NSF-REU Site Funded Student Highlight Slides
The goal of this project was to investigate the magneto-optic (MO) response of Gd-doped CdO by measuring its Verdet constant for various wavelengths near the plasma frequency. Materials with a large MO response make great candidates for integrated photonics.

I contributed to the project by helping to implement a set-up to measure the Faraday rotation of the material as a function on magnetic field. Participating in this project was an honor. It gave me insight into the research process and confirmed my interest in research.
The experiment that was conducted during the REU session was encoding and retrieving memory in a liquid contact line on glass. Understanding the type of memory involved will help determine where it can be used. My contributions to this project were finishing the apparatus and obtaining results that show there is memory involved with a liquid contact line on glass.

My contribution to the project were the finalization of the apparatus setup, cleaning techniques for the glass substrate, technique to remove bubbles, and development of code for automation of experiment. The goals of the experiment were met, and I will be able to take the experience and knowledge learned for future work in researching.
This project was aimed to use a drift correction algorithm and investigate its drift maps and to see if we could find local strain within these maps to look at impurities of in lattice structure of superconducting material. My specific contribution would help rewrite the algorithm from IDL to python.

For this project I was able to rewrite the original algorithm from IDL to Python. After we analyzed the distortion map by using a set of fake data to see how the distortion maps work. This will help me in my future career path either with graduate school or a more industry focus path since this has provide me with a great coding experience and with real research experience.
First-Principles Study of Transition Metal Sulfides for Lithium Sulfur Batteries

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Lithium sulfur batteries offers an attractive alternative to lithium-ion batteries in order to meet the need for higher energy density. However, the life cycle of LiS batteries is limited by the loss of active cathode material due to the shuttling of polysulfides. My project investigated the polysulfide anchoring effect of TaS$_2$, WS$_2$, and ReS$_2$ as the cathode material with the aim to enhance the redox mechanism.

I contributed to my project by calculating surface and binding energies in order to determine the best of these transition metal dichalcogenides for the cathode. Through this project, I got a better understanding the work of a researcher, especially that of a computationalist. I know the both the individual effort as well as the collaboration needed for a successful project.
Simulation of Carbon Nanothreads for Structure Control

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A **nanothread** is a new 1D form of carbon. Aromatic molecules such as furan (C₄H₄O) can bond in stacks under high pressure. Two possible configurations are *syn* (oxygen are aligned) and *anti*. The *syn* thread is conductive and thus has many possible applications, but is higher energy and hence less likely to form. The goal was to modify the furan molecule such that *syn* was lowest in energy.

I successfully constructed multiple nanothreads wherein *syn* was lower in energy than *anti*. This helped improve my research skills via presenting unsolved problems and demanding thorough reading of scientific articles.
Lyotropic chromonic liquid crystals have received a wide interest in recent years because their fundamental viscoelastic properties are not very well understood. These materials, which include common compounds like dyes and drugs, are composed of self-assembled, plank-like molecules that stack into linear aggregates when dissolved in water. The self-assembled stacks form nematic and columnar liquid crystal phases at varying concentrations and are uniquely characterized by their huge viscoelastic anisotropies, which give rise to fascinating behavior including spontaneous chiral symmetry breaking in their bulk molecular organization and sub-diffusivity of suspended colloidal inclusions. In our work, we studied the structural response of chromonic LCs to shear flow in a quasi 2D, freely suspended, thin film geometry and how the changing structure in turn affects the effective viscosity.

In the lab, I prepared our DSCG mixtures, did film thickness calibrations, helped with the setup of the magnetic thin film rheometer, and took images using polarized optical microscopy to study our thin films. Our data showed that at low shear rates, the film’s long-range molecular order was mostly unaffected. However, a higher shear rate greatly disordered the film and induced many disclinations. This project was a great opportunity for me to discover more about how a lab and research environment works and what I can expect in graduate school. It has also allowed for me to develop new technical and personal skills as well as improve on existing skills. I learned more to program in python and ImageJ, communicate and present research, setup an experiment from scratch and more. Overall, it was a very positive and exciting experience.
Two dimensional (2D) materials have recently demonstrated to have outstanding properties and endless applications in the field of nanocatalysis. One of these 2D materials is hexagonal Boron Nitride (hBN), a layered material with an atomic structure of alternating Boron and Nitrogen atoms in a hexagonal geometry in each layer with outstanding thermal and chemical stability. hBN, although it is an insulator, has similar properties to graphite and other carbon material that are used as supports of metals catalysts. A promising alternative for new catalysts with non-carbon supports is the use of hBN as the support material for metals nanoparticles.

