Personal and Research Overview/Intellectual Merit: As a mechanical engineer, I greatly appreciate the integrative nature of the discipline. Many research projects within mechanical engineering overlap with other disciplines, such as bioengineering and environmental engineering, and by collaborating across disciplines, mechanical engineers have the potential to directly impact society and uniquely contribute to the body of knowledge in their sub-discipline. While studying at Caltech, I have had the opportunity to conduct research in different sub-disciplines within mechanical engineering. My research experiences have led me towards fluid mechanics, an area of study almost as diverse as its parent discipline. I have greatly enjoyed working on three interdisciplinary research projects and sharing my results with both scientific and general audiences. I thus plan to pursue a career as an academic researcher after completing my Ph.D. and apply my interdisciplinary skillset to address real-world problems involving fluid mechanics.

Although my current research is in fluid mechanics, my first research experience was in solid mechanics and involved working for nine months in Professor Pellegrino's lab at Caltech to design an origami-inspired base for a set of antenna tiles. I sought out this research opportunity to pursue one of my long-standing interdisciplinary interests: applications of origami to engineering. As part of the project, I researched and developed bistable hinges to connect the antenna tiles, conducted a parametric study to optimize the hinge widths and lengths, arranged the hinges in CAD and laser-cut them in polypropylene to form the antenna base, and independently designed and built a device to manually actuate the base. The final antenna base had robust hinges, was easy to actuate, and morphed between flat, spherical, and cylindrical configurations. At the conclusion of my project, I presented my work at Caltech's Summer Undergraduate Research Fellowship (SURF) conference and **placed third out of over 200 Caltech students in the Doris S. Perpall Speaking Competition**. It was satisfying to make the connection between origami and engineering for my audience members and see that they too understood and were excited about the interdisciplinary nature of the project after watching my presentation. I was also **a co-author on the resulting research paper** and gained experience in the process of writing a peer-reviewed journal article. My experience working on this project **contributed to my interdisciplinary skillset and gave me a greater appreciation for the design considerations an engineer must account for** when developing a model for a specific application. The skills I gained in engineering design will aid me greatly in future research projects when I apply my theoretical knowledge to real-world problems and account for relevant factors either in a model or in a prototype. I also **gained invaluable practice in communicating my research to both a scientific and a general audience.**

After spending almost a year on a solid mechanics-related project, I wanted to diversify my experience within mechanical engineering and immerse myself in a project involving fluid mechanics. My interest in fluids was piqued by the breadth of intriguing and interdisciplinary research in the field; I came across papers studying bioinspired wind energy, ocean dynamics, filtration, airborne disease transmission, and the atmosphere. I found the sub-discipline of fluid mechanics particularly appealing because it has applications to health, the environment, and sustainability, impact areas I would like to focus on to address real-world problems in society. To further investigate research in fluid mechanics, I initiated work with Professor Bourouiba at MIT and spent a summer studying incoming air flow past a woven cloth mask under her supervision. During the summer, I independently researched components of analytical filter models and taught myself relevant filter theory. I then synthesized a filter model in MATLAB that plotted the trajectory of a particle as it moved through a grid of filter fibers. The model accounted for the effects of Brownian motion, electrostatic forces, and the flow field itself. After programming the analytical model, I taught myself to use OpenFOAM, an open-source computational fluid dynamics (CFD) program, and developed an analogous numerical model for the flow past a grid of filter fibers. In comparing my numerical and analytical models, I gained a much deeper understanding of the interactions between particles and fibers and what my analytical model did not account for. I also

developed my ability to work with open-source CFD code and independently communicate with the community of code developers to troubleshoot errors in simulations of specific physical phenomena.

At the end of the summer, I presented my work at Caltech's SURF conference and was a **semifinalist in the Perpall Speaking Competition.** I continued work on this project through the academic year and investigated the dynamics on the outgoing side of the mask by tracking sneeze clouds over time. Here, I taught myself to use image-processing software (ImageJ) to identify properties of the clouds such as their position and radius. I also researched the distortion produced by camera lenses and developed a procedure to manually correct distortion in measured sneeze trajectories. In completing two projects related to disease transmission, I gained experience both in developing simulations to predict the movement of fluids through filters and analyzing experimental data that characterized the fluids. I greatly enjoyed working independently on these interdisciplinary projects and cemented my desire to conduct research in fluid mechanics. Currently, I am **working with Professor Bourouiba and other lab group members to prepare two papers for journal submissions; the papers will include components of my analysis of sneeze clouds**.

