

# 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  $\alpha$ -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 collaborative research center (CRC) 1394 “Structural and chemical atomic complexity - from defect phase diagrams to material properties”
- Funding: 160k Euro
- 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: \$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: \$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: \$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: \$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: \$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, 02/25: Citations: 263

- 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*. Citations: 0 doi:[10.1038/s41524-024-01388-2](https://doi.org/10.1038/s41524-024-01388-2).  
• Code:  [pyiron/pyiron-dft-uncertainty](https://github.com/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*. Citations: 2 doi:[10.1021/jacsau.4c00770](https://doi.org/10.1021/jacsau.4c00770).
- 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*. Citations: 1 doi:[10.1038/s41524-024-01441-0](https://doi.org/10.1038/s41524-024-01441-0).  
• Code:  [pyiron/potential\\_publication](https://github.com/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*. Citations: 3 doi:[10.1039/D4DD00089G](https://doi.org/10.1039/D4DD00089G).  
• Code:  [lanl/minervachem](https://github.com/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](https://doi.org/10.1038/s41467-023-38169-2). Citations: 25  
• Code:  [lanl/Architector](https://github.com/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](https://doi.org/10.21105/joss.05118). Citations: 35  
• Code:  [FitSNAP/FitSNAP](https://github.com/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](https://doi.org/10.1016/j.commatsci.2020.110065). Citations: 39  
• Code:  [pyiron/pyiron\\_meltingpoint](https://github.com/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](https://doi.org/10.1103/PhysRevB.102.100101). Citations: 8  
• Code:  [tomswinburne/BLaSA](https://github.com/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](https://doi.org/10.1016/j.commatsci.2018.07.043). Citations: 113  
• Code:  [pyiron](https://github.com/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](https://doi.org/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](https://doi.org/10.1080/14786435.2016.1170224). Citations: 13


## PUBLICATIONS IN REVIEW

2024 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](https://doi.org/10.48550/arXiv.2212.04804).


Sk. Md. A. A. Alvi, **J. Janssen**, D. Khatamsaz, D. Perez, D. Allaire and R. Arroyave. Hierarchical Gaussian Process-Based Bayesian Optimization for Materials Discovery in High Entropy Alloy Spaces. doi:[10.48550/arXiv.2410.04314](https://doi.org/10.48550/arXiv.2410.04314).

## 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](https://github.com/pyiron/pyiron)


2018 – present **Conda-forge** - community-led software distribution for the conda package manager

- Role: Maintainer for materials science software
- Contribution: over 800 packages with a total of over 200 million downloads
- Code:  [conda-forge/staged-recipes](https://github.com/conda-forge/staged-recipes)


2024 **LangSim** - Large language model for atomistic simulation

- Contribution: Lead the team of international researchers
- Code:  [jan-janssen/LangSim](https://github.com/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](https://github.com/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](https://github.com/fitsnap/fitsnap)

## WORKSHOPS

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](https://github.com/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](https://github.com/pyiron-workshop/phasediagram-workshop-2020)

## SUPERVISION

- 2024 – present **Haitham Wael Ali Awad Gaafer** (PhD student): Potentials for chemo-mechanics
- Role: Supervisor - acquiring the funding and leading the supervision of the PhD student
- 2023 – present **Ilgar Baghishov** (intern): Multi-fidelity machine learned interatomic potentials
- Role: Primary Supervisor - acquiring the funding and leading the supervision of the intern
- 2023 – present **Ahnaf Akif Alvi** (PhD student): Autonomous in silico processing and materials discovery
- Role: Co-Supervisor - in collaboration with Prof. Arroyave at Texas A&M University
- 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

- 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, 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, 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, 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, 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**, 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, J. Neugebauer. Uncertainty quantification for *ab initio* thermodynamics, *Group Seminar Professor R. Drautz*, Bochum, Germany (online).

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

2019 **J. Janssen**, T. Hickel, 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, J. Neugebauer. pyiron - an integrated development environment for computational materials science, *Group Seminar Professor G. Kresse*, Vienna, Austria.

## TALKS AT INTERNATIONAL CONFERENCES

2024 **J. Janssen**, J. Neugebauer and 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. Neugebauer and 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 analysis 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.