ADRIANA J. LADERA

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RESEARCH INTERESTS

Computational science for materials design, large-scale accelerated materials discovery, and electronic characterization of functional materials, with emphasis on first-principles simulation and machine-learning–assisted workflows.

EDUCATION

Ph.D. in *Computational Science and Engineering* — February 2025 – present
Massachusetts Institute of Technology (MIT)

S.M. in *Computational Science and Engineering* — September 2022 – February 2025
Massachusetts Institute of Technology (MIT)

B.S. Honors in *Computer Science* — August 2018 – May 2022
University of South Florida (USF), Minor in *Physics*

HONORS AND AWARDS

MITEI Society of Energy Scholar, MIT Energy Initiative (*sponsor: ExxonMobil*) — September 2025 – present
NSF Graduate Research Fellowship, National Science Foundation — September 2022 – present
USF Directors Award, University of South Florida, *merit-based financial award* — August 2018 – May 2022
Florida Academic Scholarship, Bright Futures, *merit-based full tuition coverage* — August 2018 – May 2022
Dean's List, College of Engineering, University of South Florida — May 2019

PUBLICATIONS

- *Optical Gap in Single Crystal Quantum Wire Lattices.*
  A. Ladera*, V. Quirós-Cordero*, Q. Fan*, M. C. Willson*, *et al.* (2026). In preparation.
- *1-Dimensional Metal-organic Chalcogenolates with Hydration-tunable Chiroptical Emission.*
  A. Ladera*, Q. Fan*, D. W. Paley, D. M. Tchon, A. Rasamsetty, H. Nyiera, D. W. Mittan-Moreau, C. D. Liyanage, M. C. Willson, M. Aleksich, E. A. Schriber, et al. (2026). Submitted.
- *Stabilizing Structural Transitional States between 1- and 2-Dimensional Topologies via Hydrogen Bond-Mediated Crystal Engineering.*
  A. Ladera*, M. Aleksich*, A. LaMonica, K. Christensen, D. Paley, *et al*. (2026). Revised and resubmitted.
- *Strain phase equilibria and phase-field method of ferroelectric polydomain: A case study of monoclinic $K_xNa_{1-x}NbO_3$ films.*
  B. Wang, M.J. Zhou, **A. Ladera**, L.Q. Chen (2024). Journal of the American Ceramic Society, **107**(12), 7692-7710 (https://doi.org/10.1111/jace.20072).
- *Phonon Calculations (In "Artificial Intelligence for Science in Quantum, Atomistic, and Continuum Systems").*
  A. Ladera and T. Smidt (2023). arXiv, 2307.08423, 144-146 (https://doi.org/10.48550/arXiv.2307.08423).
- *Machine learning reveals memory of the parent phases in ferroelectric relaxors $Ba(Ti_{1-x}, Zr_x)O_3$.*
- **A. Ladera**, R. Kashikar, S. Lisenkov, and I. Ponomareva (2023). Advanced Theory and Simulations, **6**(3), 2513-0390 (https://doi.org/10.1002/adts.202200690).
- *Exploiting Ligand Additivity for Transferable Machine Learning of Multireference Character across Known Transition Metal Complex Ligands.*
  C. Duan, **A. Ladera**, J. C.-L. Liu, M. G. Taylor, I. R. Ariyarathna, and H. J. Kulik (2022). Journal of Chemical Theory and Computation, **18**(8), 4836–4845 (https://doi.org/10.1021/acs.jctc.2c00468).
- *Phase diagrams, superdomains, and superdomain walls in $(K_x,Na_{1-x})NbO_3$ epitaxial thin films.*
  M.J. Zhou, B. Wang, **A. Ladera**, L. Bogula, H.X. Liu, L.Q. Chen, and C.W. Nan (2021). Acta Materialia, **215**, 117038 (https://doi.org/10.1016/j.actamat.2021.117038).
- *$Ba(Ti_{1-x}, Zr_x)O_3$ relaxors: Dynamic ferroelectrics in the gigahertz frequency range.*
  S. Lisenkov, **A. Ladera**, and I. Ponomareva. (2020). Physical Review B, **102**(22), 224109 (https://doi.org/10.1103/PhysRevB.102.224109).
- *Temperature Dependence of Three-Dimensional Domain Wall Arrangement in Ferroelectric $K_{0.9}Na_{0.1}NbO_3$ Epitaxial Thin Films*
  M. Schmidbauer, L. Bogula, B. Wang, M. Hanke, L. von Helden, **A. Ladera**, J.J. Wang, L.Q. Chen, and J. Schwarzkopf. (2020). J. Appl. Phys. 128 (https://doi.org/10.1063/5.0029167).

