Workshop on Theoretical Chemistry 2024

27 February – 1 March 2024, Bad Hofgastein (Austria)

Machine Learning for Chemistry

Scientific Organizer: Alexandre Tkatchenko, University Luxembourg

Lectures and Topics

Alexandre Tkatchenko, University Luxembourg	Introduction into ML / ML for Exploring Chemical Spaces
Gabor Csanyi , University Cambridge	Machine Learning Potentials and Force Fields
Mariana Rossi, MPI Hamburg	Machine Learning for Electronic Structure Properties
Nongnuch Artrith, Utrecht University	Neural Networks and Materials Modeling

Schedule for the Workshop

Time	Tuesday, 27 Feb.	Wednesday, 28 Feb.	Thursday, 29 Feb.
8:45 – 9:00	Welcome		
9:00 – 10:30	Tkatchenko	Csanyi	Rossi
10:30 – 11:00	Coffee Break	Coffee Break	Coffee Break
11:00 – 12:00	Rossi	Artrith	Csanyi
12:00 – 16:00	Break	Break	Break
16:00 – 17:00			Poster Session
17:00 – 18:00	Rossi	Tkatchenko	Artrith
18:00 – 19:00	Csanyi	Artrith	Tkatchenko
19:30 – 21:30			Dinner

Program of the Minisymposium

Time	Friday, 1 March	Title
9:00 – 9:20	Andreas J. Achazi	Effective Screening Procedure for Redox-Active Molecules in Organic Batteries
9:25 – 9:45	Nina Strasser	Predicting Spin-Dependent Phonon Band Structures of HKUST-1 with Machine-Learned Interatomic Potentials
9:50 – 10:10	Lukas Legenstein	Calculating Thermal Conductivities of Crystalline Polymers using Machine-Learned Potentials with close to DFT accuracy
10:15 – 10:45	Coffee Break	
10:45 – 11:05	Kajjana Boonpalit	Pre-training Strategy for Antiviral Drugs Screening with Low-Data Graph Neural Network: Case Study in HIV-1 K103N Reverse Transcriptase
11:10 – 11:30	Charlotte Rickert	Tensor-decomposed iterative distinguishable cluster triples
11:35 – 11:55	Michał Tomza	Phase Detection with Neural Networks: Interpreting the Black Box
12:00	End of the Workshop	

Workshop site: Kongresszentrum, Tauernplatz 1, 5630 Bad Hofgastein

Scientific Organizer: Alexandre Tkatchenko (University Luxembourg)

Local Organizer: Anne-Marie Kelterer (TU Graz), kelterer@tugraz.at

https://www.tugraz.at/institute/ptc/conferences/wtc-mariapfarr

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General Information

Workshop on Theoretical Chemistry 2024, 27 February – 1 March, Bad Hofgastein

Machine Learning for Chemistry

The workshop takes place from 27 February til 1 March 2024 in the seminar room Lichtung at the Kongresszentrum, Tauernplaatz 1, 5630 Bad Hofgastein, Austria.

We thank our scientific organizer Alexandre Tkatchenko for planning the workshop, and our lecturers for their lectures.

This year, we have a total of 70 participants.

Lecture Notes Booklet: The Lecture Notes booklet contains black&white copies of the lectures in smaller format. Printed booklets will be distributed at the workshop to those who have ordered it.

The slides can be downloaded with a password (see your email) via: https://www.tugraz.at/institute/ptc/conferences/wtc-mariapfarr/previous-workshops/wtc-2024-1

Poster Session: on Thursday, 29 February 2024, a poster session will take place from 16:00 – 17:00. Posters in A0 portrait format can be presented during the whole workshop.

Minisymposium: on Friday, 1 March 2024, the Minisymposium with six short talks from participants takes place from 9:00-12:00. Talks last 20 minutes plus max. 5 min. discussion. We kindly ask the speakers to bring their presentation on a USB stick in the break before their session.

Social Program:

At Monday, 26 February 2024, we will meet for an optional Get-Together at the *Hotel Alte Post* in the Stube „Post-Schmiede“ (upper floor), Kirchplatz 4, 5630 Bad Hofgastein. Meeting time is from 18:30 – 21:30, the kitchen orders are possible until ca. 20:30. The dinner and drinks must be paid by the participants themselves, it is not included in the registration fee.

