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(generated on April 19, 2024)

Jan Hermann

Employment

Microsoft, Berlin
Nov 2022– Principal research manager · MSR AI4Science

Free University of Berlin
Nov 2020–Oct 2022 Junior research group leader · Department of Mathematics
Jan 2019–Oct 2020 Postdoctoral researcher · AI4Science group

University of Luxembourg
Jan–Dec 2018 Postdoctoral researcher · Theoretical Chemical Physics group

Fritz Haber Institute, Berlin
Oct 2013–Dec 2017 Graduate research assistant · Theory department

Institute of Organic Chemistry and Biochemistry, Prague
Mar 2010–Sep 2013 Undergraduate research assistant · Non-Covalent Interactions group

Education

Humboldt University of Berlin
Dec 2017 **Ph.D.** in **Physics** · *summa cum laude*

Charles University, Prague
Sep 2013 **M.S.** in **Molecular Modeling**
Sep 2011 **B.S.** in **Physics**
Jun 2011 **B.S.** in **Chemistry**

Secondary appointments

Jul 2021–Oct 2022 Junior Fellow · BIFOLD, Berlin
Jan 2019–Oct 2020 Postdoctoral research fellow · Machine Learning group, TU Berlin
Sep–Dec 2016 Visiting graduate researcher · IPAM, UCLA
(long program "Understanding Many-Particle Systems with Machine Learning")

Awards

Feb 2021 **Marie Skłodowska-Curie Individual Fellowship** *[relinquished]*
Jan 2014 **Heyrovsky Prize for the best science graduate** · Charles University
Jul 2008 **Gold Medal** · 39th International Physics Olympiad

Funding

Apr 2021–Mar 2024 MATH+ AA2-8 (co-PI) · "Deep backflow for accurate solution of the electronic Schrödinger equation" · **€160k**

Professional activities

- Peer-reviewed 43 manuscripts for *Phys. Rev. X*, *Nat. Commun.*, *Nat. Mach. Intell.*, *Phys. Rev. Lett.*, *J. Chem. Phys.*, and other journals
- Reviewed 1 grant proposal for *U. S. Department of Energy*

Teaching & mentoring

Professional mentorship

Sep 2022– U. C. Kaya, Master student
Mar–Sep 2022 E. Trushin, Postdoc (with F. Noé)
Sep 2021–Oct 2022 B. Szabó, Phd student (with F. Noé)
May 2021–Dec 2022 P. del Mazo, Postdoc
Apr 2021–Apr 2022 M. Höfler, Master student
Jul 2019–Jul 2020 J. Lederer, Phd student, TU Berlin (with K.-R. Müller)
Jan 2019–Oct 2022 Z. Schätzle, Master/Phd student (with F. Noé)

Lectures for students

2022 "Machine Learning in Quantum Chemistry" · IMPRS Summer School (Berlin, Germany)
• "Basic principles of application of machine learning in quantum chemistry" (VŠCHT, Prague)
2019 "Message-passing neural networks for modeling many-particle systems" · CECAM Summer School (Mainz, Germany)

Doctoral committees

2022– B. Ames, University of Luxembourg
2021 M. Wilson, University of Bristol, UK

Public outreach

Sep 2019 Public lecture in the Six Minute Challenge series, Czech Center, Berlin
2018 Mentored a student in the LEAF program, accepted to University of Edinburgh
Sep 2008–Jun 2010 Co-organized FYKOS, physics competition for high school students

Software

- **DeepQMC** · creator *https://github.com/deepqmc/deepqmc (324 stars)*
  Deep learning quantum Monte Carlo for electrons in real space (Python)
- **libMBD** · creator *https://github.com/libmbd/libmbd (48 stars)*
  Many-body dispersion library (Fortran)
- **Pyberny** · creator *https://github.com/jhrmnn/pyberny (103 stars)*
  Molecular structure optimizer (Python)
- **FHI-aims** · core contributor *https://aimsclub.fhi-berlin.mpg.de*
  All-electron electronic-structure calculations (Fortran)
- **PySCF** · contributor *https://pyscf.org*
- **DFTB+** · contributor *https://dftbplus.org*
- **QCEngine** · contributor *https://github.com/MolSSI/QCEngine*

