break

11:00 - 11:40 Sergei Tretiak, Los Alamos National Laboratory, New Mexico (USA)
Multiple cloning and polaritons in excited state non-adiabatic molecular dynamics

11:40 - 12:20 Gotthard Seifert, Technical University of Dresden (Germany)
Bridging scales in materials simulations - quantum versus classical simulations

12:20 - 12:25 Closing words and departure



Conference Organisers

Thomas Frauenheim — University of Bremen, Germany
Department of Physics, BCCMS
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Marcus Elstner — Karlsruhe Institute of Technology, Germany
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www.ipc.kit.edu/tcb/Mitarbeiter_51.php

Benjamin Hourahine — University of Strathclyde, Glasgow, UK
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Benjamin Nebgen — Los Alamos National Laboratory, New Mexico, USA
Theoretical Division
https://cnls.lanl.gov/~serg/group.html

Anatole von Lilienfeld — University of Basel, Switzerland
Department of Chemistry
https://chemspacelab.org/head-of-lab/

http://www.bccms.uni-bremen.de/veranstaltungen/2019/cecam-outbox

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