Martin Stöhr

Postdoctoral Scholar

Dept. of Chemistry, The PULSE Institute,
& SLAC National Accelerator Laboratory

Stanford University, CA, USA

martin.stoehr@stanford.edu
martin.stoehr.research@gmail.com

ORCID: 0000-0002-4068-4692
Google scholar ID: MyoZPDAAAAAJ
martin-stoehr.github.io

About my work:

My research aims to advance our understanding of the microscopic origins of emergent phenomena in realistic, complex systems from biomolecules to nano-structures. This involves the development of efficient electronic structure methods and new tools for the characterization and conceptual understanding of many-particle systems. To this end, my work combines insights and approaches from (quantum) chemistry, (bio)physics, applied mathematics, and data science with smart computational solutions.

About myself:

I consider myself a positive, open-minded and sociable person. My hobbies include football/soccer, ice hockey, volleyball, alpine sports and general outdoor activities, but I also enjoy traveling, web & graphic design, music, cooking, and trivia.

Professional Experience

07/2022- Postdoctoral Scholar, Stanford University, CA, USA
Advisor: Prof. Todd J. Martínez (Theoretical Chemistry, Dept of Chemistry)

03-06/2022 Visiting Scholar, University of California, Los Angeles
Institute for Pure and Applied Mathematics
Long program: Advancing quantum mechanics with mathematics and statistics

2021 Postdoctoral Researcher, University of Luxembourg
Advisor: Prof. Alexandre Tkatchenko (Theoretical Chemical Physics, Department of Physics and Materials Science)

2018-19 Teaching Assistant, University of Luxembourg
Thermodynamics | *Mathematical Physics I: Classical Mechanics*

04/2018 Scientific Consultant
Avant-garde Materials Simulation Deutschland GmbH, Merzhausen, Germany

2016 Visiting Graduate Researcher, University of California, Los Angeles
Institute for Pure and Applied Mathematics
Long program: Understanding Many-Particle Systems with Machine Learning

03-06/2015 Visiting Assistant in Research, Yale University
Advisor: Prof. John C. Tully (Theoretical Chemistry, Department of Chemistry)

2014-16 Research Assistant, Technical University of Munich
Advisor: Prof. Notker Rösch (Theoretical Chemistry, Department of Chemistry)

2013-15 Teaching Assistant, Technical University of Munich
Measurement, Analysis, and Simulation | *Mathematical Methods in Chemistry*

Education

11/2020 Ph.D. in Physics, University of Luxembourg
"van der Waals dispersion interactions in biomolecular systems: Quantum-mechanical insights and methodological advances"
Supervisor: Prof. Alexandre Tkatchenko (Theoretical Chemical Physics)

04/2016 M.Sc. in Chemistry, Technical University of Munich
Focus: Physical & Theoretical Chemistry, Final grade: 1.3 (3.62 on GPA 4.0)
"*Simulation of hybrid organic-inorganic interfaces with dispersion-corrected semi-empirical electronic structure methods*"
Supervisor: Prof. Karsten Reuter (Theoretical Chemistry)

08/2013 B.Sc. in Chemistry, Technical University of Munich
Final grade: 1.7 (3.27 on GPA 4.0)
"*(Co)adsorption effects on the work function of coinage metal surfaces*"
Supervisor: Prof. Karsten Reuter (Theoretical Chemistry)

Awards & Grants

07/2022 Rolf Tarrach Award | Les Amis d'Université du Luxembourg
Awarded annually to the best PhD thesis across all disciplines in Luxembourg

12/2021 DSSE Excellent Thesis Award
Doctoral School in Science and Engineering (DSSE), University of Luxembourg

10/2021 FNR Award "Outstanding PhD Thesis" (shortlist)
Luxembourg National Research Fund (FNR)

2016-20 FNR-AFR PhD grant | Luxembourg National Research Fund (FNR)

2015 DAAD-PROMOS scholarship | German Academic Exchange Service

04/2011 Award for the year's best graduates in chemistry
Gesellschaft deutscher Chemiker (German Chemical Society)

Scientific Expertise:

- van der Waals interactions
- Electronic structure theory *(density-functional theory, tight binding)*
- Atomistic modeling *(structure prediction, molecular dynamics)*
- High-performance computing
- Biomolecular systems
- Hybrid organic-inorganic interfaces

Language Proficiency:
German (native language), English (C1)

Coding & Typesetting:
Python, Fortran (including MPI, BLACS/ScaLAPACK), bash, HTML/CSS, LaTeX

