Jan Janssen

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PROFESSIONAL APPOINTMENTS

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

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

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: 1.0 excellent

FUNDED PROPOSALS

2022 **Principal Investigator** of the "transferability of interatomic machine learning potentials" as part of the summer school for applied machine learning at Los Alamos National Laboratory.
- Funding: $19k

Co-Principal Investigator of the "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

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 biennially 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, 10/22: Citations: 85

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: 13
- 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: 1
- 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: 45
- 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. Citations: 15

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: 11

PUBLICATIONS IN REVIEW

2022 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*.

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.
- 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 80+ 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

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

2022 **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

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*, Gaitgersburg, 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

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. High throughput 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 analyis 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.