Jan Janssen

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PROFESSIONAL APPOINTMENTS

2023 – present **Group leader for Materials Informatics** - Computational Materials Design
Research topic: foundation models for sustainable materials
Max Planck Institute for Sustainable Materials, Düsseldorf, Germany

2024 **Invited Fellow** - Institute for Mathematical and Statistical Innovation (IMSI)
Research topic: data-driven materials informatics
University of Chicago, Chicago, IL, USA

2022 – 2023 **Director's Postdoctoral Fellowship** - Theoretical Division (T-1)
Research topic: long-timescale simulations of materials with *ab initio* accuracy
Los Alamos National Laboratory, Los Alamos, NM, USA

2023 **Invited Postdoctoral Fellow** - Institute for Pure and Applied Mathematics (IPAM)
Research topic: new mathematics for the exascale: applications to materials science
University of California, Los Angeles, CA, USA

2021 – 2022 **Postdoctoral Research Associate** - Theoretical Division (T-1)
Research topic: exascale atomistic capability for accuracy, length, and time
Los Alamos National Laboratory, Los Alamos, NM, USA

2017 **Invited Fellow** - Institute for Pure and Applied Mathematics (IPAM)
Research topic: complex high-dimensional energy landscapes
University of California, Los Angeles, CA, USA

2015 – 2021 **PhD Candidate** - Computational Materials Design
Research topic: computational phase studies and *ab initio* thermodynamics
Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany

EDUCATION

2015 – 2021 **PhD in Theoretical Physics** - Paderborn University, Germany
- Thesis: pyiron - an integrated development environment for *ab initio* thermodynamics
- Advisor: Prof. Jörg Neugebauer
- Grade: summa cum laude

2009 – 2015 **Advanced Degree in Physics** - Technical University of Kaiserslautern, Germany
- Thesis: carbon in α-iron-grainboundaries - an atomistic study of elastic properties
- Advisor: Prof. Herbert Urbassek
- Grade: thesis 1.0 (excellent) - total 1.6 (good)

FUNDED PROPOSALS

2024 **Principal Investigator** as part of the International Max Planck Research School for Sustainable Metallurgy - from Fundamentals to Engineering Materials
- Funding: EUR 150k

Co-Principal Investigator as part of the collaborative research center (CRC) 1394 "Structural and chemical atomic complexity - from defect phase diagrams to material properties"
- Funding: EUR 160k

2023 **Principal Investigator** of "workflows for machine learned interatomic potentials" as part of an internal call for funding for Postdoctoral Fellows at Los Alamos National Laboratory
- Computing Hardware Funding: USD 13k

Co-Principal Investigator of "uncertainty propagation for multi-fidelity machine learned interatomic potentials" as part of the summer school for applied machine learning at Los Alamos National Laboratory
- Funding: USD 25k

2022 **Co-Principal Investigator** of "development and deployment of a fully autonomous in *silico* processing and materials discovery platform" in collaboration with the department of Mechanical Engineering at Texas A&M University
- Funding: USD 176k

Co-Principal Investigator of "transferability of interatomic machine learning potentials" as part of the summer school for applied machine learning at Los Alamos National Laboratory
- Funding: USD 25k

Principal Investigator of "helping users build workflows with ontological typing" project funded by a NumFOCUS small development grant to hire an independent contractor
- Funding: USD 6k

AWARDS & HONORS

2024 Winner of the "2nd Annual Large Language Model Hackathon for Applications in Materials Science and Chemistry" coupling a large language model to atomistic simulation

Invited fellow at the Institute for Statistical and Mathematical Innovation (IMSI)

2023 Invited postdoctoral fellow at the Institute for Pure and Applied Mathematics (IPAM)

2022 Los Alamos National Laboratory (LANL) director's postdoctoral fellowship

2021 PhD with highest distinction - summa cum laude

2019 Runner-up for the Heinz Billing Award - a national biennial award for outstanding contributions to computational science by younger scientist without tenure