Software Development:
DFTB+, libmbd, ASE, Hotbit, FHI-aims

Software Experience:
GROMACS, CASTEP, VMD, PyMol, GIMP

Collaborations:

University of Luxembourg, Luxembourg
Howard University, Washington, D.C.
Technical University Berlin, Germany
University of South Florida, Tampa, FL
University of Torino, Italy
University of Warwick, United Kingdom
Google Brain Berlin/Zürich
Luxemb. Centre for Systems Biomedicine
Vienna University of Technology, Austria

Voluntary Activities/Outreach:

2018 Mentor for High School Student
"M-ProJ" program, Luxembourg

2009-11 Tutor for freshmen classes and member of the school council
Werdenfels Gymnasium Garmisch-Partenkirchen, Germany

2007-10 Member of the youth committee and youth leader
Evangelische Kirche Mittenwald, Germany

Publications

Quantum-mechanical force balance between multipolar dispersion and Pauli repulsion in atomic van der Waals dimers O. Vaccarelli, D. V. Fedorov, M. Stöhr and A. Tkatchenko, *Physical Review Research* **3**, 033181 (2021); doi: 10.1103/PhysRevResearch.3.033181

Coulomb Interactions between Dipolar Quantum Fluctuations in van der Waals Bound Molecules and Materials M. Stöhr, M. Sadhukhan, Y. S. Al-Hamdani, J. Hermann and A. Tkatchenko, *Nature Communications* **12**, 137 (2021); doi: 10.1038/s41467-020-20473-w

Accurate many-body repulsive potentials for density-functional tight binding from deep tensor neural networks M. Stöhr, L. Medrano Sandonas and A. Tkatchenko, *The Journal of Physical Chemistry Letters* **11**, 6835–6843 (2020); doi: 10.1021/acs.jpclett.0c01307

DFTB+, a software package for efficient approximate density functional theory based atomistic simulations B. Hourahine *et al.*, *The Journal of Chemical Physics* **152**, 124101 (2020); doi: 10.1063/1.5143190

Quantum mechanics of proteins in explicit water: The role of plasmon-like solute-solvent interactions M. Stöhr and A. Tkatchenko, *Science Advances* **5**, eaax0024 (2019); doi: 10.1126/sciadv.aax0024

Theory and practice of modeling van der Waals interactions in electronic-structure calculations M. Stöhr, T. Van Voorhis and A. Tkatchenko, *Chemical Society Reviews* **48**, 4118–4154 (2019); doi: 10.1039/C9CS00060G

Quantum-mechanical relation between atomic dipole polarizability and the van der Waals radius D. V. Fedorov, M. Sadhukhan, M. Stöhr and A. Tkatchenko, *Physical Review Letters* **121**, 183401 (2018); doi: 10.1103/PhysRevLett.121.183401

Communication: Charge-population based dispersion interactions for molecules and materials M. Stöhr, G. S. Michelitsch, J. C. Tully, K. Reuter and R. J. Maurer, *The Journal of Chemical Physics* **144**, 151101 (2016); doi: 10.1063/1.4947214

Dynamics of spatially confined Bisphenol A trimers in a unimolecular network on Ag(111) J. A. Lloyd *et al.*, *Nano Letters* **16**, 1884–1889 (2016); doi: 10.1021/acs.nanolett.5b05026

Reviewing experience for the German Research Foundation (DFG), Communications Chemistry, Journal of Chemical Theory and Computation, The Journal of Physical Chemistry Letters

Conferences & Workshops

Invited Talks/Seminars IPAM Program *"Advancing Quantum Mechanics with Mathematics and Statistics"*, Los Angeles (2022); CECAM Flagship Workshop *"Non-Covalent Interactions in Large Molecules and Extended Materials"*, Lausanne (2021); DPG BP-CPP-DY-SOE Spring Meeting, Virtual (2021); Atomistic Modeling Webinar, ICTP Trieste, Virtual (2021); DFTB Developers Meeting *"Supporting Machine Learning in DFTB"*, Virtual (2020).

Contributed Talks/Posters APS March Meeting (2017-2021); DPG Spring Meeting (2016, 2019); *"Bose-Einstein condensation in inorganic and organic molecules"*, Marseille (2019); IPAM Program *"Understanding Many-Particle Systems with Machine Learning"*, Los Angeles (2016, 2018, 2019); *"Physics meets Biology"*, Luxembourg (2018); *"Frontiers of Multiscale Modeling in Materials, Energy, and Catalysis"*, Monte Isola (2016); CECAM/Psi-k workshop *"Simulation of chemistry-driven growth phenomena for metastable materials"*, Ebsdorfergrund (2015).