Program of the International CECAM-Workshop

Thinking outside the box - beyond machine learning for quantum chemistry

Bremen Center for Computational Materials Science – BCCMS
University of Bremen, October 7th - 11th 2019
Conference site: House of Science, Downtown

Monday, October 7th 2019 (Radisson Blu Hotel Bremen**)**

18:00 – 21:00 **Registration**

Tuesday, October 8th 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)**

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Wednesday, October 9th 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*
11:40	**–**	**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
19:00	**–**	**22:30**	**Conference Dinner (Restaurant Juergenshof)**

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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)**

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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**	Olexandr Isayev, University of North Carolina, Chapel Hill, USA *Accurate and transferable multitask prediction of chemical properties with an atoms-in-molecule neural network*
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: Thomas Frauenheim***
12:25			**Departure**