2017 Invited fellow at the Institute for Pure and Applied Mathematics (IPAM)

2015 Scholarship of the Technical University of Kaiserslautern

PUBLICATIONS

Google Scholar, 10/25: Citations: 363

2025

Y. Zimmermann, A. Bazgir, A. Al-Feghali, M. Ansari, L.C. Brinson, Y. Chiang, D. Circi, M.-H. Chiu, N. Daelman, M.L. Evans, A.S. Gangan, J. George, H. Harb, G. Khalighinejad, S.T. Khan, S. Klawohn, M. Lederbauer, S. Mahjoubi, B. Mohr, S.M. Moosavi, A. Naik, A.B. Ozhan, D. Plessers, A. Roy, F. Schöppach, P. Schwaller, C. Terboven, K. Ueltzen, S. Zhu, **J. Janssen**, C. Li, I. Foster, B. Blaiszik. 32 examples of LLM applications in materials science and chemistry: towards automation, assistants, agents, and accelerated scientific discovery. *Machine Learning: Science and Technology* doi:10.1088/2632-2153/ae011a. Citations: 10
- Code: jan-janssen/LangSim

J. Janssen, M.G. Taylor, P. Yang, J. Neugebauer and D. Perez. Executorlib – Up-scaling Python workflows for hierarchical heterogenous high-performance computing. *Journal of Open Source Software*. doi:10.21105/joss.07782. Citations: 1
- Code: pyiron/executorlib

Sk Md A.A. Alvi, **J. Janssen**, D. Khatamsaz, D. Perez, D. Allaire and R. Arróyave. Hierarchical Gaussian process-based Bayesian optimization for materials discovery in high entropy alloy spaces. *Acta Materialia*. doi:10.1016/j.actamat.2025.120908. Citations: 10
- Code: sheikhahnaf/DGP-BO

2024

J. Janssen, E. Makarov, T. Hickel, A.V. Shapeev and J. Neugebauer. Automated optimization and uncertainty quantification of convergence parameters in plane wave density functional theory. *npj Computational Materials*. doi:10.1038/s41524-024-01388-2. Citations: 4
- Code: pyiron/pyiron-dft-uncertainty

T.J. Summers, M.G. Taylor, L.J. Augustine, **J. Janssen**, D. Perez, E.R. Batista, and P. Yang. On the Importance of Configuration Search to the Predictivity of Lanthanide Selectivity. *JACS Au*. doi:10.1021/jacsau.4c00770. Citations: 7

S. Menon, Y. Lysogorskiy, A. L. M. Knoll, N. Leimeroth, M. Poul, M. Qamar, **J. Janssen**, M. Mrovec, J. Rohrer, K. Albe, J. Behler, R. Drautz, and J. Neugebauer. From electrons to phase diagrams with classical and machine learning potentials automated workflows for materials science with pyiron. *npj Computational Materials*. doi:10.1038/s41524-024-01441-0. Citations: 12
- Code: pyiron/potential_publication

M. Tynes, M.G. Taylor, **J. Janssen**, D. Burrill, D. Perez, P. Yang, and N. Lubbers. Linear graphlet models for accurate and interpretable cheminformatics. *Digital Discovery*. doi:10.1039/D4DD00089G. Citations: 4
- Code: lanl/minervachem

2023

M.G. Taylor, D.J. Burrill, **J. Janssen**, E. Batista, D. Perez, and P. Yang. Architector: high-throughput cross-periodic table 3D complex builder. *Nature Communications*. doi:10.1038/s41467-023-38169-2. Citations: 43
- Code: lanl/Architector

A. Rohskopf, C. Sievers, N. Lubbers, M. A. Cusentino, J. Goff, **J. Janssen**, M. McCarthy, D. Montes de Oca Zapiain, S. Nikolov, K. Sargsyan, E. Sikorski, L. Williams, D. Sema, A. P. Thompson, and M. A. Wood. FitSNAP: Atomistic machine learning in LAMMPS. *Journal of Open Source Software*. doi:10.21105/joss.05118. Citations: 44

- Code: FitSNAP/FitSNAP

2021 L.F. Zhu, **J. Janssen**, S. Ishibashi, F. Körmann, B. Grabowski and J. Neugebauer. A fully automated approach to calculate the melting temperature of elemental crystals. *Computational Materials Science*. doi:10.1016/j.commatsci.2020.110065. Citations: 45