This summer I made 2D hBN with supported Fe, Ni, FeNi, Pt, and Pd nanoparticles using a novel intercalation/exfoliation method. This materials where characterized using the MSC facilities. Subsequently, I focused on the electrochemical characterization of the different materials as well as teaching some graduate student on the technique. The materials were tested for their catalytic activity for producing hydrogen through the Hydrogen Evolution Reaction.
The Rechtsman group studies the properties of light in complex photonic structures. My specific project was to optimize the parameters of a 45-degree chiral woodpile photonic crystal for experimentally observing Fermi arcs. I chose to optimize the parameters by running my own simulations and provided the group with a fabricable crystal design that has the potential for observing Fermi arcs with the FTIR. In parallel, I took data with the FTIR to verify the results of a paper the group previously published. This summer, I learned to push through disappointment and technical frustration on the path to interesting results. In short, I became a more disciplined researcher.
NSF-MRSEC REU Students participating in REU-Site Sponsored Professional Development
Characterizing Hidden Tunable Monoclinic Phases in Barium Titanate

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For this project, I created and observe intermediate monoclinic phases in tetragonal Barium Titanate (BaTiO$_3$), a common ferroelectric. These phases have ~4x higher second harmonic generation (SHG) coefficients than the parent phase, and they are reproducible, reversible, and tunable with a relatively low applied voltage (~400 V/cm). The characterization of these phases that I performed with SHG microscopy will be useful for fundamental science and in potential device applications; manipulating BaTiO$_3$ domains and phases with voltage allows for tunable optical properties and possibly piezoelectric properties as well.

My contribution to the project was the optimization and operation of an SHG microscopy setup with a scanning piezo stage. I was able to image the surface of a BaTiO$_3$ sample, confirm the identity of tetragonal domains as reported in previous literature, and create and observe monoclinic phase regions. I then increased and decreased the size of these regions in a systematic manner with applied fields of opposite polarity. These results are consistent after many voltage cycles. The experiments I took part in were a huge step in my development as a physics researcher – I am now more knowledgeable, capable, and able to work independently. I am also now confident in my decision to pursue a doctorate degree in a related field.
Increasing evidence points to the presence of unregulated labile Cu$^{2+}$ in regions of the brain affected by neurodegeneration, as a root cause for neurodegenerative diseases such as Alzheimer’s. It is hypothesized that Cu$^{2+}$ can bind to the negatively charged phosphatidylserine (PS) presented on the surface of cells undergoing apoptosis, thus catalyzing membrane oxidation, halting controlled cell death, and instead inducing necrosis, a type of cell death that can harm surrounding healthy cells. This study was conducted to gain a better understanding of the factors which govern the interaction between Cu$^{2+}$ ions and PS.

I aided in exploring how altering the ionic strength, solution acidity, membrane composition, and vesicle curvature affects the binding of Cu$^{2+}$ ions to heterogeneous as well as homogenous synthetic membrane systems.
The snowball chamber is a new technology with the potential to become a novel particle detector. The chamber is aimed at detecting dark matter, but it can also aid in particle detection at large. My contributions helped in understanding how the chamber works on an atomic level.

My project was to simulate the chamber and analyze the simulation's output to investigate how environmental neutrons affect it. This information is critical to the snowball chamber so that it detects only specific particles. This experience has showcased to me what research entails and has confirmed my interest in pursuing a career in particle physics.
This project aims to find a way to computationally predict the catalytic performance of compositionally rich perovskite oxygen evolution catalysts based on their comprising prototypical unary perovskites to guide subsequent synthetic work. To this end, I performed preliminary work to confirm that these methods could recapitulate the performance of known single-phase materials. Improved oxygen redox turnover is of paramount importance in ensuring that hydrogen is readily and cheaply available for fuel cells to ensure its use as a renewable energy source for vehicle and grid applications. In the latter case, the availability of electrochemical energy storage ensures the viability of intermittent alternative energy sources (e.g., solar and wind) versus fossil fuels.

