

## ADRIANA J. LADERA

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### RESEARCH INTERESTS

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numerical methods, high-performance scientific computing, modeling, simulation, graphics, algorithms

### EDUCATION

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**University of South Florida**, Tampa, FL

Bachelor of Science, Computer Science; Minor in Physics, GPA: 3.69 / 4.00

Expected May 2022

### RESEARCH EXPERIENCE

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**University of South Florida, Department of Physics**

*Undergraduate Research Assistant*, February 2020 – present

*Revealing Hidden Dynamics of  $\text{Ba}(\text{Ti}_{1-x}\text{Zr}_x)\text{O}_3$  with Machine Learning* (Principal Investigator: Inna Ponomareva, Ph.D.)

- Construct datasets of simulations of  $\text{Ba}(\text{Ti}_{1-x}\text{Zr}_x)\text{O}_3$  (barium zirconate titanate, BZT) polarization domain structures at temperatures up to 450 Kelvin and zirconium concentrations up to 25%, with datasets separated by concentration
- Develop an unsupervised machine learning workflow that partitions the datasets using k-means clustering and plots the cluster labels as a function of temperature to show phase transitions (i.e. transition between cluster labels)
- Visualize each of the clusters by choosing a simulation from each cluster to represent its dipole dynamics
- Compare cluster-predicted phase transitions with simulation phase transitions, in which discrepancies may require more physical investigation

*Undergraduate Research Assistant*, May – August 2020

*$\text{Ba}(\text{Ti}_{1-x}\text{Zr}_x)\text{O}_3$  Relaxors in the Gigahertz Frequency Range* (Principal Investigator: Inna Ponomareva, Ph.D.)

- Learned how to use Molecular Dynamics simulations and properties of relaxor ferroelectrics
- Ran and processed simulations of BZT 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

*Undergraduate Research Assistant*, February – May 2019

*Optical Characterization of Transition Metal Dichalcogenides:  $\text{MoS}_2$*  (Principal Investigator: Dmitri Voronine, Ph.D.)

- Received training for optical and atomic force microscopy and conducted optical characterizations of  $\text{MoS}_2$
- Learned to read scientific literature, scientific communication, and presentation skills

**Massachusetts Institute of Technology, Department of Chemical Engineering**

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

*An Active Learning Approach for Exploring Transition Metal Complexes* (Principal Investigator: Heather Kulik, Ph.D.)

- 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 ANN on the set of TAEs produced by that functional
- Developed ANN active learning scheme that searches for TMCs which produce large functional disagreement

**University of South Florida, Department of Computer Science and Engineering**

*Undergraduate Research Assistant*, August – November 2019

*Functional Object-Oriented Networks* (Principal Investigator: Yu Sun, Ph.D.)

- Collected object and state data (i.e. “tomato” and “knife” with states “chopped”, “dirty”) for a functional object-oriented network composed of subgraphs of recipes, with each subgraph containing nodes of objects and states
- Practiced writing machine learning models using Tensorflow and Keras software

**Pennsylvania State University, Department of Material Science and Engineering**

*REU Intern*, May – August 2019, *Visiting Student Researcher*, August – December 2019

*Phase-Field Simulations: Phase-Diagram of  $\text{K}_{0.5}\text{Na}_{0.5}\text{NbO}_3$  Thin Films* (Principal Investigator: Long-Qing Chen, Ph.D.)

- Created and visualized phase-field simulations of  $\text{K}_{0.5}\text{Na}_{0.5}\text{NbO}_3$  (potassium sodium niobate, KNN) thin films by varying lateral tensile and compressive strain, temperature, and film size
- Arranged simulations to establish anisotropic strain phase diagrams of KNN 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 KNN thin film properties

## **PUBLICATIONS**

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Duan, C., **Ladera, A.**, and Kulik, H.J. (2021). Why do density functionals disagree the most: An active learning approach for screening experimental crystal structures. In preparation.

Zhou, M.J., Wang, B., **Ladera, A.**, Bogula, L., Liu, H.X., Chen, L.Q., and Nan, C.W. (2021). Phase diagrams, superdomains, and superdomain walls in  $(K_x, Na_{1-x})NbO_3$  epitaxial thin films. *Acta Materialia*, 215, 117038 (<https://doi.org/10.1016/j.actamat.2021.117038>).

Wang, B., Bogula, L., **Ladera, A.**, Wang, J.J., Schmidbauer, M., Schwarzkopf, J., and Chen, L.Q. (2021). Phase stability and three-dimensional structures of polydomains in orthorhombic ferroelectric thin films under anisotropic misfit strains. In review.

Lisenkov, S., **Ladera, A.**, and Ponomareva, I. (2020).  $Ba(Ti_{1-x}, Zr_x)O_3$  relaxors: Dynamic ferroelectrics in the gigahertz frequency range. *Phys. Rev. B*, 102, 224109 (<https://doi.org/10.1103/PhysRevB.102.224109>).