- Code: pyiron/pyiron_meltingpoint

2020 T.D. Swinburne, **J. Janssen**, M. Todorova, G. Simpson, P. Plechac, M. Luskin and J. Neugebauer. Anharmonic free energy of lattice vibrations in fcc crystals from a mean field bond. *Physical Review B*. doi:10.1103/PhysRevB.102.100101. Citations: 9

- Code: tomswinburne/BLaSA

2019 **J. Janssen**, S. Surendralal, Y. Lysogorskiy, M. Todorova, T. Hickel, R. Drautz and J. Neugebauer. pyiron: an integrated development environment for computational materials science. *Computational Materials Science*. doi:10.1016/j.commatsci.2018.07.043. Citations: 137

- Code: pyiron/pyiron

Y. Lysogorskiy, T. Hammerschmidt, **J. Janssen**, J. Neugebauer and R. Drautz. Transferability of interatomic potentials for molybdenum and silicon. *Modelling and Simulation in Materials Science and Engineering*. doi:10.1088/1361-651X/aafd13. Citations: 24

2016 **J. Janssen**, N. Gunkelmann and H. M. Urbassek. Influence of C concentration on elastic moduli of $\alpha' - Fe_{1-x}C_x$ alloys. *Philosophical Magazine*. doi:10.1080/14786435.2016.1170224. Citations: 13

PUBLICATIONS IN REVIEW

2025 Sk Md A.A. Alvi, B. Vela, V. Attari, **J. Janssen**, D. Perez, D. Allaire, and R. Arróyave. Deep Gaussian Process-based Cost-Aware Batch Bayesian Optimization for Complex Materials Design Campaigns. doi:10.48550/arXiv.2509.14408.

Z. Wang, H. Huang, H. Zhao, C. Xu, S. Zhu, **J. Janssen** and V. Viswanathan. DREAMS: Density Functional Theory Based Research Engine for Agentic Materials Simulation. doi:10.48550/arXiv.2507.14267.

- Code: BattModels/material_agent

I. Baghishov, **J. Janssen**, G. Henkelman and D. Perez. Application-specific Machine-Learned Interatomic Potentials: Exploring the Trade-off Between Precision and Computational Cost. doi:10.48550/arXiv.2506.05646.

J. Janssen, J. George, J. Geiger, M. Bercx, X. Wang, C. Ertural, J. Schaarschmidt, A.M. Ganose, G. Pizzi, T. Hickel and J. Neugebauer. A Python workflow definition for computational materials design. doi:10.48550/arXiv.2505.20366.

- Code: pythonworkflow/python-workflow-definition

2022 M. Stricker, L. Banko, N. Sarazin, N. Siemer, **J. Janssen**, L. Zhang, J. Neugebauer and A. Ludwig. Computationally accelerated experimental materials characterization - drawing inspiration from high-throughput simulation workflows. doi:10.48550/arXiv.2212.04804.

OPEN-SOURCE SOFTWARE

2015 – present **pyiron** - an integrated development environment for computational materials science
- Role: Lead developer for a team of eight core developers
- Code: pyiron

2018 – present **Conda-forge** - community-led software distribution for the conda package manager
- Role: Maintainer for materials science software
- Contribution: over 1000 packages with a total of over 400 million downloads
- Code: conda-forge/staged-recipes

2025 **executorlib** - Up-scale python functions for high performance computing (HPC)
- Contribution: Lead the development
- Code: pyiron/executorlib

2024 **LangSim** - Large language model for atomistic simulation
- Contribution: Lead the team of international researchers
- Code: jan-janssen/LangSim

2022 **Architector** - high-throughput cross-periodic table 3D complex builder
- Contribution: Parallelization of the chemical complex building using mpi4py
- Code: lanl/Architector

2021 **FitSNAP** - Software for generating SNAP machine-learning interatomic potentials
- Contribution: Implemented a python library interface for the Exascale computing project
- Code: fitsnap/fitsnap

WORKSHOPS

2025 **Co-organizer** for the workshop on "Machine Learning" as part of the International Max Planck Research School for Sustainable Metallurgy. *ICAMS, Ruhr University*, Bochum, Germany

