ADRIANA J. LADERA

Massachusetts Institute of Technology, Bldg. 36-647, Cambridge, MA 02139
aladera@mit.edu ♦ ORCID: 0000-0002-5538-5011 ♦ LinkedIn ♦ Website

RESEARCH INTERESTS

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

EDUCATION

Doctor of Philosophy in *Computational Science and Engineering* — 2025 - present
Massachusetts Institute of Technology (MIT), Cambridge, MA

Master of Science in *Computational Science and Engineering* — 2022 - 2025
Massachusetts Institute of Technology (MIT), Cambridge, MA

Bachelor of Science with Honors in *Computer Science*, Minor in *Physics* — 2018 - 2022
University of South Florida (USF), Tampa, FL

HONORS AND AWARDS

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

PUBLICATIONS

Topological Crystal Engineering via Hydrogen Bond-Mediated Lattice Distortion of Inorganic Component of Silver Metal Organic Chalcogenolates
A. Ladera*, M. Aleksich*, A. LaMonica, K. Christensen, D. Paley, et al (2025). Revised and resubmitted.
*Denotes equal authorship.

Unveiling the origins of fluorescent 1D metal organic chalcogenolates
(2025). In preparation.

Bio-Chiral Metal-Organic Chalcogenolates with Optical Asymmetry
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. (2025). In preparation.
*Denotes equal authorship.

Strain phase equilibria and phase-field method of ferroelectric polydomain: A case study of monoclinic KxNa1-xNbO3 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, (pp 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). J. Chem. Theory Comput. 2022, 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). Phys. Rev. B, 102, 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).

PRESENTATIONS

- *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 Materials Research Society Fall Meeting and Exhibit (November 2023), Boston, MA.
- *Density Functional Theory in the Design of Novel Metal Organic Chalcogenolates*
  A. Ladera, A. M. Tehrani, and T. Smidt. Oral presentation at MOCha Madness Collaboration (July 2023), University of Connecticut, Storrs, CN.
- *Ferroelectric Phase Transitions in Strained K0.9Na0.1NbO3 Epitaxial Films Studied by in situ X-Ray Diffraction and Three-Dimensional Phase-Field Simulations*
  M. Schmidbauer, L. Bogula, B. Wang, M. Hanke, L. von Helden, **A. Ladera**, J.J. Wang, L.Q. Chen, and J. Schwarzkopf. Oral presentation at the International Conference on Advances in Functional Materials (AAAFM) (August 2021), Los Angeles, CA.
- *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 $Ba(Ti_{1-x}, Zr_x)O_3$ Relaxor Ferroelectric via Machine Learning*
  A. Ladera, and I. Ponomareva. Poster presented at the University of South Florida Undergraduate Research Conference (April 1, 2021), Tampa FL.
- *Phase-Field Simulations: Anisotropic Misfit Strain Phase Diagram of $K_{0.5}Na_{0.5}NbO3$ 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.

RESEARCH AND WORK EXPERIENCE

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

Perform first-principles density functional theory (DFT) calculations on novel metal organic chalcogenolates, including geometry optimization and electronic structure analysis (band structures, densities of states, partial charge densities at band edges), resulting in co-first author manuscripts submitted or in preparation to major peer-reviewed journals. Develop a machine-learning–assisted workflow for accelerated materials discovery that integrates generative models with DFT to propose novel material geometries and predict target properties. Design equivariant deep learning models to learn mappings from atomic systems to electronic Hamiltonians, enabling surrogate electronic-structure prediction.

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

Developed an unsupervised clustering workflow within a latent representation framework of 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). Workflow successfully identified phases and phase transitions in $BaTiO_3$ (BTO), the parent compound of BZT. Applying the workflow to BZT with Zr concentrations ≤ 0.25 revealed (i) that some of the compounds bear a subtle memory of BTO phases beyond the point of the pinched phase transition, which could contribute to their enhanced electromechanical response, (ii) the existence of peculiar phases with delocalized precursors of nanodomains—likely candidates for polar nanoregions, and (iii) nanodomain phases for the largest concentrations of Zr.