My work confirmed that some material properties of interest could be adequately recapitulated with the given computational methods to compare some of the performance predictions to actual electrochemical experiments to soon follow. The project also illuminated additional considerations for executing subsequent calculations where these failed to recapituate known behaviors in some prototypical materials. Furthermore, it served as a comprehensive pedagogical exercise in density functional theory that will allow me to better understand literature and methodology in a field to which I had little exposure. The software in question also improved my ability to use auxiliary software, notably the underlying operating system in which Quantum Espresso runs (i.e., Linux).
High-entropy materials make up a relatively new class of materials in which five or more elements are combined in nearly equimolar concentrations with the hopes of stabilizing the product into a phase pure material. These materials can have a variety of interesting properties including interesting magnetic ordering and high thermoelectric performance. In this project, a polycrystalline sample of a novel spinel oxide was synthesized, its magnetic ordering was measured, and a possible synthesis method for a single crystalline sample was explored. The discovery and ability to synthesize high-entropy materials is important if they are to be used in future applications.

My responsibilities in this project included high temperature solid-state synthesis of the polycrystalline sample, X-ray diffraction to determine if the sample was phase pure, and energy dispersive spectroscopy to identify the composition of the compound. I also synthesized a couple of the material's parent compounds for comparison. This program was my first experience doing research, and it has helped me build a solid foundation for my work in the future. Not only did I learn the basics of research, but I also picked up valuable laboratory skills such as X-ray diffraction, energy dispersive spectroscopy, and various materials synthesis techniques.
My research for the summer REU characterized the limiting component of Zn ion rechargeable batteries using Impedance spectroscopy. The importance of this project is to optimize this affordable battery to be used as energy storage for renewable energy producers to reduce harmful fossil fuel production.

I was tasked with developing the testing parameters and assembling battery coin cells for testing in this project. I was also performing the data analysis to characterize and identify the performance of the battery. As a researcher, I will continue using this newly learned technique across all my electrochemical systems.
The goal of this project was to find out how layer thickness, aggregation, and doping effects the nonlinear optical properties of MoS$_2$. This is important in a global context because tuning these properties can advance applications in light and energy. I took data of second harmonic generation (SHG) and multi-photon photoluminescence (MPPL) of MoS$_2$.

I learned how to use the Fourier-Transform nonlinear optical microscope, which interferes laser pulses with each other to measure the excitation spectrum of the sample, making it possible to measure MPPL and SHG. This summer, my project allowed me to learn about something new and I got to experience a lab that mainly works with optics and phenomena happening on a small scale. I also learned more about how to problem solve and what to do when something isn’t working or going as planned.
Implementing SABARSI (Statistical Approach of Background Removal and Spectrum Identification) To Uncover Raman Spectrums

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Biomarkers for diseases can be used to further drug development and early detection. Alzheimer’s disease still faces challenges in terms developing early diagnosis and effective treatment. Biomarkers can be found using the technique of surface-enhanced Raman spectroscopy (SERS) to obtain a biomarker’s Raman spectrum. A molecule’s Raman spectrum is often described as a type of “fingerprint” as each molecule has a unique Raman spectrum. This research implements SABARSI (Statistical Approach of Background Removal and Spectrum Identification) to identify Raman signals from SERS spectra taken from a brain slice with Alzheimer’s to identify Raman signals reliably and accurately.

The method of SABARSI was originally on the programming language R and then I translated it into MATLAB. By the end of the ten weeks, I had implemented SABARSI and detected multiple Raman spectra for my group. SABARSI was the method of choice because it has been shown to detect Raman spectra accurately and reliably from biomolecules in complex samples. Unlike most methods, SABARSI can also be implemented on a large data set. Using this algorithm along with machine learning methods, our research group will look to find biomarkers for Alzheimer’s disease. This research experience has helped me become better at coding and science communication. The experience also allowed me to see what work can be like in a dedicated research group. I am thankful to the research group I worked with, everyone who served as a program coordinator for this REU, and the National Science Foundation (NSF).
MnBi$_6$Te$_{10}$ (MBT) is a possible magnetic topological insulator (MTI). MTI's have attracted interest due to their applications in spintronics, which would increase electronics efficiency. Due to past difficulties in working with MBT, testing methods are needed to determine its status as an MTI. Over the summer my mentor and I have experimented with exfoliation and transport testing methods, which will be used in the future to characterize MBT.

My contributions to this project were straightforward: I researched other group’s processes on working with MBT and similar materials, ran them by my mentor, attempted them, and then recorded the results. I also wrote documentation on our lab’s techniques for those who come after me. I went into this program expecting to find the characteristics of MBT by the end but spending the whole summer working on forming methods taught me to appreciate the often-overlooked but ever-vital process of carefully forming methods before the actual testing can begin.
Investigating Cobalt Valence in Entropy Stabilized Oxides through Density Function Theory Calculations

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Entropy stabilized oxides (ESO) are a new class of ceramics that show great promise for a vast number of future applications, including energy storage. Recent experimental studies on J14, a specific ESO composed of equiatomic amounts of Mg, Co, Cu, Ni, and Zn, showed that under different growth conditions, cobalt can charge compensate by oxidizing, leading to enhanced properties. Due to the compositional degrees of freedom of ESOs, experimental studies cannot determine what is structurally happening in the material when cobalt oxidizes, although it has been suggested that this oxidation is due to cation vacancies, which is why computational methods are needed. It was my role to explore whether cation vacancies could result in cobalt oxidation and how the local environment of the vacancy effects this.