2021 **Co-organizer** for the workshop on "workflows for atomistic simulation".
Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany (online)
- Code: pyiron-workshop/potentials-workshop-2021

2020 **Co-organizer** for the workshop on "software tools from atomistics to phase diagrams".
Pennsylvania State University, Pennsylvania, USA (online)
- Code: pyiron-workshop/phasediagram-workshop-2020

TEACHING

2025 **Shared lecture with Prof. G. Sutmann** on "Programming Concepts in Materials Science" for master students in materials science and simulation. *Ruhr University Bochum*, Bochum, Germany

Single lecture on "Extension of Density Functional Theory: From Molecules to Solids" as part of the lecture on "Molecular Photonics and Excited-State Processes (MPESP)" for master students in chemistry. *Heinrich Heine University*, Düsseldorf, Germany

2024 **Single lecture** on "Density Functional Theory" as part of the International Max Planck Research School for Sustainable Metallurgy lecture series on Thermodynamics. *Max Planck Institute for Sustainable Materials*, Düsseldorf, Germany

2023 **Single lecture** on "Introduction to Materials Informatics" as part of the Graduate Autumn School of the CRC1349. *Rheinisch-Westfälische Technische Hochschule (RWTH)*, Aachen, Germany

SUPERVISION

2025 – present **Prabhath Chilakalapudi** (PhD student): Machine-learned interatomic potentials combining theoretical predictions and experimental references
- Role: Supervisor - acquiring the funding and leading the supervision of the PhD student

2024 – present **Haitham Wael Ali Awad Gaafer** (PhD student): Machine-learned interatomic potentials for chemo-mechanics balancing computational efficiency and accuracy
- Role: Supervisor - acquiring the funding and leading the supervision of the PhD student

2023 – present **Sk Md Ahnaf Akif Alvi** (PhD student): Autonomous in silico processing and materials discovery for additive manufacturing
- Role: Co-Supervisor - in collaboration with Prof. Arroyave at Texas A&M University

2023 – 2025 **Ilgar Baghishov** (intern): Multi-fidelity machine-learned interatomic potentials
- Role: Primary Supervisor - acquiring the funding and leading the supervision of the intern

2022 – 2023 **Jason Blake Gibson** (intern): Transferability of interatomic machine learning potentials
- Role: Primary Supervisor - acquiring the funding and leading the supervision of the intern

2018 **Ankita Biswas** (student assistant): Calculation of vacancy formation energies with pyiron
- Role: Primary Supervisor - for a student research project

2017 **Martin Böckmann** (student assistant): Monte Carlo sampling with pyiron
- Role: Primary Supervisor - guiding the student as the first user of the pyiron software

PRESENTATIONS

INVITED TALKS

2025 **J. Janssen**. Up-scale Python Functions for High-Performance Computing with Executorlib, *Department of Energy Python Exchange*, New York, NY, USA (online).

J. Janssen. Predict the chemistry of sustainable materials with machine learning, *Seminar in department of Chemistry at the University of Utah*, Salt Lake City, UT, USA.

J. Janssen. Accelerating Materials Discovery with Machine Learning, *Nanomaterials: Computation, Theory, Machine Learning and Experiment*, Telluride, CO, USA.

J. Janssen. Large Language Model Agents Towards Autonomous Materials Discovery, *Center for Nonlinear Studies (CNLS) Seminar at Los Alamos National Laboratory*, Los Alamos, NM, USA.

J. Janssen. Machine Learned Interatomic Potentials for Extreme Environments, *Workshop on Models and Data for Plasma-Material Interactions in Fusion*, Vienna, Austria.

J. Janssen. Predicting Sustainable Materials with Machine Learned Interatomic Potentials, *AAPALI-Psi-K*, Pune, India.

J. Janssen. pyiron – Workflows for data-driven Materials Science, *NHR4CES Community Workshop*, Darmstadt, Germany (online).

J. Janssen. Predicting Sustainable Materials with Machine Learning, *Machine learning with computational materials science data for modelling nanocrystal catalysts*, Freiburg, Germany.

2024 **J. Janssen**. How to use machine learning in the discovery and design of materials for the future?, *Michigan Institute for Computational Discovery & Engineering*, Michigan, MI, USA.

