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Jan Hermann

My research focuses on the development of computational methods for efficient modeling of the electronic structure of molecules and materials. The goal is to enable straightforward multi-scale simulations of complex electronic environments, which I am pursuing through tight integration of machine learning into first-principles approaches.

Employment

Free University of Berlin
Nov 2020– Head of Junior Research Group, Department of Mathematics
Jan 2019–Oct 2020 Postdoctoral researcher, **Noé** group

University of Luxembourg
Jan–Dec 2018 Postdoctoral researcher, **Tkatchenko** group

Fritz Haber Institute of the Max Planck Society, Berlin
Oct 2013–Dec 2017 Graduate researcher, **Tkatchenko** group, Theory Department

Institute of Organic Chemistry and Biochemistry, Prague
Mar 2010–Sep 2013 Undergraduate researcher, **Hobza** 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– Junior Fellow, BIFOLD
Jan 2019–Oct 2020 Research fellow in Müller group, TU Berlin
Sep–Dec 2016 Research fellow at 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 36 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

May 2021– P. del Mazo, Postdoc
Apr 2021– M. Höfler, Master student, FU Berlin
Jul 2019–Jul 2020 J. Lederer, Phd student in Müller group, TU Berlin
Jan 2019–Oct 2020 Z. Schätzle, Master/Phd student in Noé group, FU Berlin

Invited lectures

2019 "Message-passing neural networks for modeling many-particle systems", CECAM Summer School, Mainz, Germany

Doctoral examinations

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 (230 stars)*
  Deep learning quantum Monte Carlo for electrons in real space (Python)
- **Libmbd**, creator *https://github.com/libmbd/libmbd (32 stars)*
  Many-body dispersion library (Fortran)
- **Pyberny**, creator *https://github.com/jhrmnn/pyberny (75 stars)*
  Molecular structure optimizer (Python)
- **FHI-aims**, core contributor *https://aimsclub.fhi-berlin.mpg.de*
  All-electron electronic structure theory (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

2022 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, Atlanta, USA *[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, Beijing, China
2018 "Modeling van der Waals interactions in molecules and materials", Molecular Simulations Meets Machine Learning and Artificial Intelligence, Leiden, Netherlands
• "Modeling van der Waals interactions in materials with many-body dispersion", Electronic Structure Theory with Numeric Atom-Centered Basis Functions, Munich, Germany

- "Modeling van der Waals interactions", Python for Quantum Chemistry and Materials Simulation Software, 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, Prague, Czechia

Conference poster presentations

2021 "Solving the electronic Schrödinger equation with deep learning", Stochastic Methods in Electronic Structure Theory, Telluride, USA *[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 Computational Surface Chemistry Seminar, University of Warwick
- Lennard-Jones Centre Discussion Group, University of Cambridge *[virtual]*
2021 Molecular and Ultrafast Science Seminar, Center for Free-Electron Laser Science, Hamburg *[virtual]*
- Machine Learning seminar, Chalmers University of Technology *[virtual]*
- Grüneis group, TU Wien *[virtual]*
- (Nano)Materials Modeling Seminar, Charles University *[virtual]*
- Institute of Physics, 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, University of Pittsburgh *[virtual]*
2018 "Mona: Calculation framework for reproducible science", Theory department, Fritz Haber Institute
2016 "Nanoscale π–π stacked molecules bound by collective charge fluctuations", Aspuru-Guzik group, Harvard University
2015 DiStasio group, Cornell University

Publications

- Citation numbers (on the right) from Google Scholar

Research articles

- M. Entwistle, Z. Schätzle, P. A. Erdman, **JH** & F. Noé. Electronic excited states in deep variational Monte Carlo. *arXiv:2203.09472* (2022)
- H. Kulik et al. Roadmap on machine learning in electronic structure. *Electron. Struct.* (2022) 2
- D. G. A. Smith et al. Quantum Chemistry Common Driver and Databases (QCDB) and Quantum Chemistry Engine (QCEngine): Automation and interoperability among computational chemistry programs. *J. Chem. Phys.* **155**, 204801 (2021) 7

