

Eike Sebastian Eberhard

PhD Candidate in Machine Learning for Electronic Structure & Quantum Chemistry
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Machine-learned interatomic potentials (MLIPs) and force fields simulate proteins, materials, and reactive chemistry at a fraction of the cost of quantum mechanics, but they are fundamentally bounded by their training data. That data is the bottleneck in AI4Science: gold-standard coupled cluster cannot scale past small molecules, while standard Kohn-Sham DFT (KS-DFT) trades away accuracy. I attack this bottleneck by rethinking electronic structure modeling itself. I train equivariant neural exchange-correlation (XC) functionals end-to-end through GPU-accelerated differentiable self-consistent field (SCF) solvers, unlocking hybrid-level quantum chemistry accuracy where hybrids are computationally out of reach. Then I make these calculations fast. Learned SCF initializations slash the iterations needed to converge, while direct density-matrix and Hamiltonian prediction bypasses the solver loop entirely. My goal is to make coupled-cluster-quality reference data cheap enough to generate at the scale modern force fields demand.

KEY PUBLICATIONS

* equal contribution

- 2026 Oct **Physics-Aligned Electronic Ground-State Learning Improves Generalization**
E. S. Eberhard*, X. Kainz*, V. Kotsev, A. Aldossary, S. Günnemann
Preprint 2026 · ROCKET, GROOT, ON-Loss · Cuts OOD energy/force MAE by 79%/83% (QM9→QM40)
- 2026 Jun **Derivative Informed Learning of Exchange-Correlation Functionals**
E. S. Eberhard, L. A. Thiede, A. Aldossary, A. Burger, N. Gao, V. Bhethanabotla, A. Aspuru-Guzik, S. Günnemann
ICML 2026 · DI-XC, DI-Loss · Grassmannian derivative supervision distilling $\mathcal{O}(N^4)$ B3LYP into $\mathcal{O}(N^3)$ ML-XC
- 2026 Apr **Transferable SCF-Acceleration through Solver-Aligned Initialization Learning**
E. S. Eberhard*, V. Kotsev*, T. Güthle, S. Günnemann
NeurIPS 2026 · SAIL, ERIC · Differentiable SCF cutting iterations by 37% and wall-time by 1.35× on QMugs
- 2026 Jan **3D Molecule Generation from Rigid Motifs via SE(3) Flows**
R. Poletukhin, M. Kollovieh, **E. S. Eberhard**, S. Günnemann
NeurIPS 2026 · MotiFlow · SE(3)-equivariant flow matching with 3.5× compression and 2–10× fewer steps
- 2025 Apr **Force Generation by Enhanced Diffusion in Enzyme-Loaded Vesicles**
E. S. Eberhard*, L. Burger*, C. L. Pastrana*, H. Seyed-Allaei, G. Giunta, U. Gerland
Nano Letters · GPU-accelerated multiscale Brownian dynamics of active-matter vesicles in JAX-MD
- 2024 Oct **Learning Equivariant Non-Local Electron Density Functionals**
E. S. Eberhard*, N. Gao*, S. Günnemann
ICLR 2025 (Spotlight) · EG-XC · SO(3)-equivariant GNN capturing non-local exchange-correlation interactions

EDUCATION

GPA's on the German scale from 1.0 (best) to 4.0 (passed).

- 2025 Jan – present **PhD Candidate in Computer Science (AI4Science & Quantum Chemistry)**
Data Analytics and Machine Learning Group, TUM · Munich Data Science Institute (MDSI)
Architecting GPU-accelerated differentiable KS-DFT solvers, equivariant GNNs, and electronic structure foundation models in JAX/PyTorch
- 2026 Jun – Sep **Visiting Researcher**
University of Toronto & Vector Institute · MatterLab (Prof. Alán Aspuru-Guzik)
Research on derivative-informed neural exchange-correlation functionals and hybrid functional distillation for large-scale molecular systems
- 2022 Oct – 2024 Aug **M. Sc. Computer Science & Engineering** GPA 1.1
Technical University of Munich (TUM) · Best of class 2024
Thesis: *Machine Learning for Density Functional Theory* (Prof. S. Günnemann) — developed the EG-XC equivariant functional and JAX-based DFT framework
- 2021 Oct – 2023 Oct **M. Sc. Physics** GPA 1.2
Technical University of Munich (TUM) · Specialization in Theoretical & Computational Biophysics
Thesis: *Effects of Enhanced Diffusion in Enzyme-Loaded Vesicles: A Multiscale Simulation Study* — custom GPU molecular dynamics in JAX-MD
- 2017 Oct – 2021 Oct **B. Sc. Physics** GPA 1.8
Technical University of Munich (TUM)
Thesis: *Extending Dispersive Bounds to Include Sub-threshold Branch Cuts* (Mathematical Particle Physics)