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

Performed large-scale first-principles calculations of energy properties for over 1,000 transition metal complexes using 23 density functional approximations to generate a diverse electronic-structure dataset, and found that ligand additivity is inversely correlated with high multireference (MR) character in TMCs, which complicates property evaluation. To address this, trained functional-specific neural networks derived from functional-specific energy properties, and co-developed an active learning framework that predicts MR character of TMCs from its constituent ligands, 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 which classify and localize signals at given frequencies for the user to gain better understanding of the device-mapping around them.

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

Created and visualized phase-field simulations of $K_{0.5}Na_{0.5}NbO_3$ thin films. By varying lateral tensile and compressive strain, temperature, and film size, arranged phase-field simulations by strain parameters to develop anisotropic strain phase diagrams of $K_{0.5}Na_{0.5}NbO_3$ at different temperatures and film sizes. After REU, continued simulation work with Penn State in collaboration with the Leibniz-Institut für Kristallzüchtung group to demonstrate great agreement in computational and experimental results of $K_{0.5}Na_{0.5}NbO_3$ thin film properties.

Undergraduate Research Assistant, Voronine Lab, **USF** February - May 2019

Received training for optical and atomic force microscopy and conducted optical characterizations of MoS_2. Learned to read scientific literature, scientific communication, and presentation skills.

TEACHING

Peer Leader, Dept. of Computer Science & Engineering, **USF** 2021 – 2022

Expanded the learning experience for Program Design (COP 3514) students 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 a retention of underrepresented gender groups in STEM.

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

Aided in-class lectures and grade weekly programming projects, quizzes, and exams for Program Design. Guided students in understanding class concepts and answer programming project questions through email and office hours.

Research Project Mentor, Computational Nanoscience Group, **USF** 2020 – 2021

Trained a high school student to learn aspects of machine-learning relaxor research project with Prof. Inna Ponomareva. Outlined biweekly project plans and demonstrated data visualization tasks.

LEADERSHIP AND SERVICE

Application Review Committee, **MIT Summer Research Program** 2023 – present

As a 2021 MSRP alumna, co-review undergraduate applications for the 2023, 2024, and 2025 MSRP cohorts. Rank admission scores based on quality of application, commitment to diversity, equity, and inclusion in STEM, and advocacy for students in recommendation letters.

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 for serving days.

Vice President, Women in Computer Science and Engineering (WICSE), **USF** 2020 – 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 USF Engineering Expo and the Grace Hopper Conference.

SKILLS

- **Programming and Scientific Computing:** Python, Julia, scikit-learn, C, Euclidean neural networks in 3D (e3nn), PyTorch, Keras
- **Modeling and Simulation:** Vienna Ab initio Simulation Package (VASP), Atomic Simulation Environment (ASE), Python Materials Genomics (pymatgen), density functional theory (DFT), first-principles electronic structure calculations (band structure, density-of-states, band edge partial charge densities) and geometry optimization, phase-field simulations
- **Machine Learning for Materials Science:** machine learning property prediction and surrogate modeling, representation learning to unveil features in materials, physically-informed machine learning
- **Algorithms & Optimization:** Gurobi, mixed-integer linear optimization, stochastic and deterministic gradient-based optimization

- **Scientific Domains:** computational materials science, semiconductor physics, hybrid and functional materials, condensed matter group theory
- **Languages:** English (*native*), Ilocano (*native*), French (*fluent*), Spanish (*conversational*)

MISCELLANEOUS

Powerlifting PRs: deadlift- 2.26x BW, squat- 2x BW, bench- 1.05x BW
Rock climbing (indoor boulder): level v4-v5
Photography: https://www.instagram.com/materialiaphoto/