ADRIANA J. LADERA

Massachusetts Institute of Technology, Cambridge, MA 02139

aladera@mit.edu ♦ ORCID: 0000-0002-5538-5011 ♦ adrianaladera.github.io ♦ buildingstemcells.github.io

RESEARCH INTERESTS

Modeling and simulation, ML-accelerated tools (generative models, machine-learned interatomic potentials) for materials design, density functional theory, condensed matter group theory, characterization and property evaluation of functional materials

EDUCATION

Massachusetts Institute of Technology (MIT), Ph.D. *in Computational Science and Engineering* 2025 - present
Massachusetts Institute of Technology (MIT), S.M. *in Computational Science and Engineering* 2025
University of South Florida (USF), B.S. Honors in *Computer Science* with minor in *Physic*s 2022

HONORS AND AWARDS

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
International Baccalaureate Diploma, Largo High School 2018
State-Level Superior with Distinction, Florida Bandmasters Association (piano solo: *Toccata*, Aram Khachaturian) 2016

PUBLICATIONS

Functional group identity drives the structural topology of silver benzenethiolate Metal Organic Chalcogenolates
A. Ladera*, M. Aleksich*, A. LaMonica, T. Smidt, and J.N. Hohman (2024). In preparation.
*Denotes equal authorship.

Fluorescent 1D Metal Organic Chalcogenolates: Insight into thiolated ligands that drive inorganic distortion and optoelectronic properties
(2024) 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 (2024). 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. Accepted 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

Conduct density functional theory (DFT) calculations to understand the electronic properties of experimentally-realized metal organic chalcogenolates (MOChas), as well as evaluate and relax the geometries of experimental and hypothetical structures. Create a machine learning (ML)-accelerated design workflow to generate and optimize novel MOCha geometries, which will enable fast feedback loops between ML design, experimental synthesis, and DFT characterization of MOChas and other functional materials.

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

Developed an unsupervised machine learning workflow within a framework of first-principles-based atomistic simulations to investigate phases, phase transitions, and their structural origins in ferroelectric relaxors, $Ba(Ti_{1-x}, Zr_x)O_3$. Demonstrated applicability of workflow by first using it to identify phases and phase transitions in the parent compound of $Ba(Ti_{1-x}, Zr_x)O_3$, $BaTiO_3$, a well-known prototypical ferroelectric, then applying the workflow to $Ba(Ti_{1-x}, Zr_x)O_3$ with $x \leq 0.25$. Revealed that (i) some of the compounds bear a subtle memory of $BaTiO_3$ 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 *x*.

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

Calculated energy properties for each transition metal complex (TMC) using 23 different density functional approximations for over 1000 TMCs. For each functional, trained a separate artificial neural network on the set of

TAEs produced by that functional. Developed an artificial neural network active learning scheme that searches for TMCs which produce large functional disagreement.

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 simulations by strain parameters to develop a phase-field simulation based anisotropic strain phase diagram 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

Learned properties of relaxor ferroelectrics and how to use Molecular Dynamics simulations. Ran and processed simulations of $Ba(Ti_{1-x}, Zr_x)O_3$ at temperatures up to 450 Kelvin, zirconium concentrations up to 25%, and frequencies up to 5.0 GHz to demonstrate the frequency dependence of phase transition temperature and remnant polarization.

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 Dr. Inna Ponomareva. Outlined biweekly project plans and demonstrated data visualization tasks.

SKILLS

Programming Languages: Python, CSS/HTML/Javascript, Julia, C/C++, Java, MATLAB, Processing,
Software: VASP 5/6, Rhino7/Grasshopper, Pymatgen, Atomic Simulation Environment, e3nn, Gurobi, AIRSS, Keras, Sci-Kit Learn, molSimplify, NequIP,
Computational: first-principles calculations, phase-field simulations, efficient algorithm design, 2D polygon triangulation algorithms, mixed-integer linear optimization, (stochastic) gradient descent, machine learning workflow design, machine learning clustering algorithms, data analysis and visualization, generative models for inorganic structures
Topics: semiconductor physics, linear optimization methods, density functional theory, hybrid materials, condensed matter group theory
Experimental: optical microscopy, atomic force microscopy
Languages: English *(native),* Ilocano *(native),* French *(fluent),* Spanish *(basic conversation),* Tagalog *(basic conversation)*

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 in STEM, and advocacy for students in recommendation letters.

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

Co-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.

*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.

MISCELLANEOUS

Weightlifting (max set x 5) – deadlift: 2.23x BW, squat: 1.73x BW, bench: 0.81x BW
Rock climbing (indoor boulder): level v4-v5
Photography: https://www.instagram.com/aladeraphoto/