

## 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  
**IB Diploma**, International Baccalaureate Program July 2018  
**State-Level Superior with Distinction**, Florida Bandmasters Association (piano solo: Khachaturian – Toccata) March 2017

### 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). In preparation.
- *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). Accepted pending minor revisions.
- *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>).
- *Section 7.6: Phonon Calculations (In "Artificial Intelligence for Science in Quantum, Atomistic, and Continuum Systems").*  
**A. Ladera** and T. Smidt (2023). Foundations and Trends in Machine Learning, **18**(4), 385–849, (<https://doi.org/10.1561/22000000115>).
- *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. Ariyaratna, 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  $(K_xNa_{1-x})NbO_3$  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  $\text{Ba}(\text{Ti}_{1-x}\text{Zr}_x)\text{O}_3$  (BZT), and parent compound  $\text{BaTiO}_3$  (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  $\text{K}_x\text{Na}_{1-x}\text{NbO}_3$  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 presented at the 36th Annual MIT Summer Research Program Research Forum (August 2021), Cambridge, MA.
- Investigating the Structure-Property Relationship of the  $\text{Ba}(\text{Ti}_{1-x}\text{Zr}_x)\text{O}_3$  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  $\text{K}_{0.5}\text{Na}_{0.5}\text{NbO}_3$  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

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- **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

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- 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](https://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

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**Powerlifting PRs:** deadlift- 2.39x BW, squat- 1.96x BW, bench- 1.05x BW

**Piano:** Khachaturian – *Toccata* (received "*Superior With Distinction*" at State-Level Solo and Ensemble); Beethoven – *Sonate Pathétique* No. 8 Op. 13 (performed and won at IB Talent Show 2018); Chopin – *Winter Wind Op. 25 No. 11* (first and last page)

**Rock climbing (indoor boulder):** level v4-v5

**Photography:** <https://www.instagram.com/materialiaphoto/>