J. Janssen. Foundation Models for Materials Discovery, *Summer School at Center for Scientific Foundation Models*, Michigan, MI, USA (online).

J. Janssen. pyiron: Simulation Workflows for Data-Driven Materials Design, *Center for Nonlinear Studies (CNLS) Seminar Los Alamos National Laboratory*, Los Alamos, NM, USA.

J. Janssen. pyiron: workflows for the development and assessment of interatomic potentials, *Workshop on Machine Learning Force Fields at the institute for mathematical and statistical innovation (IMSI)*, Chicago, Il, USA.

2023 **J. Janssen** and J. Neugebauer. Rapid prototyping and up-scaling atomistic workflows with pyiron , *Ab initio Description of Iron and Steel (ADIS): Digitalization and Workflows*, Kreuth, Germany.

J. Janssen. Packaging Scientific Software with Conda-Forge, *Workshop at the Institute for Pure and Applied Math (IPAM)*, Los Angeles, CA, USA.

J. Janssen and D. Perez. Up-scaling atomistic simulation workflows with pyiron, *Workshop at the Institute for Pure and Applied Math (IPAM)*, Los Angeles, CA, USA.

J. Janssen, M. G. Taylor, P. Yang and D. Perez. Tutorial on high-throughput screening for chemical science with pyiron, *2nd International Workshop on Theory Frontiers in Actinide Science : Chemistry & Materials*, Santa Fe, NM, USA.

2022 **J. Janssen**, T. Hickel and J. Neugebauer. Automated atomistic calculation of thermodynamic and thermophysical data, *DPG Fall Meeting*, Regensburg, Germany.

J. Janssen. pyiron - an integrated development environment (IDE) for scientific workflows at scale, *Department of Energy Python Exchange*, New York, NY, USA (online).

J. Janssen. Up-scaling simulation protocols with pyiron, *Platform Material Digital Workflow Meeting 2022*, Berlin, Germany (online).

J. Janssen. pyiron - an integrated development environment (IDE) for materials science, *Special Interest Group Data Infrastructure (SIGDIUS) Seminar*, Stuttgart, Germany (online).

2021 **J. Janssen** and J. Neugebauer. pyiron - an integrated development environment for materials science, *CECAM Workshop: Simulation Workflows in Materials Modelling (SWiMM)*, Lausanne, Switzerland (online).

2020 **J. Janssen**, T. Hickel and J. Neugebauer. Uncertainty quantification for *ab initio* thermodynamics, *Group Seminar Professor R. Drautz*, Bochum, Germany (online).

J. Janssen, T. Hickel and J. Neugebauer. Automated *ab initio* determination of materials properties at finite temperatures with pyiron, *NIST Workshop: Atomistic simulations for industrial needs*, Gaitgersburg, MD, USA (online).

2019 **J. Janssen**, T. Hickel and J. Neugebauer. Automated *ab initio* determination of materials properties at finite temperatures with pyiron, *Center for Nonlinear Studies (CNLS) Seminar at Los Alamos National Laboratory*, Los Alamos, NM, USA.

J. Janssen, T. Hickel and J. Neugebauer. pyiron - an integrated development environment for computational materials science, *Group Seminar Professor G. Kresse*, Vienna, Austria.

TALKS AT INTERNATIONAL CONFERENCES

2025 **J. Janssen** and J. Neugebauer. Automated Workflows for Fitting Machine Learned Interatomic Potentials on the Exascale with pyiron, *Psi-k conference*, Lausanne, Switzerland.

J. Janssen and J. Neugebauer. Large Language Model Agents for Atomistic Simulation Workflows, *MSE Research Data Forum*, Siegburg, Germany.

J. Janssen and J. Neugebauer. Inverse Materials Design with Large Language Models, *DPG Spring Meeting*, Regensburg, Germany.

2024 **J. Janssen**, J. Neugebauerand D. Perez. Potential in a day - up-scale the fitting of machine learning potentials for the Exascale, *IPAM Workshop*, Los Angeles, CA, USA.

J. Janssen and J. Neugebauer. pyiron - Simulation Workflows for the Design of Sustainable Materials, *MRS Fall Meeting*, Boston, MA, USA.