Presentations

- Includes future presentations

Invited conference talks

2023 "Solving the electronic Schrödinger equation with deep learning" · SIAM Conference on Computational Science and Engineering (Amsterdam, Netherlands)

2022 "Libmbd: A general-purpose package for scalable many-body dispersion calculations" · Electronic Structure Software Development (Lausane, Switzerland) *[virtual]*

• "Neural-network wave functions for quantum chemistry" · MLQC4DYN (Institut Pascal, Paris, France)

• "Neural-network wave functions for quantum chemistry" · Monte Carlo and Machine Learning Approaches in Quantum Mechanics (IPAM, Los Angeles, USA)

2021 "Deep-learning solution to the electronic many-body problem" · Non-Covalent Interactions in Large Molecules and Extended Materials (EPFL, Lausanne, Switzerland)

• "Solving the electronic Schrödinger equation with deep learning" · ACS Fall Meeting *[virtual]*

2020 "Density-functional model for van der Waals interactions: Unifying atomic approaches with nonlocal functionals" · Electronic Structure Theory with Numeric Atom-Centered Basis Functions *[virtual]*

2019 "Unifying density-functional and interatomic approaches to van der Waals interactions" · Frontiers in Density Functional Theory and Beyond (Kavli ITS, Beijing, China)

2018 "Modeling van der Waals interactions in molecules and materials" · Molecular Simulations Meets Machine Learning and Artificial Intelligence (Lorentz Center, Leiden, Netherlands)

• "Modeling van der Waals interactions in materials with many-body dispersion" · Electronic Structure Theory with Numeric Atom-Centered Basis Functions (TU Munich, Germany)

• "Modeling van der Waals interactions" · Python for Quantum Chemistry and Materials Simulation Software (Caltech, Pasadena, USA)

Contributed conference talks

2021 "Approaching exact solutions of the electronic Schrödinger equation with deep quantum Monte Carlo" · APS March Meeting *[virtual]*

2020 "Deep neural network solution of the electronic Schrödinger equation" · APS March Meeting (Denver, USA) *[cancelled]*

2018 "Unified many-body approach to van der Waals interactions based on semilocal polarizability functional" · APS March Meeting (Los Angeles, USA)

2017 "What is the range of electron correlation in density functionals?" · APS March Meeting (New Orleans, USA)

2016 "First-principles approaches to van der Waals interactions" · Many-Body Interactions (Telluride, USA)

2015 "Many-body dispersion meets non-local density functionals" · Modeling Many-Body Interactions (Lake La Garda, Italy)

• "Many-body dispersion meets non-local density functionals" · DPG March Meeting (Berlin, Germany)

• "Many-body dispersion meets non-local density functionals" · APS March Meeting (San Antonio, USA)

2014 "Non-local density functionals meet many-body dispersion" · DPG March Meeting (Dresden, Germany)

2013 "Adsorption in zeolites investigated by dispersion-corrected DFT" · Layered Materials (Liblice, Czechia)

• "Modeling of surface properties of lamellar zeolites" · Molecular Sieves (Heyrovsky Institute, Prague, Czechia)

Conference poster presentations

2021 "Solving the electronic Schrödinger equation with deep learning" · Stochastic Methods in Electronic Structure Theory *[virtual]*

2020 "Convergence to the fixed-node limit in deep variational Monte Carlo" · NeurIPS workshop Machine Learning and the Physical Sciences *[virtual]*

2019 "Deep neural network solution of the electronic Schrödinger equation" · NeurIPS workshop Machine Learning and the Physical Sciences (Vancouver, Canada)

2017 "Balancing semilocal and nonlocal energy contributions in van der Waals systems" · Intermolecular Interactions (Arenas de Cabrales, Spain)

2016 "Python interface to FHI-aims" · Electronic Structure Theory with Numeric Atom-Centered Basis Functions (Munich, Germany)

2015 "Non-local density functionals meet many-body dispersion" · Psi-k Conference (San Sebastian, Spain)

• "Many-body dispersion meets non-local density functionals" · Congress of Theoretical Chemists (Torino, Italy)

• "Non-local density functionals meet many-body dispersion" · Frontiers of First-Principles Simulations: Materials Design and Discovery (Berlin, Germany)

2014 "Non-local density functionals meet many-body dispersion" · Addressing Challenges for First-Principles Based Modeling of Molecular Materials (Lausanne, Switzerland)

