

Jan Janssen

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PROFESSIONAL APPOINTMENTS

- 2022 – present **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 Department
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

- 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

- 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, 03/23: Citations: 102

- 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* (accepted).
- Code:  [lanl/Architector](#)
- 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: 17
- 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: 3
- 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: 54
- Code:  [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: 17

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: 11

PUBLICATIONS IN REVIEW

2022 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*.


- Code:  [FitSNAP/FitSNAP](#)

2021 **J. Janssen**, E. Makarov, T. Hickel, A.V. Shapeev and J. Neugebauer. Automated optimization of convergence parameters in plane wave density functional theory calculations via a tensor decomposition-based uncertainty quantification. *npj Computational Materials*. doi:[10.48550/arXiv.2112.04081](https://doi.org/10.48550/arXiv.2112.04081).


- Code:  [pyiron/pyiron-dft-uncertainty](#)

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: 500+ packages with a total of 100+ million downloads
- Code:  [conda-forge/staged-recipes](#)

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

2021 **Co-organizer** for the workshop on “workflows for atomistic simulation“ *Max-Planck-Institut für Eisenforschung*, Düsseldorf, Germany (online)

- Code:  [pyiron/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/phasediagram-workshop-2020](#)

SUPERVISION

- 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 – present **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

- 2023 **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**, D. Perez. Enabling long timescale molecular dynamics simulation with ab initio precision, *TMS Spring Meeting*, San Diego, 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, *CLNS Seminar 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

2023 **J. Janssen**, D. Perez. Enabling long timescale molecular dynamics simulation with ab initio precision, *MRS Spring Meeting*, San Francisco, CA, USA.

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

2022 **J. Janssen**, T. Hickel, 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, 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, J. Neugebauer. Automated uncertainty quantification for *ab initio* thermodynamics, *MRS Fall Meeting*, Boston, MA, USA.

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

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

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

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

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

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

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

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

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