M. Stricker, L. Banko, N. Sarazin, **J. Janssen**, N. Siemer, J. Neugebauerand A. Ludwig. Computationally Accelerated Experimental Materials Characterization Using pyiron, *Multiscale Materials Modelling (MMM) conference*, Prague, CZ.

J. Janssen and J. Neugebauer. Automated Workflows to Construct and Validate Machine-Learned Interatomic Potentials, *Multiscale Materials Modelling (MMM) conference*, Prague, CZ.

I. Baghishov, **J. Janssen**, G. Henkelman and D. Perez. Investigating the uncertainty in multi-fidelity machine learning interatomic potentials, *TMS Spring Meeting*, Orlando, Fl, USA.

J. Janssen and D. Perez. Transferable Machine Learning Potentials for Extreme Environments, *TMS Spring Meeting*, Orlando, Fl, USA.

2023 **J. Janssen** and D. Perez. Parameter studies for interatomic potentials using LAMMPS and pyiron, *LAMMPS Virtual Workshop and Symposium 2023*, Philadelphia, PA, USA (online).

J. Janssen and D. Perez. Enabling long timescale molecular dynamics simulation with ab initio precision, *MRS Spring Meeting*, San Francisco, CA, USA.

J. Janssen and D. Perez. pyiron an integrated development environment for the development and assessment of interatomic models, *11th Annual Mach Conference*, Baltimore, MD, USA.

J. Janssen and D. Perez. Enabling long timescale molecular dynamics simulation with ab initio precision, *TMS Spring Meeting*, San Diego, CA, USA.

2022 **J. Janssen**, T. Hickel and J. Neugebauer. Predicting melting temperatures from bulk properties with pyiron, *Multiscale Materials Modelling (MMM) conference*, Baltimore, MD, USA.

J. Janssen, M. G. Taylor, P. Yang and D. Perez. Screening of ligand-metal-complexes for separation science with pyiron, *ACS Fall Meeting*, Chicago, IL, USA.

J. Janssen. pyiron – an integrated development environment (IDE) for scientific workflows, *Scientific Computing with Python (SciPy)*, Austin, TX, USA.

J. Janssen. Predicting melting temperatures from bulk properties with pyiron, *Artificial Intelligence for Materials Science (AIMS)*, Gaithersburg, MD, USA (online).

2019 **J. Janssen**, T. Hickel and J. Neugebauer. Automated uncertainty quantification for *ab initio* thermodynamics, *MRS Fall Meeting*, Boston, MA, USA.

J. Janssen, T. Hickel and J. Neugebauer. Automated sensitivity analysis for high-throughput *ab initio* calculations, *IPAM Workshop*, Los Angeles, CA, USA.

J. Janssen, T. Hickel and J. Neugebauer. Automated error analysis and control for *ab initio* calculations, *DPG Spring Meeting*, Regensburg, Germany.

J. Janssen, T. Hickel and J. Neugebauer. Automated sensitivity analysis for high-throughput *ab initio* calculations, *TMS Spring Meeting*, San Antonio, TX, USA.

2018 **J. Janssen**, T. Hickel and J. Neugebauer. Generation of *ab initio* datasets with predefined precision using uncertainty quantification, *DPG Spring Meeting*, Berlin, Germany.

2017 **J. Janssen**, T. Hickel and J. Neugebauer. Towards an uncertainty quantification for *ab initio* thermodynamics, *MRS Fall Meeting*, Boston, MA, USA.

J. Janssen, T. Hickel and J. Neugebauer. Sensitivity analyis for large sets of density functional theory calculations, *DPG Spring Meeting*, Dresden, Germany.

J. Janssen, T. Hickel and J. Neugebauer. Automated convergence and error analyses for high-precision DFT calculations, *TMS Spring Meeting*, San Diego, CA, USA.

2016 **J. Janssen**, T. Hickel and J. Neugebauer. Automated convergence checks with the python based library pyiron, *DPG Spring Meeting*, Regensburg, Germany.

J. Janssen, T. Hickel and J. Neugebauer. Automated convergence checks with the python based workbench pyiron, *TMS Spring Meeting*, Nashville, TN, USA.