Levi Felix, Ph.D.

Postdoctoral Research Associate • Computational Materials Scientist
lf33@rice.edu | levicfelix.github.io | levi-felix | 0000-0001-5928-0885

My research aims to elucidate the role of defects in materials behavior using computational atomistic simulations under conditions inaccessible to experiments, such as confined spaces and extreme environments. I approach rare events through enhanced-sampling free-energy methods to overcome the limited timescales of conventional molecular dynamics simulations. For processes at length scales inaccessible to quantum-mechanical calculations, I employ machine-learning techniques such as deep neural network potentials.

Experience

Rice University — *Houston, TX, USA*
Postdoctoral Research Associate, Department of Materials Science and NanoEngineering — Oct. 2022 – Present
Research in nanomechanics, corrosion, thermal transport, and machine learning interatomic potentials.

State University of Campinas (UNICAMP) — *Campinas, SP, Brazil*
Graduate Teaching Assistant — Aug. 2019 – Dec. 2019
Taught General Physics IV, covering optics, special relativity, and quantum physics.

Federal University of Ceará (UFC) — *Fortaleza, CE, Brazil*
Graduate Teaching Assistant — Aug. 2017 – Dec. 2017
Supervised laboratory sessions and taught experimental electricity and magnetism.

Education

State University of Campinas (UNICAMP) — *Campinas, Brazil*
Ph.D. in Physics — 2018 – 2022
Thesis: *Computational Mechanics of Porous and Two-Dimensional Carbon Nanomaterials*.

Federal University of Ceará (UFC) — *Fortaleza, Brazil*
M.Sc. in Physics — 2016 – 2018
Dissertation: *Wave-Packet Propagation in Phosphorene in the Presence of Grain Boundaries*.

Federal University of Ceará (UFC) — *Fortaleza, Brazil*
B.S. in Physics, Magna Cum Laude — 2013 – 2016
Monograph: *Landau Levels in Graphene Influenced by One-Dimensional Potentials*.

Technical Skills

Methods	Machine learning force fields; molecular dynamics; density functional theory; density functional tight-binding; nudged elastic band; umbrella sampling; metadynamics
Software	DeePMD-kit, MACE, LAMMPS, SIESTA, Quantum ESPRESSO, CP2K, VASP, DFTB+, VMD, VESTA, OVITO
Programming	Python, C++, LaTeX
Languages	Portuguese (native), English (fluent), Spanish (intermediate)

Selected Publications

[1] **L. C. Felix**, E. S. Penev, M. Sun, and B. I. Yakobson, "Topochemistry of Ammonium Perchlorate: How Surface Morphology Mediates Its Sublimation," *The Journal of Physical Chemistry Letters* **17**(31), 9031–9037 (2026). [DOI]

[2] **L. C. Felix**, Q.-K. Li, E. S. Penev, and B. I. Yakobson, "Ab Initio Molecular Dynamics Insights into Stress Corrosion Cracking and Dissolution of Metal Oxides," *Materials* **18**(3), 538 (2025). [DOI]

[3] **L. C. Felix**, C. F. Woellner, and D. S. Galvão, "Mechanical and Energy-Absorption Properties of Schwarzites," *Carbon* **157**, 670–680 (2020). [DOI]

Conferences and Proceedings

2022	MRS Spring Meeting, oral presentation	*Honolulu, HI*
2021	MRS Fall Meeting, poster presentation	*Boston, MA*
2019	MRS Fall Meeting, poster presentation	*Boston, MA*
2019	MRS Brazil Meeting, poster presentation	*Balneário Camboriú, Brazil*

Awards and Honors

2022	Recognition Award from NIST, MRS Spring Meeting	*Honolulu, HI*
2021	Best Poster Award, MRS Fall Meeting	*Boston, MA*
2016	Magna Cum Laude, B.S. in Physics	*Fortaleza, Brazil*