

# 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](https://orcid.org/0000-0001-9948-7119)  
email: [jan.janssen@outlook.com](mailto:jan.janssen@outlook.com)  
Research group: [lanl.gov](http://lanl.gov)  
Website: [jan-janssen.com](http://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



## 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](https://doi.org/10.1016/j.commatsci.2020.110065).  
• 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).  
• Code:  [tomswinburne/BLaSA](https://github.com/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](https://doi.org/10.1016/j.commatsci.2018.07.043).  
 • Code:  [pyiron](https://github.com/pyiron/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](https://doi.org/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](https://doi.org/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](https://github.com/pyiron/pyiron)  
 • Website: [www.pyiron.org](http://www.pyiron.org)

## WORKSHOPS

- 2021 Workflows for Atomistic Simulation  
*Max-Planck-Institut für Eisenforschung*, Düsseldorf, Germany (online).  
 • Code:  [pyiron/potentials-workshop-2021](https://github.com/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](https://github.com/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*, 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

- 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.