Throughout the summer, I performed density functional theory calculations through VASP on simpler oxide structures that can be used as a basis for future computational studies on the five-component J14. To understand cobalt oxidation, I also performed Bader charge analysis, density of states calculations, and generated electron charge density difference diagrams through VESTA. My structures with cation vacancies were able to induce cobalt oxidation and showed similar properties as seen experimentally, such as smaller lattice parameter and band gap. Before coming to Penn State, I had never been given the opportunity to do computational materials research, so I had little to no computer skills. This summer I learned so many state-of-the-art computational techniques and worked with some amazing faculty. I now feel confident enough and plan to pursue a Ph.D. after completion of my undergraduate degree and focus on computational materials research in graduate school.
Ferroelectric thin films are ubiquitous for their use in microsystems, computer memory, and high-frequency electrical components. A cornerstone of ferroelectric thin films is the ability to manipulate phase transitions and ferroelectric domains leading to enhanced control of ferroelectric properties. Compositionally manipulating phase transitions leverages a strain-based spinodal decomposition between in-plane and out-of-plane superdomain polarization states to achieve unique properties, including a tunable piezoresponse. However, in lead-free ferroelectric thin films, this superdomain decomposition has yet to be found.

For this project, I ran hundreds of phase-field simulations using high-performance computing resources from the XSEDE, performed data analysis, and utilized thermodynamic theory to predict material properties like the piezoelectric coefficient. As a researcher, I gained real-world experience and developed essential skills in programming, thermodynamics, computational modeling, and scientific communication.
Physics Department Undergraduate Research "hosts" participating in REU-Site hosted professional development programs
A new measure of localization and coherence in localized wavefunctions

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Contrary to our classical intuition, a finite amount of disorder can localize a particle irrespective of how large its kinetic energy is. This surprising quantum phenomenon, known as Anderson localization, is the result of wave function interference in the presence of disorder. The effect carries the name of P. W. Anderson, whose prediction was widely confirmed experimentally. We proposed a new metric $L_n$ based on distance between coherent sites of a given wavefunction to measure localization.

My contributions are to explore our new metric as a tool to study localization and to compare it with well-known metrics, such as participation ratio and von Neumann entropy. During this research, I have learned many fundamental physics ideas such as quantum coherence, density matrix, and tight-binding model. Also, since this project is also about numerical simulation, I have learned how to construct a cubic lattice model in python and studied new techniques to minimize time to generate data. For professional development, I have learned how to communicate through writing and discussion effectively. All experiences inspire me to pursue a graduate school in Physics.

$$L_n = \sum_{RR'} P_R P_{R'} |R - R'| = \sum_{RR'} (|c_R^n|^2)(|c_{R'}^n|^2) |R - R'|$$
Simulating Light Curves of Core-collapse Supernovae with Dense Circumstellar Material

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The study is carried out by using radiation hydrodynamics simulations code SNEC to model the light curve. The SNEC code solves Lagrangian hydrodynamics equations which are coupled with radiation transport in the flux-limited diffusion approximation. Specifically, this study is aiming to reproduce theoretically a light curve of SN 2005cl. Once we successfully reproduce light curve of SN 2005cl and we believe we could produce the rest of Type II[n]Sne as well.

We determined the different parameters of explosion that will influence the light curve include, different pre-explosion energy, different full explosion energy, different time period, different $^{56}$Ni masses and so on. I gained a lot of skills during REU, using cluster to do simulation, learning python, learning hydrodynamics of supernova, learning how to write a paper and so on!
My REU project was to develop a parallel addressing method for our neutral atom quantum computer in order to perform multiple operations at once. This is part of the worldwide effort to improve the flexibility and robustness of current quantum computers. The successful completion of my project would increase the speed of our apparatus by a factor of 7.