My most recent research project with Professor Colonius at Caltech focuses on how ultrasound waves in burst-wave lithotripsy (BWL) break up kidney stones. The project refines a safer, more efficient, and noninvasive alternative to traditional treatments. Over the summer, I used an open-source multi-component flow code program (MFC) to simulate patterns of strain energy inside 2D stones of different sizes and compositions. The simulations validated the patterns of strain energy and stone responses to varied ultrasound input predicted by a 2D resolvent analysis model. I am currently continuing my research from the summer as part of a year-long senior thesis project and plan to develop an analogous resolvent analysis model in 3D that will predict the combination of ultrasound input that generates the most strain energy within the kidney stone. In working on this project, I have utilized knowledge not only from my graduate-level solid and fluid mechanics classes at Caltech but also from my minor in information and data sciences (IDS). **My graduate-level and interdisciplinary classwork in applied mathematics, electrical engineering, and computer science has enabled me to tackle problems from troubleshooting and interpreting simulation data to understanding and writing finite-difference codes.** I have also gained an introduction to the complexities of multiphase flows and the numerical tools used to approximate flows of varied compositions.

In completing three interdisciplinary research projects, I have built a strong foundation of research skills and knowledge. I recently applied for and was **one of five Caltech students to receive the 2021 Barry Goldwater Scholarship**, a scholarship recognizing undergraduates who have excelled academically and in research and who intend to pursue research-based careers. As a future graduate student, I am prepared for the demands of a Ph.D. and remain committed to a career in research.

Broader Impacts: One of the most rewarding aspects of completing a research project for me is sharing my results and enthusiasm for the project with people from both scientific and general backgrounds. My favorite part of sharing my research is **engaging a wider audience**; by motivating citizens from varied scientific and non-scientific backgrounds, I can increase awareness of the issues my research addresses and facilitate communication between people from different sectors of the workplace. My experiences with communication go beyond my three research projects. As a member of the Society of Women Engineers (SWE), I have shared my enthusiasm for engineering with young girls from underrepresented backgrounds for the past two years during Introduce a Girl to Engineering Day (IGED). The workshops I led included a short presentation on applications of origami to engineering, including my first SURF project and collapsible satellites, airbags, and heart stents, and an origami activity where participants folded intricate geometric modules. I very much enjoyed seeing the looks of surprise and excitement on participants' faces when they realized that scientists are using an ancient Japanese art form to solve engineering problems. **In linking art and engineering, I made the field of engineering more relatable to participants and encouraged them to consider an interdisciplinary career in STEM.** I have also taken my experiences with origami and engineering and presented at both Caltech's annual Summer Preview / Women in STEM Day and an event that brought prospective underrepresented students to Caltech's campus. It was satisfying to know that sharing my research experiences with students from underrepresented backgrounds could inspire them to apply to Caltech and pursue a career in STEM.

As a 2021 Goldwater Scholar, I have also shared my application experience and advice with potential applicants from underrepresented backgrounds. I recently joined the Goldwater Scholar Community Mentorship Program, an initiative that aims to **broaden participation in the Goldwater application process** and make the scholarship more accessible to students from all backgrounds. During the summer, I gave a virtual presentation on the Goldwater Scholarship to students at the University of Virgin Islands, a HBCU, and encouraged participants to consider a career in STEM research and apply for the scholarship. I am currently working with students at the University of California Riverside and providing one-on-one advice to prospective applicants to motivate interest in the Goldwater Scholarship and its career benefits and strengthen the applicants' submission to the Goldwater Foundation.

In addition to increasing the participation of women and underrepresented minorities in STEM-related fields, I am very interested in **using my communication skills to improve STEM education.** For the past two years, I have served as an at-large representative on Caltech's Academic and Research Committee (Caltech ARC). Members of the ARC act as a liaison between students and faculty and implement programs to better the educational experiences of students at Caltech. As an at-large representative, I have helped facilitate student-faculty lunches, where students may speak freely with faculty about their research interests and experiences, and the Option Buddies program, which connects underclassmen with upperclassmen willing to provide advice about their major. I have also volunteered as a class ombudsperson and provided my professors with feedback from other students enrolled in the class so that the professors better addressed the needs of the students. After my freshman year, I participated in the "How to Succeed at Caltech" panel for incoming students and contributed to the freshman guide to academics at Caltech. My work on the ARC has **given me experience in connecting faculty and students and understanding what students need to maximize their educational experience at the undergraduate level.**

