I pursued computer science because I perceive it to have the potential to open up new ways of solving problems, and I pursued physics as a minor because I sought to strengthen my understanding of the world around us. Perhaps my affinity for combining fields comes from my own identity– a state of dualities: Asian and American, classical pianist and learning scientist, living at my mother's house and then living at my father's. I found that uniting my paired worlds provided me with the advantage of a unique perspective and was determined to choose my undergraduate research experience to reflect this thinking. I carried this dual perspective into my computational projects– material science, physics, and chemical engineering– where application of my computer science studies became intertwined with the field's research. Today's most pressing questions are multifaceted in nature and require a deeper appreciation from various approaches. Nowadays, research encourages perspectives that are strengthened from crossing boundaries between disciplines. Bearing this in mind, I have taken the initiative to work toward a career that is computationally driven, but interdisciplinary in its focus, and my research journey echoes this.

Undergraduate Research: In February 2019 of my first year, I chose an experimental physics lab with Dr. Dmitri Voronine. I made optical characterizations of 2D materials called transition metal dichalcogenides (TMDs), which, due to their atomic-scale thickness and semi-conductivity, are of great intrinsic interest for potential applications in optics, flexible electronics, and personalized medicine. The TMD I conducted research on was molybdenum disulfide (MoS_2), in which I used optical microscopy to investigate samples of MoS_2 crystals grown on various substrates. This experience enabled me to read scientific literature, learn optical and atomic force microscopy, and present scientific literature in biweekly oral presentations.

My work with Dr. Voronine led me to my first **REU in computational studies of materials at Penn State University** in June of 2019. Here, my work with Dr. Long-Qing Chen in the Dept. of Material Science and Engineering revolved around potassium sodium niobate (KNN) thin films, whose piezoelectric properties could be harvested and therefore provide a more environmentally friendly alternative to their lead zirconate titanate counterparts. I ran several phase-field simulations of KNN polarization domains structures, which I used to create a phase diagram that demonstrated how polarization domains varied according to changes in applied x and y strain. **I presented my results at the Penn State REU Symposium.** We discovered that our simulations resembled experimental polarization domain structures from a paper by the IKZ Group in Germany, and so after the REU ended, I continued working with Dr. Chen's group and the IKZ Group to **co-author a paper that was published in the *Journal of Applied Physics* and was presented at the 2021 *American Association for Advances in Functional Materials* Conference at UCLA. From this work, I also co-authored a publication in *Acta Materialia*, and a manuscript that, while rejected, may eventually lead to a publication in the future.** In this project I learned to write Bash scripts, how to display and process data obtained from computational modeling, gained knowledge of ferroelectric materials and phase-field modeling, and strengthened my presentation and scientific writing abilities. This experience reinforced in my mind the value that computation brings to materials discovery.

Returning from Penn State with a newfound interest in the abilities of computing for the natural sciences, I became a member of the Computational Nanoscience Group in February 2020 under the supervision of Dr. Inna Ponomareva. I learned basics of Molecular Dynamics (MD) simulation and relaxor ferroelectric materials, which are promising transducer materials for applications like optics due to their large response to external stimuli. I processed data produced by MD simulations of the barium zirconate titanate (BZT) relaxor ferroelectric. My contributions helped demonstrate the frequency dependence of phase transition temperatures and remnant polarization in BZT and **was published in *Physical Review B.***

My most recent and ongoing work with Dr. Ponomareva is a self-directed project that employs unsupervised machine learning (ML) to reveal hidden dynamics of BZT. We turn to the nontraditional ML approach, given both the computational and experimental challenges that impede progress on the atomistic insight into the origins of relaxor dynamics. Throughout my process of searching for ML algorithms that suited this problem, I learned how to construct datasets, developed supervised and unsupervised ML models using TensorFlow and Scikit Learn packages, and statistically analyzed and optimized algorithms' performance. To test the suitability of my selected unsupervised clustering algorithm, I clustered dipole structure simulations of barium titanate (BTO), the well-studied parent compound of BZT, at various temperatures. Comparing the phase transition temperatures revealed very good agreement between the clustering predictions and the MD analysis for BTO, which suggests that the clustering algorithm will do well detecting phase transitions in the dipole structure simulations of BZT. Any new phase transitions in BZT suggested by the clustering method would require more physical explanation, and if physics successfully reveals any new BZT dynamics related to the cluster-based phase transitions, then the ML methods described can be extended to investigate the dynamics of other relaxor ferroelectric materials. **I presented my work at the 2021 USF Undergraduate Research Conference.**

As the work in the Ponomareva group progressed, I felt increasingly inspired to bring more computational fields into my repertoire. With that in mind I applied to **participate in the 2021 MIT Summer Research Program (MSRP). I was accepted by Dr. Heather Kulik in the Dept. of Chemical Engineering** to explore the chemical space of transition metal complexes (TMCs) with computational methods and ML. TMCs are interesting due to their complicated and unique electronic structure, which makes electronic structure methods like density functional theory produce inaccurate calculations of their properties. The difficulty in TMC property evaluation, however, can be used to select TMCs that can benchmark the development of new electronic structure methods. I evaluated the total atomization energy property of selected TMCs which I used to train an artificial neural network. I targeted TMCs with large density functional disagreement in atomization energy, as this suggested TMCs with a more complex electronic structure. We can then build a workflow that would identify highly complex-electronic structured TMCs and yield a benchmark set for the development of new electronic structure methods. **I presented my results at the 36th annual MIT Summer Research Program Research Forum.** From this experience, I learned how to create automated workflows that evaluated TMCs and computed density functional calculations. This project also illustrated to me the challenges of computation in the natural sciences by demonstrating disagreement across density functionals in property evaluation of TMCs. **I was invited to continue my research with Dr. Kulik's group through the Fall MSRP Expansion Program,** and have been extending my summer work to the present day. **I am also co-authoring an in-preparation manuscript based on this work with Chenru Duan, my graduate mentor at MIT.**

