Program

Monday, October 17, 2022

14:30	**Welcome Reception** Frank Glorius (Münster University)	Foyer
15:30	**SPP Organizational Meeting** Frank Glorius (Münster University)	Lecture Hall
16:00	**How can AI and Big Data Propel Developments in Catalysis?** Stephan Andreas Schunk (hte GmbH; BASF SE)	
17:00	**Molecular Machine Learning in Drug Design: Data, Algorithms & User Experience** Nils Weskamp (Boehringer Ingelheim)	
18:00	**Break**	
19:00	**Dinner**	Restaurant Wenzel

Program

Tuesday, October 18, 2022

09:00	**Project Talks** PhD Students	Lecture Hall
	Advanced Learning Strategies for Potential Energy Surfaces Applied to Organic Electrolytes Fabian Zills[1], Moritz René Schäfer[2] (Holm[1], Kästner[2])	
	AI-Empowered Universal Workflow for Molecular Design of Performant Photoswitches Robert Strothmann[1] (Reuter[1], Hecht)	
	Development and Application of Improved Ligand Descriptors and Representations for Inverse Catalyst Design Julian Löffler[1] (Däschlein-Gessner[1], Gensch)	
10:00	**Break**	Foyer
10:30	**Future of Simulation in Industry: Physics vs. Data Driven Approaches** Jan Gerit Brandenburg (Merck KGaA)	Lecture Hall
11:30	**Machine Learning for the Optimisation of Reaction Conditions** Tiago Rodrigues (imed Research Institute for Medicines; University of Lisbon)	
12:30	**Lunch**	Harzmensa
14:30	**State Museum of Prehistory**	State Museum of Prehistory

Program

Wednesday, October 19, 2022

09:00 **Project Talks** — Lecture Hall
PhD Students

Elucidating Fingerprints - Towards a Holistic Explanatory Toolbox for Molecular Machine Learning
Debanjan Rana[1], Mathias in Wolde-Lübke[2] (Glorius[1], Jiang[2])

Exploring Tailored Ru-Triphos Catalysts for Hydrogenation Reactions by Combination of Experimental, Computational, and Machine Learning Techniques
Alessandro Curra[1], Angelina Schreiber[2], Johanna Henkel[2] (Bannwarth[1], Klankermayer[2])

Multi-fidelity, Active Learning Strategies for Exciton Transfer Among Adsorbed Molecules
Dongyu Lyu[1], Matthias Holzenkamp[2] (Kleinekathöfer[1], Zaspel[2])

SAFE: Synthetically Accessible Fragment Expansion Based on Machine Learning Approaches
Malte Korn[1], Felix Katzenburg[2] (Rarey[1], Glorius[2])

10:30 **Break** — Foyer

11:00 **Project Talks** — Lecture Hall
PhD Students

Fourth-Generation Neural Network Potentials for Molecular Chemistry
Moritz Richard Schäfer[1], Jonas Finkler[2] (Behler[1], Goedecker[2])

Machine Learning Approaches for Faster Discovery and Adaptation of Enzymes for Difficult Chemical Reactions. Phase I: Providing Solutions for Regioselective Oxygenations by 2OGD-oxidases (MacBioSyn)
Fatemeh Fadaei (Davari)

Machine Learning for Developing and Understanding Novel, Asymmetric 3d Metal-catalyzed C–H Activations
Neeraj Kumar Pandit, Philipp Boos (Ackermann)

12:30 **Lunch** — Harzmensa

14:30 **Visions for SPP Workshop** — Lecture Hall

16:00 **Coffee Break** — Foyer

16:30 **Poster Session I** (Projects 1 - 9) — Foyer

Program

Thursday, October 20, 2022

09:30	**Project Talks** PhD Students **Machine Learning-guided Chemical Space Exploration: Automatic Creation and Navigation of Ultra-large Open-source Molecular Libraries** Polina Oleneva (Kolb) **Molecular Descriptors in Matrix Completion Methods** Dominik Gond[1] (Hasse[1], Jirasek[1], Leitte) **Molecular Machine Learning for Asymmetric (Organo)-Catalysis** Marcel Ruth, Oliver Pereira (Schreiner) **Neural Fingerprints as Structure and Activity-sensitive Molecular Representations** Samuel Homberg[1] (Koch[1], Risse)	Lecture Hall
11:00	**Break**	Foyer
11:30	**Project Talks** PhD Students **Quantum Chemical Molecular Representations for Machine Learning** Christian Hoelzer (Grimme) **Understanding the Interaction of Organic Molecules and Metal Ions by Robot-based High-throughput Experimentation and Molecular Machine Learning** Jyothika Pillay[1], Michael Ringleb[2] (Gräfe[1], Schubert[2]) **Virtual Drug Screening in the Chemical Space Accessible by Chemical Synthesis** Paul Eisenhuth[1], Nico Domschke[2] (Meiler, Stadler)	Lecture Hall
12:30	**Lunch**	Harzmensa
14:30	**Machine Learning for Chemical Biology Studies** Tiago Rodrigues (imed Research Institute for Medicines; University of Lisbon)	Lecture Hall
15:30	**Coffee Break**	Foyer
16:00	**Poster Session II** (Projects 10 - 18)	
18:00	**Break**	
19:00	**Dinner**	Hallesches Brauhaus

Program

Friday, October 21, 2022

09:00 **Social and Scientific Implications of AI Workshop** — Lecture Hall

Overcoming Inevitabilism: The Quest for Regulating Machine Learning
José Renato Laranjeira de Pereira (Chancellor Fellow, Alexander von Humboldt Stiftung, Berlin; in person)

Prediction as Social Action
Celestine Mendler-Dünner (MPI for Intelligent Systems, Tübingen; virtual)

Human-ML Teaming
Samira Samadi (MPI for Intelligent Systems, Tübingen; virtual)

Brainstorming and Summary

12:00 **Science Founders Talk**
Philipp Pflüger and Marius Kühnemund (ChemInnovation; Münster University)

12:30 **Lunch** — Harzmensa