Career Goals: Across my research experiences, I have thoroughly enjoyed the process of combing through the literature and creatively using the knowledge I gained to solve problems from incompatible hinges to unstable numerical simulations. Each of my research projects has had direct applications to the real world, and I have greatly appreciated the opportunity to work on projects whose outcomes have the potential to transform society for the better. My positive experiences conducting and communicating my research have reinforced my desire to pursue an academic research career in fluid mechanics. As an academic, I will continue to share my research with general and scientific audiences by teaching classes, giving talks, and writing papers. I plan to utilize the communication skills I have gained as an undergraduate to connect with researchers across fields from academia and industry and work with them to develop interdisciplinary solutions to real-world problems involving fluid mechanics. I will also ensure that as an educator, I cater to the needs of my students and implement programs to enrich their educational experience. Lastly, I will continue to organize outreach activities that encourage women and underrepresented minorities to pursue careers in STEM early in their education. Receiving the NSF GRFP award will enable me to not only contribute to the wealth of knowledge in my sub-discipline but also positively impact the lives of future STEM researchers in both graduate school and my future career.

Introduction: Multiphase flows are ubiquitous in our lives. These flows, which include any combination of thermodynamic phases of matter, govern carbon sequestration, combustion, the interaction of precipitation with vehicles, and many other important processes[1-3]. Although multiphase flows are integral to a variety of disciplines and industries, we still do not fully understand the fundamental physical interactions that take place within the flows. We also cannot simulate them with ease; many current numerical models are computationally expensive and do not account for complex, multiphase dynamics at different scales[4]. To improve technology utilizing multiphase flows and predict how flows will behave, it is imperative that we develop the computational tools to accurately simulate the interactions between the different phases of matter in multiphase flows.

One common type of multiphase flow includes particles suspended in a fluid. Fluid-particle multiphase flows have applications such as predicting the erosion and transport of sediment, the deformation of blood cells in the human body, and the movement of food in the digestive tract[5-7]. Current numerical models for fluid-particle multiphase flows use different sets of equations to model phenomena such as flow at varied length and time scales and the interface between phases of matter. These equations include, but are not limited to, the Reynolds Averaged Navier-Stokes (RANS) equations for turbulent flow and the equations in the volume of fluid (VOF) model for immiscible fluids[8]. With appropriate modifications, the equations account for two-way coupling and other multiphase interactions. However, they also include many unclosed terms that require additional modeling and thus computational cost.

Recent studies have addressed closures in numerical multiphase models by incorporating additional equations that balance the number of equations and unknowns in the model. For instance, Ouda et al. develop closures for particle stresses and viscous and turbulent stress tensors in a sediment transport model that allow them to capture a variety of sediment flows. However, the model closures do not yet accommodate smooth transitions between viscous and inertial regimes[5]. Another intriguing approach to addressing model closures involves using machine learning techniques to formulate the complex dynamics present in multiphase flows. In a recent study, Beetham and Capecelatro use sparse regression to develop a closed functional form for the RANS equations in the context of single-phase turbulent flows[9]. Beetham et al. extend this framework to gas-solid multiphase flows with solid particles in a subsequent paper, but they are still expanding their model to more complex multiphase flows and flows with different combinations of phases of matter. They also note that current applications of machine learning to multiphase flows involving neural networks are limited in that they are "black boxes" and do not provide analytical expressions that describe the complex flows[10]. Alternatives to neural networks, such as the sparse regressions described in their papers, are still being developed.

Research Plan: I aim to study the interactions between particles and their surrounding fluid in multiphase flows and improve upon computational models for fluid-particle interactions. My implementation will include numerical closures for fluid-particle flows at different length and time scales and incorporate elements of machine learning to aid in developing the closures. In modeling fluid-particle multiphase flows more accurately and efficiently, I hope to push the boundaries of current computational models and enable researchers to simulate flows from blood in human arteries to sediment-filled rivers with ease.

Research Goal 1 (Improved computational models): I will first expand upon current models for fluid-particle multiphase flows by analytically introducing closures where possible that accurately model the interactions between the particles and their surrounding fluid. To further capture the behavior of complex fluid-particle flows through numerical closures, I plan to investigate alternatives within machine learning to neural networks and implement them in my model. This will enable me to simulate flows where the functional forms of the equations involved are not fully known. In introducing closures to my model, I will ensure that the computational cost of my numerical setup is reasonable and that the simulations run with a high efficiency. I plan to assess the efficiency of my code with metrics such as the computational "grind time." To complete this phase of my research, I will need access to a computing cluster on which I can run my computational model. I plan to either use an existing cluster at my proposed graduate institution (MIT), or if selected as an awardee, the XSEDE computing allocation granted to all NSF GRFP research fellows.