WORK EXPERIENCE

2023 Nov – 2024 Feb	Research Associate · Chair of Theory of Complex Biosystems, TUM Engineered GPU-accelerated multiscale Brownian and Langevin dynamics simulations in JAX-MD for active-matter vesicle mechanics, resulting in a first-author publication in <i>Nano Letters</i>
2022 Oct – 2023 Sep	Teaching Assistant (GPU Computing & Deep Learning) · TUM Department of Physics Instructed graduate-level tutorials on <i>Parallelization of Physics Calculations on GPUs</i> (CUDA, parallel numerical algorithms) and <i>Introduction to Neural Networks</i>
2021 Sep – 2022 Jun	Working Student in Machine Learning Engineering · Deloitte Consulting GmbH Developed production machine learning pipelines and distributed data-processing workflows for enterprise analytics (<i>trufa</i>)
2020 Aug – 2021 May	Research Assistant · Chair of Theoretical Elementary Particle Physics, TUM Implemented numerical routines for flavor-physics observables and Bayesian inference in the open-source C++/Python library EOS Software
2019 Jun – 2020 Jan	Research Assistant · Walter Schottky Institute (Semiconductor Physics) Built automated data-analysis pipelines in Python correlating multi-modal experimental spectroscopy and transport measurements

RESEARCH & TECHNICAL EXPERTISE

AI4Science & QC	Quantum Chemistry, Kohn-Sham DFT (KS-DFT), Exchange-Correlation (XC) Functionals, Differentiable SCF Solvers, Electronic Structure Modeling, Hamiltonian & Density Matrix Prediction, Machine-Learned Interatomic Potentials (MLIPs), Coupled Cluster, Molecular Dynamics (MD), Hybrid Distillation (B3LYP, SCAN, PBE)
Machine Learning	SE(3)/SO(3)-Equivariant Graph Neural Networks (GNNs), Deep Equilibrium Models (DEQs), Riemannian & Grassmannian Manifold Optimization, Flow Matching & Generative Modeling, Differentiable Physics, Out-of-Distribution Generalization
Computing & Stack	JAX (Flax, Optax, JAX-MD), PyTorch, PySCF, GPU Acceleration & Parallel Computing (CUDA), Python, C++, Linux HPC Clusters

INVITED TALKS

2026 Nov	Grimme Group University of Bonn — ML Exchange-Correlation Functionals & Long-Range Interactions
2026 Nov	Learning-Based Methods in Scientific Computing RICAM, Austrian Academy of Sciences, Linz
2025 Nov	AMLab Seminar Ensing & Welling Groups, University of Amsterdam
2025 May	Scientific Machine Learning Seminar University of Heidelberg
2024 Nov	Learning on Graphs Reading Group Massachusetts Institute of Technology (MIT, online)

HONOURS & AWARDS

2025 Nov	ChemAI Best Poster Award (1st Place) Amsterdam, Netherlands
2025 Jan	ICLR 2025 Spotlight (Top ~5% of Submissions) <i>Learning Equivariant Non-Local Electron Density Functionals</i> (EG-XC, Master's Thesis Work)
2024 Aug	Best of Class 2024 (M. Sc. Computer Science & Engineering) Technical University of Munich (TUM)
2016 Jun	Abitur Award for Outstanding Achievements in Physics German Physical Society (DPG)