Arnimallee 6, 141 95 Berlin, Germany
jan.hermann@fu-berlin.de
+49 176 43313859
https://jan.hermann.name
ORCID: 0000-0002-2779-0749

(generated on May 12, 2021)

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, BIFOLD, 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

Jan 2019–Oct 2020 Research fellow in Müller group, Technical University of Berlin
Sep–Dec 2016 Research fellow at the Institute for Pure and Applied Mathematics, UCLA (long program "Understanding Many-Particle Systems with Machine Learning")

Awards

2021 **Marie Skłodowska-Curie Individual Fellowship** *[relinquished]*
2014 **Best science graduate**, Charles University, Prague
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**

Teaching & mentoring

Mentorship

May 2021– P. del Mazo, Postdoc
Apr 2021– M. Höfler, Master student, FU Berlin
Jul 2019– J. Lederer, Phd student in Müller group, TU Berlin
Jan 2019– 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, Meinz, 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

Professional activities

- Peer-reviewed 22 manuscripts for impact-factored journals including *Nat. Commun.*, *J. Phys. Chem. Lett.*, *J. Chem. Theory Comput.*, *Phys. Rev. B*, and *J. Chem. Phys.*

Software projects

- **DeepQMC**, creator *https://github.com/deepqmc/deepqmc (182 stars)*
  Deep learning quantum Monte Carlo for electrons in real space (Python)
- **Libmbd**, creator *https://github.com/libmbd/libmbd (27 stars)*
  Many-body dispersion library (Fortran)
- **Pyberny**, creator *https://github.com/jhrmnn/pyberny (61 stars)*
  Molecular structure optimizer (Python)
- **FHI-aims**, core contributor *https://aimsclub.fhi-berlin.mpg.de*
  All-electron electronic structure theory (Fortran)
- **PySCF**, contributor *http://pyscf.org*
- **DFTB+**, contributor *https://www.dftbplus.org*

Presentations

- Includes future accepted presentations

Invited conference talks

2021 "Solving the electronic Schrödinger equation with deep learning", ACS Fall Meeting, Atlanta, USA
• Non-Covalent Interactions in Large Molecules and Extended Materials, Lausanne, Switzerland
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", Python for Quantum Chemistry and Materials Simulation Software, Pasadena, USA
• "Modeling van der Waals interactions in materials with many-body dispersion", Electronic Structure Theory with Numeric Atom-Centered Basis Functions, Munich, Germany

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", 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", APS March Meeting, San Antonio, USA
• "Many-body dispersion meets non-local density functionals", DPG March Meeting, Berlin, Germany
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

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", Ψ-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 faujasite: A theoretical investigation", Molecular Sieves, Prague, Czechia
• "Silver clusters in zeolites: Structure, stability and photoactivity", British Zeolite Association Meeting, Chester, UK

Invited seminars

2021 "Solving the electronic Schrödinger equation with deep learning", CC4S group, TU Wien *[virtual]*
• "Some new methods in electronic structure theory", (Nano)Materials Modeling seminar, Charles University *[virtual]*
• "Solving the electronic Schrödinger equation with deep learning", 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]*
• "Solving the electronic Schrödinger equation with deep learning", MLDG, University of Cambridge *[virtual]*
• "Deep neural network solution of the electronic Schrödinger equation", 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 "The unreasonable effectiveness of harmonic oscillators", DiStasio group, Cornell University

Publications

- Citation numbers on the right taken from Google Scholar

Research articles

• Z. Schätzle, **JH** & F. Noé. Convergence to the fixed-node limit in deep variational Monte Carlo. *J. Chem. Phys.* **154**, 124108 (2021)
• 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) 3
• **JH**, Z. Schätzle & F. Noé. Deep-neural-network solution of the electronic Schrödinger equation. *Nat. Chem.* **12**, 891–897 (2020) 74
• 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) 42

- **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) 13
- B. Hourahine et al. DFTB+, a software package for efficient approximate density functional theory based atomistic simulations. *J. Chem. Phys.* **152**, 124101 (2020) 90
- 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) 1
- 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) 10
- **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) 24
- 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) 18
- M. Chattopadhyaya, **JH**, I. Poltavsky & A. Tkatchenko. Tuning intermolecular interactions with nanostructured environments. *Chem. Mater.* **29**, 2452–2458 (2017) 8
- **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) 319
- **JH**, D. Alfè & A. Tkatchenko. Nanoscale π–π stacked molecules are bound by collective charge fluctuations. *Nat. Commun.* **8**, 14052 (2017) 62
- 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) 8
- **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) 16
- 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) 28

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