Michael Scherbela, PhD

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Education

Oct 2020 - Sep 2024   **PhD in mathematics at University of Vienna, Austria**
Developed codebase *DeepErwin*, which uses Deep Learning and Variational Monte Carlo to compute highly accurate energies of small molecules; supervised by Prof. Philipp Grohs (sub auspiciis)

Dec 2014 - Jun. 2017   **Master's degree in physics, Graz University of Technology, Austria**
with distinction (grade average 1.0); master thesis on *Structure Prediction at Organic/Inorganic Interfaces using Machine Learning*

Oct. 2011 - Nov. 2014   **Bachelor's Degree in physics, Graz University of Technology, Austria**
with distinction (grade average 1.0)

Oct. 2010 - Apr. 2011   **Mandatory military service**

Sep. 2002 - Jul. 2010   **High School and participation in international student competitions:**

International Physics Olympiad
2010 (Croatia): Silver Medal, 2008 (Vietnam): Honorable mention

International Young Physicists' Tournament (IYPT)
2010 (Austria): second place, 2009 (China): second place

Selected Publications

Scherbela, Gao, Grohs, Günnemann, *Accurate Ab-initio Neural-network Solutions to Large-Scale Electronic Structure Problems* (arxiv 2025)

Gerard[†], Scherbela[†], Sutterud[†] et al. *Transferable Neural Wavefunctions for Solids* (arxiv 2023)

Scherbela[†], Gerard[†], Grohs, *Variational Monte Carlo on a Budget – Fine-tuning pre-trained Neural Wavefunctions.* **NeurIPS** (2023)

Scherbela[†], Gerard[†], Grohs, *Towards a Transferable Fermionic Neural Wavefunction for Molecules.* **Nature Comm**. (2023)

Gerard[†], Scherbela[†] et al., *Gold-standard solutions to the Schrödinger equation using deep learning: How much physics do we need?* **NeurIPS** (2022)

Scherbela[†], Gerard[†] et al., *Solving the electronic Schrödinger equation for multiple nuclear geometries with weight-sharing deep neural networks.* **Nature Comp. Sci** (2022)

Scherbela et al. Leaving the Valley: *Charting the Energy Landscape of Metal/Organic Interfaces via Machine Learning*. **Phys. Rev. Materials** (2018)

Conference Contributions

DL-VMC workshop: Organized and presented at workshop on Deep Learning for VMC; participants from DeepMind, Microsoft, ByteDance and public research; 2023

CECAM conference: Bridging length scales with machine learning, 2023, Poster

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[†] Authors contributed equally

C'Est La Wien: Machine Learning Mixer, 2023, Best Poster Award

IPAM Workshop on Monte Carlo and ML in Quantum Mech., 2022, Invited Talk

EPFL: Big Data and Machine Learning for Chemistry, 2021, Poster

IMPRESS Conference, Structure Search at Interfaces using Bayesian Regression, 2017, Talk

DPG Spring Meeting: Structure Search using Machine Learning, 2017, Talk

Exemplary Software Projects

DeepErwin   Compute properties of small molecules from scratch using deep learning
github.com/mdsunivie/deeperwin

Image Search   AI tool, which finds similar picture in private photo collection
github.com/MScherbela/image_search

Professional Experience

Oct 2024 - current   **University of Vienna,** post-doctoral researcher

Nov. 2020 - Sep 2024   **University of Vienna,**
PhD student, incl. research and teaching of mathematics

Apr. 2018 - Oct. 2020   **McKinsey & Co, Vienna**
Management consultant focused on analytics and digitization;
Example projects: Optimizing assortment and logistics for
European Retailer; Analysis and forecast of profitability for
music label; Growth-strategy for major software company

Apr. 2016 - Dec. 2017   **Institute of Solid-State Physics, Graz University of Technology**
researcher and teaching assistant

Feb. 2013 - Feb. 2016   **VIRTUAL VEHICLE Research Center, Graz, Austria**
part time job in data analysis, software development, and
development of sensors for automotive applications

summer internships   **Infineon Technologies:** Automated testing of semiconductors)

2011 - 2012   **SLR Engineering**: Image recognition for traffic applications)

Anton Paar: Assembly of measurement instruments

Additional Skills and Qualifications

Languages   **German** (mother tongue), **English** (business fluent)

IT / programming   **python**: 10+ years of experience, incl. data analysis (numpy, scipy,
pandas), machine learning (JAX, tensorflow), web (flask)
linux: experience on various HPC-systems (SLURM) and operating
own home-server using e.g. docker, nginx, flask
C/C++: embedded systems
Quantum Chemistry: Orca, pySCF, ASE

Hobbies   **Being outdoors**: Hiking, Paragliding
Building things, e.g. X-ray machine and various software projects