Leopoldina Symposium on Molecular Machine Learning

DFG

SPP 2363

Leopoldina
Nationale Akademie
der Wissenschaften

Mon, 4ᵀᴴ March

12:15 pm ○ Opening

12:30 pm ● Synthesis planning, mechanistic analysis and discovery of new reaction classes in the age of computers
Bartosz Grzybowski, UNIST

1:20 pm ● Efficient Quantum Chemistry Methods
Stefan Grimme *ML, University of Bonn*

2:10 pm ○ Coffee break

2:45 pm ○ Poster session

4:45 pm ● Machine learning for traversing chemical structure space
Julia Westermayr, University of Leipzig

5:35 pm ● How to See Behind the Dark Rift of Chemical Reaction Space – A Story of Byproducts and Analytical Chemistry
Philipp Pflüger, ChemInnovation

6:05 pm ● Bringing ML to the Lab: Towards Autonomous Experimentation
Felix Strieth-Kalthoff, University of Toronto

TUE, 5TH MARCH

8:30 am — Chemistry using Computation, Machine Learning and Robots
Andy Cooper, University of Liverpool

9:20 am — Making Chemical synthesis and discovery universal
Leroy Cronin, University of Glasgow

10:10 am — Coffee break

10:40 am — Applying ML/AI to drug design in a pharmaceutical setting
Ola Engkvist, AstraZeneca

11:30 am — How NFDI4Chem's infrastructure and tools can support ML-initiatives
Nicole Jung, KIT

12:20 pm — Lunch

1:50 pm — Artificial Intelligence for Accelerated Chemical Synthesis
Philippe Schwaller, EPFL

2:40 pm — Hybrid AI for Drug Discovery
Andrea Volkamer, Saarland University

3:30 pm — Coffee break

4:00 pm — Poster session

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Wed, 6th March

8:30 am — Fully Quantum (Bio)Molecular Simulations: Dream or Reality?
Alexandre Tkatchenko, University of Luxembourg

9:20 am — Machine learning for drug discovery in low-data regimes
Francesca Grisoni, TU Eindhoven

10:10 am ○ Coffee break

10:40 am — Remembering the lab in computational materials discovery
Kim Jelfs, Imperial College London

11:30 am — Self-driving laboratories: A report from the trenches
Alán Aspuru-Guzik, University of Toronto

12:20 pm ○ Closing remarks

Poster session Mon, 4th March (2:45 pm - 4:30pm)

P1: ML/MM simulation of metal-organic frameworks in LAMMPS
Niklas Kappel

P3: Machine-learning for data-driven protein engineering
Mehdi D. Davari

P5: Exploring tailored Ru-triphos catalysts for hydrogenation reactions by combination of experimental, computational and machine learning techniques
Angelina Schreiber

P7: Synthesis Rebalancing Framework
Klaus Weinbauer

P9: Preference-Learning for De Novo Drug Design
Janosch Menke

P11: Collaborative Development of Machine Learned Potentials for Ionic Liquids
Fabian Zills

P13: Revolutionizing Molecular Docking: A Comprehensive Virtual Screening Analysis of the Colchicine Binding Site
Tieu Long Phan

P15: AI-Empowered Universal Workflow for Molecular Design of Performant Photoswitches
Robert Strothmann

P17: Desymmetrization of meso-Anhydrides
Jan Marcel Metzler

P19: Self-Organizing Maps in Drug Discovery – Revisited
Johannes Kaminski

P21: Multi-fidelity, Active Learning Strategies for Exciton Transfer Among Adsorbed Molecules
Matthias Holzenkamp

P23: Virtual Drug Screening in the Chemical Space Accessible by Chemical Synthesis
Fabian Liessmann

P25: Machine learning guided multi-objective optimization of a stereoconvergent nickel-catalyzed reaction to access trisubstituted alkenes
Daniel Min

P27: DoGSite3Scorer: Explainable Binding Site Druggability Predictions
Tobias Harren