I wrote a program for the operation of a digital micromirror device (DMD) as a source of multiple parallel addressing beams. The program consisted of multiple image generation algorithms that produced patterns to be displayed on the DMD. My summer research experience has strengthened my preference for both experimental research and the subdiscipline of AMO physics. I am still interested in future experimental condensed matter research.
Chaotic Dynamics of a Big Bang Singularity with Semiclassical Corrections

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In this project, we proposed a new way to implement semiclassical corrections to a Singularity model. We examined the dynamics and chaos to compare with the classical case – observe if essential properties were conserved. The Universe expanded from what we call the Big Bang Singularity. In the beginning things were small, and suddenly turned big. It is important to find a way to implement quantum variables to the Big Bang since this way we can understand how all things begun in a small scale.

My role in this project was to generate a solver for these dynamics using Mathematica, and understand the implications of changes to the model. I am very happy to have worked on this project, as quantum cosmology is a field of physics I would like to pursue in Grad School.
This project is important as it aims to detect the radio showers of the tau neutrino, a flavor of neutrino that has been seldom detected. My role in this project will allow for future researchers to assess signals from these cosmic events with more confidence.

I sought to determine in what region of space do we observe the maximum power using interferometric methods on ZHAires simulation results that aimed to assess the change signal by taking the travel time between the source and the antenna array. By doing so we can triangulate the point of max flux ‘Xmax’ with greater precision and limit the amount of antenna, thereby reducing noise and cost.
General Relativistic Stellar Structure Equations in Julia

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This project has us creating an equation solver for stellar structure equations in Julia. The purpose of the solver is to use its fast computational abilities to analyze neutron stars numerically. Studying neutron stars is important because it can provide insight on matter in extreme environments. For my part, I am responsible for the creation of the solver and its continual improvements.

As a part of this project, my duties revolve around creating the necessary script in the code to solve our equations and testing it to ensure it functions properly. Within this process, I analyze the data produced by our code to ensure it matches real world observations. Overall, I’d say this summer experience has helped me understand the up and down nature of research and how to approach seemingly intimidating situations.
Determining the dominant oscillation modes of proto-neutron stars allows us to better understand which modes are the most capable of producing gravitational waves, allowing for better insight for determining properties of the state of matter inside neutron stars and better guiding future observational studies. My project focuses on creating a computer simulation of the oscillations in these proto-neutron stars to determine these modes.

I created a 1-D Wave Equation Solver in Julia as the base for the proto-neutron star model. I also derived the radial equations governing the stellar structure of the proto-neutron. These steps allow for future full implementation of oscillation modeling. The experience has taught me the nature of computational and theoretical research and developed my skills with numerical integration techniques.
The long-term goal of this project is to simulate the visual and physical aspects of several different spacetimes in virtual reality using Unity 3D. For the summer, the goal was to simulate a Schwarzschild black hole. We will use this simulation software as an educational and outreach tool. Thus far, I have been the primary developer of the code.

My contribution to the project has been writing a script that solves the geodesic equations to be used as a ray tracing algorithm and a camera transformation algorithm. This is essential so that the user can both see how light is manipulated by the presence of a black hole, and how the observer themselves feel the gravitational influence of a black hole. This experience has been critical to my experience as a researcher: as my first real research experience, it gave me a good idea of what a career in this field could look like, as well as enlightened me as to what my interests are / are not. I really have found that I like computational astrophysics, simulations, and science that relies heavily on visuals.
Neutrinos are fundamental particles that are uncharged and only interact through the weak force. This makes them ideal messenger particles because they can propagate over cosmological distances undeflected and unimpeded. The highest energy neutrinos are produced in interactions involving high energy cosmic rays and therefore provide important information about the most energetic acceleration processes in the universe including the origins of ultra-high energy cosmic rays. For this reason, being able to detect ultra high energy (UHE) neutrinos is important for research in fundamental physics, astrophysics, and expanding the reach of human knowledge. In-ice radio arrays can detect UHE neutrinos in the PeV to $>10$ EeV range by detecting radio emission produced in showers when UHE neutrinos interact with the ice. This project aims to design, build, and test horizontally polarized antennas for improved gain and angular resolution in order to reconstruct neutrino arrival direction.

I compared antenna designs including helical, folded dipoles, and halo antennas, evaluating each antenna for its gain, efficiency, and reproducibility. Designs were simulated using the XFdtd electromagnetics software and constructed in the lab, enabling a comparison of the performance of the realized antenna with models. These designs were also compared with the current design. This summer project gave me familiarity with simulation methods using XFdtd as well as building and testing antenna prototypes using a virtual network analyzer (VNA). It also taught me how to compare simulated data with experimental data. Through exposure to these different aspects of research, I am better able to elucidate my preferences for the types of projects I may pursue in the future.