Each of my research experiences have spanned various areas of computational science, and I am always searching for ways to mingle my interests in computation applied to the sciences. While at the MSRP, I was looking for a fresh direction for my graduate research plan that would center around high-performance and scientific computing. I attended a talk by Dr. Adrian Lozano Duran from MIT's aeronautics and astronautics department, who shared his work on turbulence modeling, simulation, and its dynamics. I found it fascinating that a phenomenon that appears across multitude scales in nature, from blood flow to nebula motion, is notoriously difficult to simulate, let alone efficiently, and so I sought to address the problem of optimizing high-performance computing and numerical methods in turbulence simulations for the further applications that may come of it. More broadly, I am excited to begin my trajectory into high-performance computing and scientific computing algorithm design for the sciences.

Teaching Experience: I am a Teaching Assistant (TA) and a Peer Leader for Program Design, one of the mandatory gateway courses in the computer science and engineering majors at USF. As a TA, I aid in-class programming examples and help guide students in the proper direction for course and programming-specific questions. As a Peer Leader, I have more creative freedom and opportunities to directly be involved with students. My lesson plans are constructed with the intention to make recitations entertaining and engaging as I believe that learning should be a meaningful and enjoyable experience. In recitations, I further enrich and review the material that students learn in class, and occasionally provide mentoring advice to students on research positions, internships, and future CSE coursework. I am also mentoring a now-former high school student to learn data processing and visualization in my ML relaxor project with Dr. Ponomareva. These experiences lead me to understand the importance of helping to inspire a desire to learn in others by making personal connections with them and fostering an inviting and welcoming learning environment.

Community Involvement: Throughout my time in my undergraduate career, I made sure to acknowledge my social and communal responsibilities. While at the Penn State REU, I participated in Penn State's STEM Day, whose overarching theme was to inspire in children an early interest in science. There, I used household ingredients to demonstrate how to create simple lava lamps. The following semester, I joined the Grand Challenges Scholars Program because I wanted to help address the larger and millennium problems in science and engineering. Our group is completing a prototype design and component search for a picosatellite, which we hope to attach as a secondary payload to a launch vehicle in the near future. I am also participating in an online volunteering program that targets my issues of interest: racial justice, climate change awareness, and LGBTQ+ and gender rights. In August 2020**,** I was elected as the Vice President of Women in Computer Science and Engineering (WICSE), in which I aim to promote gender diversity and maintain retention of women in CSE through making connections between early-year CSE students and CSE faculty, and mentoring students with career and CSE major advice.

Intellectual Merit: My undergraduate experiences in research have equipped me with a series of useful skills: best practices in oral and written scientific communication, data analysis, and a strong grasp of the scientific method. Across my work in different computational research groups, I gained exposure to the expansive applications of computing and cutting-edge problems, and my involvement with these groups has merited in presentations and co-authorship of publications. My interdisciplinary training has provided me with multiple perspectives on the needs and goals of computation for the sciences and equipped me to move into the backend of these problems to address the next pressing questions in algorithms and computational science. During my graduate career and beyond, I want to develop accurate, efficient, and scalable numerical and high-performance computing algorithms for scientific applications, where I can refine the technical and soft skills nurtured by my past research experiences.

Broader Impacts: Having friends, family, and people at MIT, USF, and Penn State who are supportive of my endeavors and are helping to shape my path as a research scientist, I too hope that I can one day do the same for students who are just as curious as I was about the inner mechanisms of science and the universe. Being a TA and Peer Leader and working with women CSE students allowed me to see how I can directly impact and influence others to become more involved in research and CSE opportunities. In my career, I want to continue serving as a gateway for people to be inspired to pursue their passions in STEM. As a woman of intersecting minority groups, I also want to cultivate a diverse learning environment for underrepresented groups in STEM, especially for women, people of color, and LGBTQ+ scientists. Far too often, solving diversity and equity challenges becomes a play of statistics: how many students of color, how many women students and faculty and so-on. But we need to bring more of the research into diversity issues, like causes of the Leaky Pipeline as published by NSF and NAE, into practice.

As a GRF Fellow, I will hold GRF mentoring classes for underrepresented candidates and hold sessions to guide those candidates in graduate school applications. I will also devote my time in graduate school and beyond to work with stakeholders to target the challenges that cause perpetual cycles of systemic problems for minority groups. Additionally, I will collaborate with organizations, such as GirlsWhoCode and oSTEM, to promote a safe space and an interest in STEM for women and LGBTQ+ individuals. I hope to extend my commitment to cultivating a diverse and inclusive STEM environment far into my research career. Finally, I also want to bring more discussion to environmental issues. With ever-increasing climate change concerns raised by scientists around the world, I want to join organizations like Climate Group that campaign for environmentally conscious practices in people and especially in companies. Overall, I would like to find impactful ways to encourage sustainable living and a greener economy.

Future Vision: I plan to expand my interdisciplinary approach to research by carrying out my graduate work in programs focused on applied computational methods to scientific questions. Georgia Tech’s Ph.D in Computational Science and Engineering is the best fit for my goals. Their program is rich with research areas from computational theory of physical systems to large scale scientific computing problems, and has many professors that specialize in high-performance computing techniques for a host of scientific applications. With the skills and knowledge I gain from my Ph.D, I envision a career as a professor or industry research scientist, where I can hone my problem-solving skills, foster collaboration between students, faculty, and industry, and address climate and diversity challenges. Receiving the NSF Graduate Research Fellowship would allow me the flexibility to pursue my research interests while also granting me the freedom to work towards diversity, inclusivity, and environmental advocacy.