Research Goal 2 (Model validation): After developing and implementing an improved computational model for fluid-particle flows, I will validate my model by first running simple simulations for known flows and comparing my results to existing experimental and numerical results. I will then systematically vary length and time scales within my model to generate different types of fluid-particle flows. To validate my simulation results for these more complex flows, I plan to compare the results of my simulation to existing datasets for analogous flows. If no datasets exist for the flows I wish to simulate, I will collaborate with lab groups studying experimental fluid mechanics at my proposed graduate institution to generate the datasets.

Research Goal 3 (Open-source code): In addition to improving upon current models for fluid-particle interactions, I plan to make my implementation available to the public through an open-source computational fluid dynamics (CFD) platform such as OpenFOAM or the multi-component flow code (MFC) that the Colonius group has made publicly available. I will first determine whether the platform I am working with already has the capability to simulate multiphase flows with fluid-particle interactions. If the platform cannot simulate the flows, I will implement the setup from my improved computational model within the framework of the platform. If the platform is already designed to work with fluid-particle flows, I will modify the solver to account for closures and corrections from my improved model.

Intellectual Merit: The lack of closures for multiphase models is one of the most pressing issues that researchers face when working with multiphase-related CFD codes. Without numerical closure, researchers cannot accurately and efficiently simulate complex multiphase dynamics and thus cannot predict the behavior of multiphase flows in the real world. My research will address this gap in knowledge by developing closures for fluid-particle multiphase flows both analytically and with machine learning. The closures I implement will pave the way for future researchers modeling fluid-particle flows at different scales, build interdisciplinary knowledge of the flows, and provide a foundation for the application of additional machine learning techniques to finding closures for any multiphase problem.

Broader Impacts: The results of this project will make it easier for researchers across disciplines from biomedical to environmental engineering to simulate fluid-particle flows with open-source code and build upon models for other multiphase flows. With additional, readily available computational tools for fluid-particle multiphase flows, researchers can investigate real-world phenomena such as blood flow in major arteries and sediment transport in fluids. The fundamental knowledge they gain will advance science and benefit society by enabling them to develop and design technology from biomedical devices to sturdier infrastructure near bodies of water. As an NSF Graduate Fellow developing this research, I will facilitate the dissemination of my work and motivate the public by writing papers, presenting at conferences, and giving public talks. I also plan to join organizations promoting women and minorities in STEM at my proposed graduate institution, such as the Society of Women Engineers (SWE), and share my findings and applications of my work to the real world with young students. I will develop educational demonstrations and presentations with the organizations I join and coordinate fun and informational outreach events related to my field of study that encourage broader participation of women and minority groups in STEM.

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Methods Med. 2016 (2016) [8] Gibou, F. et al. *J Comput. Phys.* 380, 442-463 (2019) [9] Beetham, S. et al. *Phys. Rev. Fluids* 5, 084611 (2020) [10] Beetham, S. et al. *J. Fluid Mech.* 914 (2021)

Personal, Background, and Future Goals Statement

Motivation: Although my love for chemistry traces back to when I was first introduced to the subject, my desire to make chemistry my career is relatively new. I originally wanted to be a doctor, however, as I made my way through my first year at Berkeley, something about the path to an MD didn't quite feel right. It wasn't until my second semester organic chemistry class with Professor Richmond Sarpong that I realized why. In this class, Professor Sarpong shared how scientific discoveries shaped the world we live in, whether it was the synthesis of penicillin that redefined the future of antibiotics or the discovery of the polio vaccine that stopped a murderous epidemic in its tracks. I grew to understand that most doctors confront issues related to public health on a personal level, but these decisions and solutions are guided by *science*. Scientific discovery can help redefine what is possible for public health – the COVID pandemic and mRNA vaccine are a perfect representation of this concept – and is more important now than ever. This realization occurred at a pivotal point in my life. In my personal life, I finally accepted myself and came out to my parents; in my academic life, I earned nearly perfect grades during the Spring 2018 semester, something I thought would be impossible during my first semester at Cal. After learning in my class with Professor Sarpong the impact of chemistry on medicine, I reassessed my goals. I found myself buried in scientific literature and organic chemistry textbooks that I read out of my own interest and was soon enthralled by organic synthesis. With each turning page, my fascination grew overwhelmingly. While the elegant construction of complex natural products and well-conceived solutions to perplexing synthetic issues is *now* of great personal interest, paramount is the pursuit of knowledge and the impact it can make on the lives of others. My goal is to use the knowledge I acquire as a scientist to fuel lasting change in the world.