At Thursday, 29 February 2024, we will hold the Workshop Dinner for all participants in the *Hotel Rauscher und Paracelsus*, Kurpromenade 20, A-5630 Bad Hofgastein. The dinner is included in the registration fee. A Bauernbuffet will be served. Meeting time is 19:45.

Confirmation of Participation: Your confirmation of participation will be distributed on-site. In case you need an additional confirmation of payment, please write an email with all necessary data (name, address, VAT-no, etc.) to the local organizer, and we will provide it after the workshop.

The local organizer, Anne-Marie Kelterer, kelterer@tugraz.at, TU Graz.

Download of Lecture Notes slides:

https://www.tugraz.at/institute/ptc/conferences/wtc-mariapfarr/previous-workshops/wtc-2024-1

The password will be sent out by email at Friday, 23 February 2024 to all registered participants.

Effective Screening Procedure for Redox-Active Molecules in Organic Batteries

A.J. Achazi [1,2,3], D. Mollenhauer [2,3]

[1] Andreas.Achazi@phys.chemie.uni-giessen.de, [2] Justus-Liebig-Universität Gießen, Heinrich-Buff-Ring 17, 35392 Gießen, [3] Justus-Liebig-Universität Gießen, Zentrum für Materialforschung, 35392 Gießen

Organic radical polymer-based batteries are characterized by their high charging speed, longevity, and other advantages over lithium-ion batteries. However, suitable redox-active molecules for the anode are still lacking. For this purpose, we developed a multi-step quantum chemical screening procedure. [1,2] With each stage of screening, the process becomes more sophisticated. DFT, extended tight-binding methods as well as descriptors (orbital energies) are employed. The data obtained show interesting structure-property relationships, and will be used to train machine learning models to further accelerate the screening.

[1] A.J. Achazi, X. Fataj, P. Rohland, M.D. Hager, U.S. Schubert, D. Mollenhauer, *J. Comput. Chem.* **2024**, *accepted*

[2] X. Fataj, A.J. Achazi, P. Rohland, E. Schröter, S. Muench, R. Burges, K. L. H. Pohl, Prof. D. Mollenhauer, M.D. Hager, U.S. Schubert, *Chem.Eur.J.* **2023**, e202302

Predicting Spin-Dependent Phonon Band Structures of HKUST-1 with Machine-Learned Interatomic Potentials

N. Strasser, S. Wieser, E. Zojer

Institute of Solid State Physics, NAWI Graz, Graz University of Technology, 8010 Graz

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In this study spin-dependent vibrational properties of the metal-organic framework HKUST-1 are explored using density functional theory and reproduced using machine-learned interatomic potentials [1]. Phonon bands were reproduced with an accuracy ranging from 3 to 7 cm^{-1}. Notably, the force-field parametrization process involves the explicit consideration of spins only during the generation of reference data, which were generated using active learning approaches [2] that combine ab initio and force-field-based molecular dynamics runs.

[1] I. S. Novikov, K. Gubaev, E. V. Podryabinkin, A. V. Shapeev, *Mach. Learn.: Sci. Technol.* **2021**, *2*, 025002.

[2] R. Jinnouchi, K. Miwa, F. Karsai, G. Kresse, R. Asahi, *J. Phys. Chem. Lett.* **2020**, *11*, 6946-6955.

Calculating Thermal Conductivities of Crystalline Polymers using Machine-Learned Potentials with close to DFT accuracy

L. Reicht, L. Legenstein, S. Wieser, E. Zojer

Institute of Solid State Physics, Graz University of Technology, Austria, lukas.reicht@tugraz.at

Recent experiments revealed that highly aligned (crystalline) polymers can display extraordinarily high thermal conductivities. Emerging machine-learned potentials are ideal for studying such thermal conductivities provided that their accuracy approaches that of ab initio methods. Thus, we thoroughly benchmarked moment tensor potentials (MTPs) on phonon-related properties (phonon band structures, elastic constants, thermal expansion coefficients, and thermal conductivities). For a set of deliberately chosen polymers (polyethylene, polythiophene, and poly(3-hexyl-thiophene)), we achieved close to DFT accuracy, in particular when adapting the generation of the training data and the complexity of the potentials to the intended use case. These optimized MTPs are then used to calculate thermal conductivities via the Boltzmann transport equations and by molecular dynamics. This yields complementary atomistic insights into the factors determining heat transport in polymers.

