Jan Janssen

Theoretical Division
Los Alamos National Laboratory
Bikini Atoll Rd., SM 30
Los Alamos, NM 87545, USA

Last updated: October, 2021
ORCID: 0000-0001-9948-7119
email: jan.janssen@outlook.com
Research group: lanl.gov
Website: jan-janssen.com

PROFESSIONAL APPOINTMENTS

2021 – present **Postdoctoral Research Associate**
Theoretical Division (T-1)
Los Alamos National Laboratory
Los Alamos, NM, USA

2015 – 2021 **PhD Candidate**
Computational Materials Design
Max-Planck-Institut für Eisenforschung
Düsseldorf, Germany

2017 **Invited Fellow**
Institute for Pure and Applied Mathematics
University of California
Los Angeles, CA, USA

2013 **Intern**
Application Platform Services
Hilti
Buchs, Switzerland

EDUCATION

2015 – 2021 **PhD in Theoretical Physics**, Paderborn University, Germany

2010 – 2011 **Diplom in Theoretical Physics**, Technical University of Kaiserslautern, Germany

AWARDS & HONORS

2019 Runner-up for the Heinz Billing Award of 2019

PUBLICATIONS

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.
- 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.
- Code: tomswinburne/BLaSA

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

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

2016 **J. Janssen**, N. Gunkelmann, 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

OPEN-SOURCE SOFTWARE

2015 – present **pyiron**
An integrated development environment for computational materials science
- Role: Project Lead Developer
- Code: pyiron
- Website: www.pyiron.org

WORKSHOPS

2021 Workflows for Atomistic Simulation
Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany (online).
- Code: pyiron/potentials-workshop-2021

2020 Software Tools from Atomistics to Phase Diagrams
Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany (online).
- Code: pyiron/phasediagram-workshop-2020

PRESENTATIONS

INVITED TALKS

2021 **J. Janssen**, T. Hickel, 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, R*, 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

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.