2013 "Modeling of surface properties of lamellar zeolites" · Molecular Sieves and Catalysis (Segovia, Spain)

2012 "Silver clusters in zeolites: Structure, stability and photoactivity" · British Zeolite Association Meeting (Chester, UK)

• "Silver clusters in faujasite: A theoretical investigation" · Molecular Sieves (Prague, Czechia)

Invited seminars

2022 UCT & IOCB Theoretical Chemistry Seminar (VŠCHT, Prague, Czechia)

• Lennard-Jones Centre Discussion Group (University of Cambridge) *[virtual]*

2021 Molecular and Ultrafast Science Seminar (Center for Free-Electron Laser Science) *[virtual]*

• Machine Learning seminar (Chalmers University of Technology) *[virtual]*

- Grüneis group seminar (TU Wien) *[virtual]*
- (Nano)Materials Modeling Seminar (Charles University) *[virtual]*
- Cosmology Seminar (University of Szczecin) *[virtual]*

2020 "Solving the electronic Schrödinger equation with deep learning" · Scientific Machine Learning Mini-Course (Carnegie Mellon University) *[virtual]*

- Machine Learning in Physics, Chemistry and Materials (University of Cambridge) *[virtual]*
- Jordan group seminar (University of Pittsburgh) *[virtual]*

2018 "Mona: Calculation framework for reproducible science" · Theory Department seminar (Fritz Haber Institute, Berlin, Germany)

2016 "Nanoscale π–π stacked molecules bound by collective charge fluctuations" · Aspuru-Guzik group seminar (Harvard University, Cambridge, USA)

2015 DiStasio group seminar (Cornell University, Ithaca, USA)

Publications

- Citation numbers (on the right) from Google Scholar

Research articles

- Variational principle to regularize machine-learned density functionals: The non-interacting kinetic-energy functional · P. del Mazo-Sevillano & **JH** · *J. Chem. Phys.* **159**, 194107 (2023) — 2
- libMBD: A general-purpose package for scalable quantum many-body dispersion calculations · **JH**, M. Stöhr, S. Góger, S. Chaudhuri, B. Aradi, R. J. Maurer & A. Tkatchenko · *J. Chem. Phys.* **159**, 174802 (2023) — 2
- DeepQMC: An open-source software suite for variational optimization of deep-learning molecular wave functions · Z. Schätzle, P. B. Szabó, M. Mezera, **JH** & F. Noé · *J. Chem. Phys.* **159**, 094108 (2023) — 10
- Ab initio quantum chemistry with neural-network wavefunctions · **JH**, J. Spencer, K. Choo, A. Mezzacapo, W. M. C. Foulkes, D. Pfau, G. Carleo & F. Noé · *Nat. Rev. Chem.* **7**, 692–709 (2023) — 36
- Electronic excited states in deep variational Monte Carlo · M. T. Entwistle, Z. Schätzle, P. A. Erdman, **JH** & F. Noé · *Nat. Commun.* **14**, 274 (2023) — 30
- Roadmap on Machine learning in electronic structure · H. J. Kulik et al. · *Electron. Struct.* **4**, 023004 (2022) — 102
- Quantum Chemistry Common Driver and Databases (QCDB) and Quantum Chemistry Engine (QCEngine): Automation and interoperability among computational chemistry programs · D. G. A. Smith et al. · *J. Chem. Phys.* **155**, 204801 (2021) — 26
- Anisotropic interlayer force field for transition metal dichalcogenides: The case of molybdenum disulfide · W. Ouyang, R. Sofer, X. Gao, **JH**, A. Tkatchenko, L. Kronik, M. Urbakh & O. Hod · *J. Chem. Theory Comput.* **17**, 7237–7245 (2021) — 14
- Convergence to the fixed-node limit in deep variational Monte Carlo · Z. Schätzle, **JH** & F. Noé · *J. Chem. Phys.* **154**, 124108 (2021) — 23
- Coulomb interactions between dipolar quantum fluctuations in van der Waals bound molecules and materials · M. Stöhr, M. Sadhukhan, Y. S. Al-Hamdani, **JH** & A. Tkatchenko · *Nat. Commun.* **12**, 137 (2021) — 28
- Deep-neural-network solution of the electronic Schrödinger equation · **JH**, Z. Schätzle & F. Noé · *Nat. Chem.* **12**, 891–897 (2020) — 487
- Fluctuational electrodynamics in atomic and macroscopic systems: van der Waals interactions and radiative heat transfer · P. S. Venkataram, **JH**, A. Tkatchenko & A. W. Rodriguez · *Phys. Rev. B* **102**, 085403 (2020) — 2
- Recent developments in the PySCF program package · Q. Sun et al. · *J. Chem. Phys.* **153**, 024109 (2020) — 574
- Density functional model for van der Waals interactions: Unifying many-body atomic approaches with nonlocal functionals · **JH** & A. Tkatchenko · *Phys. Rev. Lett.* **124**, 146401 (2020) — 73
- DFTB+, a software package for efficient approximate density functional theory based atomistic simulations · B. Hourahine et al. · *J. Chem. Phys.* **152**, 124101 (2020) — 747
- Nonlocal electronic correlations in the cohesive properties of high-pressure hydrogen solids · T. Cui, J. Li, W. Gao, **JH**, A. Tkatchenko & Q. Jiang · *J. Phys. Chem. Lett.* **11**, 1521–1527 (2020) — 7
- Impact of nuclear vibrations on van der Waals and Casimir interactions at zero and finite temperature · P. S. Venkataram, **JH**, T. J. Vongkovit, A. Tkatchenko & A. W. Rodriguez · *Sci. Adv.* **5**, eaaw0456 (2019) — 8