Schmidbauer, M., Bogula, L., Wang, B., Hanke, M., von Helden, L., **Ladera, A.**, Wang, J.J., Chen, L.Q., and Schwarzkopf, J. (2020). Temperature Dependence of Three-Dimensional Domain Wall Arrangement in Ferroelectric  $K_{0.9}Na_{0.1}NbO_3$  Epitaxial Thin Films. *J. Appl. Phys.* 128 (<https://doi.org/10.1063/5.0029167>).

## **PRESENTATIONS**

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Schmidbauer, M., Bogula, L., Wang, B., Hanke, M., von Helden, L., **Ladera, A.**, Wang, J.J., Chen, L.Q., and Schwarzkopf, J. Ferroelectric Phase Transitions in Strained  $K_{0.9}Na_{0.1}NbO_3$  Epitaxial Films Studied by in situ X-Ray Diffraction and Three-Dimensional Phase-Field Simulations. Oral presentation session presented at: *International Conference on Advances in Functional Materials (AAAFM) at UCLA*; 2021 August 18-20; University of California, Los Angeles, CA.

**Ladera, A.**, Duan, C., Vennelakanti, V., and Kulik, H.J. Exploring Transition Metal Complex Space with Computation and Artificial Neural Networks. Poster session presented at: *36th Annual MIT Summer Research Program Research Forum*; 2021 August 5; Massachusetts Institute of Technology, Cambridge MA.

**Ladera, A.** and Ponomareva, I. Investigating the Structure-Property Relationship of the  $Ba(Ti_{1-x}, Zr_x)O_3$  Relaxor Ferroelectric via Machine Learning. Poster session presented at: *2021 USF Undergraduate Research Conference*; 2021 April 1; University of South Florida, Tampa FL.

**Ladera, A.**, Wang, B., Wang, J.J., and Chen, L.Q. Phase-Field Simulations: Anisotropic Misfit Strain Phase Diagram of  $K_{0.5}Na_{0.5}NbO_3$  Thin Films. Poster session presented at: *2019 Penn State REU Symposium*; 2019 August 1; Penn State University, University Park PA.

## **HONORS AND AWARDS**

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<b>USF Directors Award</b>	August 2018 – present
\$3,500 awarded per semester for four years, University of South Florida	

<b>Florida Academic Scholarship</b>	August 2018 – present
Full tuition scholarship for four years (\$25,517), Bright Futures	

<b>Dean's List</b>	Spring 2019
3.9 GPA for the semester, University of South Florida	

## **TEACHING AND WORK EXPERIENCE**

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**University of South Florida, Department of Computer Science and Engineering**

*Peer Leader*, January 2021 – present

- Expand the learning experience for Program Design (COP 3514) students by creating lesson plans for recitation sessions, held twice a week for one hour
- Demonstrate live programming examples, discuss course material, and give guidance for internships, research experiences, and the computer science major
- Provide 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

## **University of South Florida, Department of Computer Science and Engineering**

*Undergraduate Teaching Assistant*, August 2020 – present

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

## **University of South Florida, Department of Physics**

*Research Project Mentor*, December 2020 – December 2021

- Trained a now first year college student to learn aspects of machine-learning relaxor research project with Dr. Inna Ponomareva
- Outlined biweekly project plans and demonstrated data visualization tasks

## **SOFWERX, Tampa**

*Cybersecurity Intern*, 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

## **SKILLS**

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**Programming Languages and Software:** Python, C, C++, Java, MATLAB, Processing, CSS, HTML, molSimplify, TensorFlow, Keras, Sci-Kit Learn

**Computational:** machine learning workflows, unsupervised machine learning clustering algorithms, data analysis and visualization, phase-field simulations, calculating with density functional approximations, efficient algorithm design, 2D polygon triangulation algorithms

**Non-Computational:** optical microscopy, atomic force microscopy

**Languages:** English (*native*), Ilocano (*native*), French (*fluent*)

## **LEADERSHIP AND SERVICE**

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### **University of South Florida, Women in Computer Science and Engineering (WICSE)**

*Vice President and WICSE Mentor*, November 2020 – present

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

### **DoSomething.org Online Volunteering**

*Campaign Volunteer*, April 2020 – present

- Raise the impact factor and awareness of racial justice, environment, LGBTQ+ and gender rights through online volunteering campaigns, social media, and guided discussion

### **University of South Florida, National Academy of Engineering Grand Challenges Scholars Program**

*CubeSat Program Founding Member*, September 2019 – present

- Collaborate with fellow engineering students to deploy a satellite as a secondary payload to a launch vehicle
- Research funding and assemble the telecommunications components of the satellite as the Telecommunications Lead
- Develop a 3D printed model of proposed satellite design that can hold necessary components such as transceivers, solar panels and other forms of power