- W. Ouyang, R. Sofer, X. Gao, **JH**, A. Tkatchenko, L. Kronik, M. Urbakh & O. Hod. Anisotropic interlayer force field for transition metal dichalcogenides: The case of molybdenum disulfide. *J. Chem. Theory Comput.* **17**, 7237–7245 (2021) 1
- Z. Schätzle, **JH** & F. Noé. Convergence to the fixed-node limit in deep variational Monte Carlo. *J. Chem. Phys.* **154**, 124108 (2021) 5
- M. Stöhr, M. Sadhukhan, Y. S. Al-Hamdani, **JH** & A. Tkatchenko. Coulomb interactions between dipolar quantum fluctuations in van der Waals bound molecules and materials. *Nat. Commun.* **12**, 137 (2021) 10
- **JH**, Z. Schätzle & F. Noé. Deep-neural-network solution of the electronic Schrödinger equation. *Nat. Chem.* **12**, 891–897 (2020) 194
- P. S. Venkataram, **JH**, A. Tkatchenko & A. W. Rodriguez. Fluctuational electrodynamics in atomic and macroscopic systems: Van der Waals interactions and radiative heat transfer. *Phys. Rev. B* **102**, 085403 (2020)
- Q. Sun et al. Recent developments in the PySCF program package. *J. Chem. Phys.* **153**, 024109 (2020) 148
- **JH** & A. Tkatchenko. Density functional model for van der Waals interactions: Unifying many-body atomic approaches with nonlocal functionals. *Phys. Rev. Lett.* **124**, 146401 (2020) 29
- B. Hourahine et al. DFTB+, a software package for efficient approximate density functional theory based atomistic simulations. *J. Chem. Phys.* **152**, 124101 (2020) 266
- T. Cui, J. Li, W. Gao, **JH**, A. Tkatchenko & Q. Jiang. Nonlocal electronic correlations in the cohesive properties of high-pressure hydrogen solids. *J. Phys. Chem. Lett.* **11**, 1521–1527 (2020) 5
- P. S. Venkataram, **JH**, T. J. Vongkovit, A. Tkatchenko & A. W. Rodriguez. Impact of nuclear vibrations on van der Waals and Casimir interactions at zero and finite temperature. *Sci. Adv.* **5**, eaaw0456 (2019) 5
- P. S. Venkataram, **JH**, A. Tkatchenko & A. W. Rodriguez. Phonon-polariton mediated thermal radiation and heat transfer among molecules and macroscopic bodies: Nonlocal electromagnetic response at mesoscopic scales. *Phys. Rev. Lett.* **121**, 045901 (2018) 12
- **JH** & A. Tkatchenko. Electronic exchange and correlation in van der Waals systems: Balancing semilocal and nonlocal energy contributions. *J. Chem. Theory Comput.* **14**, 1361–1369 (2018) 26
- P. S. Venkataram, **JH**, A. Tkatchenko & A. W. Rodriguez. Unifying microscopic and continuum treatments of van der Waals and Casimir interactions. *Phys. Rev. Lett.* **118**, 266802 (2017) 22
- M. Chattopadhyaya, **JH**, I. Poltavsky & A. Tkatchenko. Tuning intermolecular interactions with nanostructured environments. *Chem. Mater.* **29**, 2452–2458 (2017) 9
- **JH**, R. A. DiStasio, Jr. & A. Tkatchenko. First-principles models for van der Waals interactions in molecules and materials: Concepts, theory, and applications. *Chem. Rev.* **117**, 4714–4758 (2017) 395
- **JH**, D. Alfè & A. Tkatchenko. Nanoscale π–π stacked molecules are bound by collective charge fluctuations. *Nat. Commun.* **8**, 14052 (2017) 72
- X. Liu, **JH** & A. Tkatchenko. Communication: Many-body stabilization of non-covalent interactions: Structure, stability, and mechanics of $Ag_3Co(CN)_6$ framework. *J. Chem. Phys.* **145**, 241101 (2016) 10
- **JH**, M. Trachta, P. Nachtigall & O. Bludský. Theoretical investigation of layered zeolite frameworks: Surface properties of 2D zeolites. *Catal. Today* **227**, 2–8 (2014) 24
- **JH** & O. Bludský. A novel correction scheme for DFT: A combined vdW-DF/CCSD(T) approach. *J. Chem. Phys.* **139**, 034115 (2013) 18
- M. Položij, E. Pérez-Mayoral, J. Čejka, **JH** & P. Nachtigall. Theoretical investigation of the Friedländer reaction catalysed by CuBTC: Concerted effect of the adjacent Cu^{2+} sites. *Catal. Today* **204**, 101–107 (2013) 32

Book chapters

- **JH**. Introduction to material modeling. In: K. T. Schütt et al. (eds), Machine learning meets quantum physics (Springer, Cham, 2020)
- **JH** & A. Tkatchenko. Van der Waals interactions in material modelling. In: W. Andreoni & S. Yip (eds), Handbook of Materials Modeling (Springer, Cham, 2018) 1

Theses

- **JH**. Towards unified density-functional model of van der Waals interactions (Humboldt University, 2018) 1
- **JH**. Nonlocal correlation in density functional theory (Charles University, 2013)