- Phonon-polariton mediated thermal radiation and heat transfer among molecules and macroscopic bodies: Nonlocal electromagnetic response at mesoscopic scales · P. S. Venkataram, **JH**, A. Tkatchenko & A. W. Rodriguez · *Phys. Rev. Lett.* **121**, 045901 (2018) 17
- Electronic exchange and correlation in van der Waals systems: Balancing semilocal and nonlocal energy contributions · **JH** & A. Tkatchenko · *J. Chem. Theory Comput.* **14**, 1361–1369 (2018) 36
- Unifying microscopic and continuum treatments of van der Waals and Casimir interactions · P. S. Venkataram, **JH**, A. Tkatchenko & A. W. Rodriguez · *Phys. Rev. Lett.* **118**, 266802 (2017) 31
- Tuning intermolecular interactions with nanostructured environments · M. Chattopadhyaya, **JH**, I. Poltavsky & A. Tkatchenko · *Chem. Mater.* **29**, 2452–2458 (2017) 10
- First-principles models for van der Waals interactions in molecules and materials: Concepts, theory, and applications · **JH**, R. A. DiStasio, Jr. & A. Tkatchenko · *Chem. Rev.* **117**, 4714–4758 (2017) 517
- Nanoscale π–π stacked molecules are bound by collective charge fluctuations · **JH**, D. Alfè & A. Tkatchenko · *Nat. Commun.* 8, 14052 (2017) 94
- Communication: Many-body stabilization of non-covalent interactions: Structure, stability, and mechanics of $Ag_3Co(CN)_6$ framework · X. Liu, **JH** & A. Tkatchenko · *J. Chem. Phys.* **145**, 241101 (2016) 14
- Theoretical investigation of layered zeolite frameworks: Surface properties of 2D zeolites · **JH**, M. Trachta, P. Nachtigall & O. Bludský · *Catal. Today* **227**, 2–8 (2014) 25
- A novel correction scheme for DFT: A combined vdW-DF/CCSD(T) approach · **JH** & O. Bludský · *J. Chem. Phys.* **139**, 034115 (2013) 19
- Theoretical investigation of the Friedländer reaction catalysed by CuBTC: Concerted effect of the adjacent Cu^{2+} sites · M. Položij, E. Pérez-Mayoral, J. Čejka, **JH** & P. Nachtigall · *Catal. Today* **204**, 101–107 (2013) 35

Book chapters

- Introduction to material modeling · **JH** · In *Machine learning meets quantum physics* (eds K. T. Schütt et al.) 7–24 (Springer, 2020)
- Van der Waals interactions in material modelling · **JH** & A. Tkatchenko · In *Handbook of materials modeling* (eds W. Andreoni & S. Yip) 1–33 (Springer, 2018) 3

Theses

- *Towards unified density-functional model of van der Waals interactions* · **JH** · Humboldt University (2018) 5
- *Nonlocal correlation in density functional theory* · **JH** · Charles University (2013)