EXPERIENCE

Graduate Research Fellow, Atomic Architects Lab, **MIT** — September 2022 – present

- Perform density functional theory (DFT)–based geometry optimization and electronic structure analysis of metal organic chalcogenolates.
- Lead scientific communication of DFT simulation work with experimental collaborators to ensure that experimental and theoretical findings are complementary.
- Design efficient equivariant deep learning models and train models to predict electronic Hamiltonians of atomistic systems, enabling forward property prediction of electronic structure and accelerated target property screening.
- Co-develop a polyhedral generation network to propose novel material geometries and periodic packing.

Undergraduate Research Assistant, Computational Nanoscience Group, **USF** February 2020 – September 2022

- Designed and implemented an unsupervised representation-learning workflow for first-principles atomistic simulations to investigate phases, phase transitions, and their structural origins in the ferroelectric relaxor $Ba(Ti_{1-x}, Zr_x)O_3$ (BZT), and parent compound $BaTiO_3$ (BTO). This analysis revealed persistent memory of BTO phases beyond the pinched phase transition and uncovered nanodomain phases at high Zr concentrations.
- Developed a physics-informed vector embedding of BZT/BTO supercell simulations and an intuitive visualization of local polarization behavior via 3D color-mapped representations of polarization directions across entire supercells.
- Built a complete machine learning and analysis pipeline, including data preprocessing, dimensionality reduction (principal component analysis), unsupervised clustering (*k*-means), and post-processing visualization.

Program Design Peer Leader, Dept. of Computer Science & Engineering, **USF** January 2021 – May 2022

- Expanded the learning experience for the Program Design (COP 3514) class in the C programming language by creating lesson plans for recitation sessions, held twice a week for one hour.
- Demonstrated live programming examples, discussed course material, and gave guidance for internships, research experiences, and the computer science major.
- Provided outreach and individualized course guidance to students in Program Design, especially women and nonbinary students, to promote retention of underrepresented gender groups in STEM.

Undergraduate Teaching Assistant, Dept. of Computer Science & Engineering, **USF** August 2020 – May 2022

- Aided in-class lectures and graded weekly programming projects, quizzes, and exams for the Program Design (COP 3514) class in the C programming language.
- Guided students in understanding class concepts and programming project questions through email and office hours.

Research Intern, Kulik Research Group*,* **MIT Summer Research Program (MSRP)** June – November 2021

- Executed large-scale first-principles calculations for over 1,000 transition metal complexes (TMCs) across 23 density functional approximations to build a diverse electronic-structure dataset.
- Identified limitations of ligand additivity in systems with high multireference character, informing model selection and uncertainty considerations.
- Trained density functional-specific neural networks and co-developed an active learning framework to predict multireference character from ligand composition, enabling high-throughput virtual screening of TMCs.

Cybersecurity Intern, **SOFWERX** August – December 2020

- Collected samples of various frequencies of wireless communication signals to train a machine learning model.
- Employed machine learning techniques to identify signals detected using a software-defined radio.
- Developed fully automated devices that classify and localize signals at given frequencies for the user to gain better understanding of the device-mapping around them.

Computer Services Employee, **USF Student Government Computer Services** January 2019 – August 2020

- Calibrated printers, assisted in user support of computer tasks, and restocked supplies and storage within the student center computer labs.

REU Intern, *Continued Collaborator,* Chen Research Group, **Pennsylvania State University** May – December 2019

- Computed hundreds of phase-field simulations of $K_xNa_{1-x}NbO_3$ thin films to study polarization phase dependence on strain, temperature, film thickness, and potassium (K) concentration.
- Categorized phase-field simulations into different polarization phases based on dominant concentrations of polarization domains in simulations.
- Constructed anisotropic strain phase diagrams from simulations and validated computational predictions through continued collaboration with experimental partners at the Leibniz-Institut für Kristallzüchtung.