Pre-training Strategy for Antiviral Drugs Screening with Low-Data Graph Neural Network: Case Study in HIV-1 K103N Reverse Transcriptase

K. Boonpalit[1)], H. Chuntakaruk[2)], J. Kinchagawat[1)], S. Nutanong[1)], T. Rungrotmongkol[2)]

[1)] School of Information Science and Technology, VISTEC, Thailand
[2)] Program in Bioinformatics and Computational Biology, Chulalongkorn University, Thailand

In this research, the focus is on tackling the challenge of identifying potent inhibitors for resistance-associated mutations (RAM), which is a low-data scenarios in machine learning (ML)-based high-throughput screening, by pre-training graph neural networks (GNN). The case study is focus on screening K103N HIV reverse transcriptase (RT) inhibitors. In this task, the conventional supervised learning encounter difficulties due to the limited availability of bioactivity data related to specific mutations. This study introduces a GNN continual pre-training pipeline, that can leverage the knowledge form unlabeled dataset and wild-type HIV dataset to enhance model performance in K103N downstream tasks.

[1] H. Chuntakaruk, K. Boonpalit, J. Kinchagawat, et al., J. Comput. Chem., 2024.

Tensor-decomposed iterative distinguishable cluster triples

Charlotte Rickert [1)*], Denis Usvyat [1)], Daniel Kats [2)]

[1)]Theoretische Chemie, HU Berlin, Brook-Taylor-Straße 2, Berlin, Germany, *rickertc@hu-berlin.de,
[2)] Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany

Obtaining sufficient quality of the benchmark data in machine learning is one of the big challenges in quantum chemistry. We present a technique that allows one to reach a very high methodological level – distinguishable cluster with singles, doubles and iterative triples [1] – at a substantially reduced computational cost. This is achieved by tensor decomposing the triples amplitudes [2], which leads to a considerable compression of the amplitude space and reduction of both the scaling and prefactor. The energy differences calculated with the presented technique are on average within 0.5 kJ/mol from the CCSDT(Q) results.

[1] D. Kats and A. Köhn, "*On the distinguishable cluster approximation for triple excitations*", J. Chem. Phys. **150**, 151101 (2019)
[2] M. Lesiuk, "*Implementation of the coupled-cluster method with single, double, and triple excitations using tensor decompositions*", J. Chem. Theory Comput. **16**, 453 (2020)

Phase Detection with Neural Networks: Interpreting the Black Box

A. Dawid[1,2,3)], P. Huembeli[3)], M. Lewenstein[3)], A. Dauphin[3)], M. Tomza[1)]

[1)] Faculty of Physics, University of Warsaw, Poland, michal.tomza@fuw.edu.pl
[2)] Flatiron Institute, NYC, USA [3)] Institute of Photonic Sciences, Barcelona, Spain

Neural networks (NNs) usually hinder any insight into the reasoning behind their predictions [1]. We demonstrate how influence functions can unravel the black box of NN when trained to predict the phases of the one-dimensional extended spinless Fermi–Hubbard model at half-filling [2]. Our results provide strong evidence that the NN correctly learns an order parameter describing the quantum transition in this model. We demonstrate that influence functions allow to check that the network, trained to recognize known quantum phases, can predict new unknown ones within the data set [3].

[1] A. Dawid, … , M. Tomza, M. Lewenstein, A. Dauphin, Machine learning in quantum sciences, Cambridge University Press in press (2024) / arXiv:2204.04198
[2] A. Dawid, P. Huembeli, M. Tomza, M. Lewenstein, A. Dauphin,, New J. Phys. 22, 115001 (2020)
[3] A. Dawid, P. Huembeli, M. Tomza, Lewenstein, A. Dauphin, Mach. Learn.: Sci. Technol. 3, 015002 (2022)

List of Posters
Workshop on Theoretical Chemistry 2024 – Machine Learning for Chemistry

