Rodrigo Freitas

Department of Materials Science and Engineering, Massachusetts Institute of Technology
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Education

University of California Berkeley
Ph.D. in Materials Science and Engineering, 2013–2018
M.Sc. in Materials Science and Engineering, 2013–2015
Dissertation: *"Atomistic Simulations of Extended Defects in Metals"*
Advisors: Mark Asta and Vasily Bulatov

University of Campinas (Brazil)
M.Sc. in Physics, 2011–2013
B.Sc. in Physics, 2007–2010
Dissertation: *"Molecular Simulation: methods and applications"*
Advisor: Maurice de Koning

Employment

Massachusetts Institute of Technology
Department of Materials Science and Engineering
AMAX Assistant Professor, starting in January 2021

Stanford University
Department of Materials Science and Engineering
Postdoctoral Researcher, 2018–2020
Supervisor: Evan Reed

Fellowships

Livermore Graduate Scholar Program, Lawrence Livermore National Laboratory, 2015 – 2018.

Research Internships Abroad, FAPESP (Brazil), 2012–2013.

Master Degree Scholarship, FAPESP (Brazil), 2011–2013.

Undergraduate Research Scholarship, CNPq (Brazil), 2009.

Invited Talks and Seminars

TMS Annual Meeting, Orlando FL, 2021.
Computational Thermodynamics and Kinetics Symposium
Title: "Uncovering atomistic mechanisms of crystallization using Machine Learning"

Telluride Science Research Center, Telluride CO, 2020.
Workshop: "Multi-Scale Quantum Mechanical Analysis of Condensed Phase Systems"
Title: "Uncovering atomistic mechanisms of crystallization using Machine Learning"

Massachusetts Institute of Technology, Cambridge MA, 2020.
Institute for Data, Systems, and Society
Title: "Uncovering atomistic mechanisms of crystallization using Machine Learning"

University Pennsylvania, Philadelphia PA, 2020.
Department of Materials Science and Engineering

Title: “Uncovering atomistic mechanisms of crystallization using Machine Learning”

University of California Los Angeles, 2019.
Department of Materials Science and Engineering (Samueli Future Faculty Lectures)
Title: “Uncovering atomistic mechanisms of crystallization using Machine Learning”

Gordon Research Conference on Crystal Growth and Assembly, Manchester NH, 2019.
Title: “Uncovering atomistic mechanisms of crystallization using Machine Learning”

University of California Irvine, 2019.
Department of Materials Science and Engineering
Title: “Modern atomic-scale simulation approaches to investigate materials solidification”

TMS Annual Meeting, San Antonio TX, 2019.
Hume-Rothery Award Symposium
Title: “Interface and defect free energies from atomistic simulations”

Stanford University, 2017.
Department of Materials Science and Engineering (Materials Computation and Theory Group)
Title: “Quantum effects on dislocation mobility from Ring-Polymer Molecular Dynamics”

University of California Berkeley, 2013.
Department of Materials Science and Engineering (Asta Research Group)
Title: “Thermodynamics and kinetics of martensitic phase transformations”

Lawrence Livermore National Laboratory, Livermore CA, 2013.
Materials Science Division
Title: “Thermodynamics and kinetics of martensitic phase transformations”

Other Talks and Presentations

NNSA Stewardship Science Academic Programs Symposium, Washington DC, 2020.
Poster: “Uncovering mechanisms of solidification from atomistic simulations using Machine Learning”

APS March Meeting, Boston MA, 2019.
Talk: “Atomistic mechanisms of phase transitions from Machine Learning”

NNSA Stewardship Science Academic Programs Symposium, Albuquerque NM, 2019.
Poster: “Atomistic mechanisms of phase transitions from Machine Learning”

TMS Annual Meeting, San Diego CA, 2017.
Talk: “The effects of quantum dynamics of atomic motion on dislocation mobility”

TMS Annual Meeting, Nashville TN, 2016.
Talk: “Quantum dynamics of atomic motion in Beryllium”

APS March Meeting, Baltimore MD, 2016.
Talk: “Free energy of steps using atomistic simulations”

Berkeley Statistical Mechanics Meeting, 2015.
Poster: “Free energy of steps on the surface of faceted solids”

7th International Conference on Multiscale Materials Modeling (MMM), Berkeley CA, 2014.
Poster: “Free energy of steps on the surface of faceted solids”

Berkeley Statistical Mechanics Meeting, 2013.

Poster: “Efficient Free Energy Calculation in LAMMPS”

Unicamp Internal Congress of Undergraduate Research, Campinas, Brazil, 2010.
Poster: “Computational Physics Models for Earthquakes”

Workshops and Summer Schools

Dynamic Compression Summer School, Chicago IL, 2018.

Telluride School on Time-Dependent Density Functional Theory, Telluride CO, 2017.

MICCoM Computational School, Chicago IL, 2017.

Purdue Prospective Faculty Workshop, Purdue IN, 2016.