PRESENTATIONS

- *Stabilizing Structural Transitional States between 1- and 2-Dimensional Topologies via Hydrogen Bond-Mediated Crystal Engineering*
  A. Ladera and T. Smidt. Oral presentation accepted at American Physical Society Global Physics Summit (March 2026), Denver, CO.
- *Towards an ML-Accelerated Workflow for the Design of Novel Metal Organic Chalcogenolates*
  A. Ladera and T. Smidt. Oral presentation at American Physical Society Global Physics Summit (March 2025), Anaheim, CA.
- *The Design Space of Novel Metal Organic Chalcogenolates*
  A. Ladera, A. M. Tehrani, and T. Smidt. Oral presentation at American Physical Society March Meeting (March 2024), Minneapolis, MN.
- *Leveraging Density Functional Theory and Geometric Tunability in the Design of Novel Metal Organic Chalcogenolates*
  A. Ladera, A. M. Tehrani, and T. Smidt. Oral presentation at the Materials Research Society Fall Meeting (November 2023), Boston, MA.
- *Exploring Transition Metal Complex Space with Computation and Artificial Neural Networks*
  A. Ladera, C. Duan, V. Vennelakanti, and H.J. Kulik. Poster resented at the 36th Annual MIT Summer Research Program Research Forum (August 2021), Cambridge, MA.
- *Investigating the Structure-Property Relationship of the Ba(Ti1-x, Zrx)O3 Relaxor Ferroelectric via Machine Learning*
  A. Ladera, and I. Ponomareva. Poster presented at the University of South Florida Undergraduate Research Conference (April 2021), Tampa FL.
- *Phase-Field Simulations: Anisotropic Misfit Strain Phase Diagram of K0.5Na0.5NbO3 Thin Films*
- **A. Ladera**, B. Wang, J.J. Wang, and L.Q. Chen. Poster presented at: Penn State University REU Symposium (August 2019), University Park, PA.

SKILLS

- **Programming Languages:** Python, Julia, C, HTML, CSS, C++
- **Technical Skills:** Density Functional Theory, First Principles Calculations, Electronic Structure Analysis, Physics-Informed Machine Learning, Phase-Field Simulations, Machine Learning Workflow Design, Website Design, Computational Materials Science, Hybrid Material Semiconductor Physics, Condensed Matter Group Theory, Linear Optimization
- **Frameworks / Libraries:** Vienna Ab initio Simulation Package (VASP), Python Materials Genomics (pymatgen), Atomic Simulation Environment (ASE), PyTorch, Euclidean neural networks in 3D (e3nn), scikit-learn, Gurobi Optimization Solver

SERVICE

Application Review Committee, **MIT Summer Research Program (MSRP)** January 2023 – present

- As a 2021 MSRP alumna, co-review undergraduate applications for the upcoming MSRP cohorts.
- Rank admission scores based on research involvement, commitment to diversity, equity, and inclusion in STEM, applicant recommendation letters, and application quality.

Founder, **STEM Cells (buildingstemcells.github.io)** 2022 – present

- Founder of a website aimed at helping to provide guidance for undergraduate students who are interested in research careers.
- Write pages on graduate school, fellowships, research, general application advice, and DEI resources.
- Recruit fellow graduate students or undergraduate research program alumni at other universities to contribute their successful application materials or writing skills or update the website.

Volunteer, Citizens' Climate Lobby, **CCL District 14** January – May 2022

- Worked with fellow CCL volunteers in Florida's district 14 to encourage political environmental action.
- Held a CCL lobby meeting with Congresswoman Kathy Castor to discuss local solutions for mitigating environmental impact.

Volunteer, **Feeding Tampa Bay** January – May 2022

- Helped package and serve food pantry care packages for those in need.
- Organized and sorted food pantry care packages.

Vice President, Women in Computer Science and Engineering (WICSE), **USF** August 2020 – May 2022

- Co-hosted weekly general body meetings with WICSE President.
- Mentored women students with career, internship, research, and major study advice.
- Advised WICSE participation in the USF Engineering Expo and the Grace Hopper Conference.

MISCELLANEOUS

Powerlifting PRs: deadlift- 2.39x BW, squat- 1.96x BW, bench- 1.05x BW
Rock climbing (indoor boulder): level v4-v5
Photography: https://www.instagram.com/materialiaphoto/