Poster Session: Thursday, 29 February 2024, 16:00-17:00

No	Authors	Poster Title
1	M. Duszka, M.F. Rode, A.L. Sobolewski	Organic molecules with the excited-state singlet-triplet inversion: Beyond BN-based structures
2	J. Martinka	A simple approach to rotationally invariant machine learning of a vector quantity
3	T. Abdurakhmonov, O. Kühn	Molecular Dynamics insight into Adsorption properties: Interlayer Potential parametrization for dye molecules on Hexagonal Boron Nitride layers
4	M. Martyka, K. Szychta, J. Jankowska	Ultrafast Separation of Photogenerated Charges in a Donor-Polarized Molecular Wire-Acceptor Triad
5	A.J. Achazi, D. Mollenhauer	Effective Screening Procedure for Redox-Active Molecules in Organic Batteries
6	A.L. Ptaszek, G. Platzer, J. Böttcher, J.E. Fuchs, L. Geist, D. Braun, D.B. McConnell, R. Konrat, P.A. Sánchez-Murcia, M. Mayer	Ligand 1H NMR Chemical Shifts as Accurate Reporters for Protein-Drug Binding Interfaces
7	E. Stocco, C. Carbogno, M. Rossi	First-principles light-driven molecular dynamics through equivariant neural networks
8	B. Tyrcha, F. Brzęk, P.S. Żuchowski	Second Quantization-based Symmetry-Adapted Perturbation Theory: Generalizing Exchange Beyond Single Electron Pair Approximation
9	S.Sharma, M. Rossi	Machine-learned Potentials for Vibrational Properties of Acene-based Molecular Crystals
10	L. Steiner, A.J. Achazi, A.-M. Kelterer, B.Paulus, H.-U. Reissig	Diastereoselective Dearomatizing Cyclizations of 5-Arylpentan-2-ones by Samarium Diiodide – A Computational Analysis
11	T. Henkes, I. Poltavskyi, A. Tkatchenko	Towards Automated Active Learning for Interatomic Potentials
12	K.M. Draijer, N. Artrith	Computational Screening of Earth Abundant Catalyst Materials for Seawater Splitting
13	F. Eilers, S. Erdmann, H.I. Sözen, T. Klüner	Exploration of Rare-Earth-Free Magnetic Materials via Active Learning from First-Principle Calculations
14	P. Lazar, K. Skladanová, T. Bučko	Can machine-learned force field reproduce unusual thermal expansion of ScF3 and ReO3?
15	N. Goncharova, J. Hoja, A.D. Boese	Polymorphic Transitions via First-Principles Nudged Elastic Band Calculations
16	EPEE NDONGUE Jules César	Enzymatic reactions transition networks: Toward an optimal choice of degree of freedoms

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No	Authors	Poster Title
17	A. List, J. Hoja, A. D. Boese	Recent Developments in Multimer Embedding for Molecular Crystals
18	M. Nachtigall, D. Wing, A. Tkatchenko, D. Firaha, H. Dietrich, M. Neumann	Machine-learned force-fields for crystal structure prediction
19	M. Ćosićová, R. Kalus	Testing of diabatization methods using neural networks on model examples
20	Munavvar Husain, T. Korona	Quantum topology study for unveiling the excitation properties of porphene and fluorine-substituted porphene
21	A. Tucholska, K. Pernal	Correlation energy with the Particle-Particle Adiabatic Connection Formalism for Strongly Correlated Systems
22	C. Wachter, O.T. Hofmann	In Search of Organic Improvements to Ab Initio Thermodynamics
23	M. Modrzejewski, K.N. Pham, J. Klimeš	Contributions beyond direct random-phase approximation in the binding energy of solid ethane, ethylene, and acetylene
24	Filip Sagan	Machine-Learning Assisted ReaxFF simulations for accurate computational pKa estimations of organic molecules
25	C. Wachter, O.T. Hofmann	In Search of Organic Improvements to Ab Initio Thermodynamics
26	R. van der Kruit, T. Morawietz, N. Artrith	Developing efficient computational workflows for the stability assessment of molecular crystal structures
27	D. Platero-Rochart, P.A. Sánchez-Murcia	Prediction of enzymatic energy barriers using steered molecular dynamics trajectories as training data