The Summer School for Integrated Computational Materials Education, Berkeley CA, 2016.

Computational Chemistry and Materials Science Summer Institute, Livermore CA, 2015.

Berkeley Statistical Mechanics Meeting, 2014 and 2016.

Computer Programming and Advanced Tools for Scientific Research Work, Trieste, Italy, 2013.

Hermes Summer School on Materials Modeling, London, England, 2012.

Summer School on Atomistic Simulation Techniques, Trieste, Italy, 2011.

USP Physics Summer School, São Paulo, Brazil, 2011.

Brazilian Center for Physics Research Winter School, Rio de Janeiro, Brazil, 2008 and 2010.

Teaching experience

Teaching Assistant, UC Berkeley, Phase Transformations and Kinetics, Spring 2015.

Teaching Assistant, Unicamp (Brazil), Statistical Mechanics (graduate class), 2013.

Teaching Assistant, Unicamp (Brazil), Experimental Physics III: Electromagnetism, 2012.

High-school level course “Wave-Particle Duality” at “Physics on Vacation” Winter School (Brazil), 2012.

Teaching Assistant, Unicamp (Brazil), Quantum Mechanics I and II, 2010.

Teaching Assistant, Unicamp (Brazil), Physics III: Electromagnetism, 2009.

Journal publications

Google Scholar: tinyurl.com/GS-Freitas

1. **Rodrigo Freitas**, Mark Asta, and Maurice de Koning
   “Nonequilibrium free-energy calculation of solids in LAMMPS”
   Computational Materials Science, 2016.
   Selected as “Editor’s Choice”.
   DOI: 10.1016/j.commatsci.2015.10.050
2. Rodolfo Leite, **Rodrigo Freitas**, Rodolfo Azevedo, and Maurice de Koning
   “The Uhlenbeck-Ford model: Exact virial coefficients and application as a reference system in fluid-phase free-energy calculations”
   The Journal of Chemical Physics, 2016.
   DOI: 10.1063/1.4967775
3. **Rodrigo Freitas**, Timofey Frolov, and Mark Asta
   “Step free energies at faceted solid surfaces: Theory and atomistic calculations for steps on the Cu(111) surface”

Physical Review B, 2017.
DOI: 10.1103/PhysRevB.95.155444

4. **Rodrigo Freitas**, Timofey Frolov, and Mark Asta
"Capillary fluctuations of surface steps: An atomistic simulation study for the model Cu(111) system"
Physical Review E, 2017.
DOI: 10.1103/PhysRevE.96.043308

5. Peyman Saidi, **Rodrigo Freitas**, Timofey Frolov, Mark Asta, and Jeff Hoyt
"Free energy of steps at faceted (111) solid-liquid interfaces in the Si-Al system calculated using capillary fluctuation method"
Computational Materials Science, 2017.
DOI: 10.1016/j.commatsci.2017.03.044

6. Pedro A. Moreira, Roberto G. Veiga, Ingrid A. Ribeiro, **Rodrigo Freitas**, Julian Helfferich, and Maurice de Koning
"Glassy dynamics at a pre-melted grain boundary in ice I_h"
Physical Chemistry Chemical Physics, 2018.
DOI: 10.1039/C8CP00933C

7. **Rodrigo Freitas**, Mark Asta, and Timofey Frolov
"Free energy of grain-boundary phases: Atomistic calculations for $\Sigma5(310)[001]$ grain boundary in Cu"
Physical Review Materials, 2018.
DOI: 10.1103/PhysRevMaterials.2.093603

8. **Rodrigo Freitas**, Mark Asta, and Vasily Bulatov
"Quantum effects on dislocation mobility from Ring-Polymer Molecular Dynamics"
npj: Computional Materials, 2018.
DOI: 10.1038/s41524-018-0112-9

9. Enze Chen, Qian Yang, Vincent D. Decieux, Carlos A. Sing-Long, **Rodrigo Freitas**, and Evan J. Reed
"Transferable kinetic Monte Carlo models with thousands of reactions learned from Molecular Dynamics simulations"
The Journal of Physical Chemistry A, 2019.
DOI: 10.1021/acs.jpca.8b09947

10. **Rodrigo Freitas** and Evan J. Reed
"Uncovering the effects of interface-induced ordering of liquid on crystal growth using Machine Learning"
Nature Communications, 2020.
DOI: 10.1038/s41467-020-16892-4

11. Luis A. Zepeda-Ruiz, Alexander Stukowski, Tomas Oppelstrup, Nicolas Bertin, Nathan Barton, **Rodrigo Freitas**, Vasily V. Bulatov
"Atomistic insights into metal hardening"
Nature Materials, 2020.
DOI: 10.1038/s41563-020-00815-1

12. Heejung Chung, **Rodrigo Freitas**, Gowoon Cheon, Evan J. Reed
"A data-centric framework for crystal structure identification in atomistic simulations using machine learning"
arXiv: 2010.04815