P29: Enabling OF-DFT with Machine Learning
Tobias Kaczun

P31: Prediction of 1H and 13C NMR Chemical Shifts of Transition Metal Complexes Using Machine Learning
Jyothika Pillay

P33: Machine learning potentials for molecular dynamics simulations of deep eutectic systems
Omid Shayestehpour

P35: A deep learning approach to study translatability of molecular fingerprints
Debanjan Rana

P37: CBS in the Age of Machine Learning
Oliver Pereira

P39: Predicting the reactivity of acyclic silylenes and germylenes in hydrogen activation
Henning Remm

P41: Machine-Driven Exploration of Electrostatics for Highly Charged Biopolymers in confined environments
Horacio V. Guzman

P43: Polymer fingerprint - decoding of polymeric structures for Machine learning
Yannik Köster

P45: Explainable Methods for Graph Neural Networks with Application to Chemistry
Ali Can Kara

P47: Utilizing Machine Learning for the Approximation of Hessian Matrices based on GFN2-xTB derived Features
Gereon Feldmann

P49: From Local Atomic Environments to Molecular Information Entropy
Alexander Croy

Postersession Tue, 5th March (4:00 pm - 5:45pm)

P2: Modern Experiment Design for Protein Design
Mojmir Mutny

P4: Machine Learning for Developing and Understanding Asymmetric 3d Metal-Catalyzed C−H Activations
Philipp Boos

P6: Multifidelity Machine Learning for Quantum Chemistry
Vivin Vinod

P8: Expert-based machine learning model for docking evaluation
Polina Oleneva

P10: Molecular Machine Learning via Efficient Quantum Chemistry Methods – Development and Application
Marcel Mueller

P12: Predicting the biochemical activities of unidentified chemicals from MS2 spectra to pinpoint potential toxic agents
Ida Rahu

P14: Explainability in AI-Driven Early-Phase Drug Discovery - Bridging Machine Learning and Matched Molecular Pair Analysis by Network Balance Scaling
Malte Holmer

P16: Prediction of Activity Coefficients with Hybrid GE Models
Dominik Gond

P18: Estimation of hydrogen atom transfer reaction barriers in peptides by learning full radical potential energy surface
Marlen Neubert

P20: Reaction-Agnostic Featurization of Bidentate Ligands for Bayesian Ridge Regression of Enantioselectivity
Alexandre Schoepfer

P22: Explainable AI for Graph Neural Network Applications in Computational Drug Discovery
Malte Laurids Modlich

P24: Accelerated First-Principles Exploration of Structure and Reactivity in Graphene Oxide
Zakariya El-Machachi

P26: Investigating charge densities of electronic structure methods
Moritz Gubler

P28: Machine learning for faster discovery and adaptation of oxidases for challenging chemical reactions
Lilly Eger

P30: Advanced Learning Strategies for Machine Learned Potentials
Moritz Schäfer

P32: Towards accelerated closed-loop discovery of porous liquids
Austin Mroz

P34: Synthetically Accessible Fragment Space Extensions by Machine Learning-Based Approaches (SAVE)
Malte Korn

P36: CIn-silico generated reagents for detection of pesticides using mass spectrometry: An out-of-distribution task
Henrik Hupatz

P38: EnTdecker – A machine learning-based platform for guiding substrate discovery in energy transfer catalysis
Jan Spies

P40: Deep interactome learning for de novo drug design
Kenneth Atz

P42: MolBar: A Molecular Identifier for Inorganic and Organic Molecules with Full Support of Stereoisomerism
Nils van Staalduinen

P44: Bayesian Optimisation to Efficiently discover large molecules for organic photovoltaic application
Mohammed Azzouzi

P46: Reactivity prediction of highly flexible catalysts using conformationally enriched machine learning
Stefan Schmid

P48: Uncertainty-Aware Genetic Optimization for the Discovery of Singlet Fission Materials
Luca Schaufelberger