Intellectual Merit: My time as a researcher in the Maimone lab was a time of grit and intense learning. There, I was introduced to the long hours of organic synthesis and became an expert in synthetic organic chemistry techniques, handling very sensitive and often dangerous chemistry (if handled inappropriately). My work built on a 2016 report in *Science* from our lab, where we utilized a reductive 8-*endo*/5-*exo* radical cascade to achieve the total synthesis of (-)-6-*epi*-ophiobolin N.

My project focused on (+)-6-*epi*-ophiobolin A, where we sought to develop a redox-neutral radical cascade instead of a reductive cascade used previously (Figure 1A). This was achieved via a Cu^{I}/Cu^{II} cycle where metal to ligand charge transfer generates Cu^{II}, which abstracts chlorine to form an alkyl radical. The tertiary radical formed upon cyclization is trapped by Cl•, which eliminates. Following a singlet oxygen ene and hydroformylation reaction, one problem I focused on was the addition of a 2-methyl propenyl nucleophile to a hemiacetal to form the final stereocenter of (+)-6-*epi*-ophiobolin A (Figure 1B). Addition of 2-methyl propenyl magnesium bromide in the presence of BF_3•OEt_2 gave low yields and low diastereoselectivity. In contrast, the use of [(2-methyl-propenyl)$_4$In]MgBr forged the final stereocenter in 64% yield with 20:1 *dr*. We believe the anionic, bulky complex creates a contact ion pair with the in-situ generated oxocarbenium to give the desired selectivity.

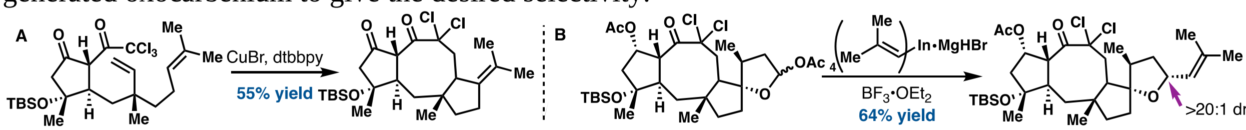


Figure 1. **A)** redox-neutral radical cascade **B)** unusual indate nucleophile.

This work was published in 2019 in ACIE. I was also awarded the *ACS SURF Fellowship* and presented my research in Boston to scientists at Merck and the extended scientific community. I also presented my research at the *College of Chemistry's* Spring Poster Session, where I won best poster. Based on this presentation, Professor Maimone asked me to present a talk to organic chemistry students at Berkeley Community College who were interested in transferring to UC Berkeley. The objective of the event was to increase engagement from community college transfer students with College of Chemistry research and in doing so inspire transfer-student interest in research. The event was a huge success. Many students were intrigued by the idea of total synthesis and making medicinally relevant molecules. One of the undergraduates at this presentation later became a member of the Maimone group. Upon completion of the ophiobolin project, I then turned my attention to a different synthetic target, rameswaralide. I was independently able to develop a succinct, effective route to the western half of the molecule. The project I began is still ongoing today. Leading my own total synthesis was invaluable and affirming.

Since starting in the Reisman Lab in January 2021, I joined an NIH funded project working with Postdoctoral Scholar Dr. Conner Farley. Since the project was still at an early stage, Dr. Farley and I investigated different routes to a key intermediate. Working independently, I investigated the plausibility of a butenolide γ-alkylation and discovered an interesting vinylogous Mukaiyama aldol reaction to form a challenging quaternary center in >20:1 dr at the γ-carbon and 8:1 dr at the alcohol (Figure 2). Remarkably, no α-alkylation was observed despite steric hindrance from the neighboring quaternary center, and the only isolatable side-product is recovered butenolide (resulting from hydrolysis) in 40% yield. Although mechanistic studies are required, one possibility is that the reaction proceeds by a hetero-Diels-Alder reaction. Recently, I was able to form the central 7-membered ring by an intramolecular enolate-arylation sequence. Optimization is currently underway. These preliminary studies allow rapid access into intermediates resembling the natural product. Due to the significant progress I've made since starting this project in January, I was nominated to present my progress at the Division of Chemistry and Chemical Engineering's Seminar Day and recently found out I was selected as the faculty's choice for best poster.

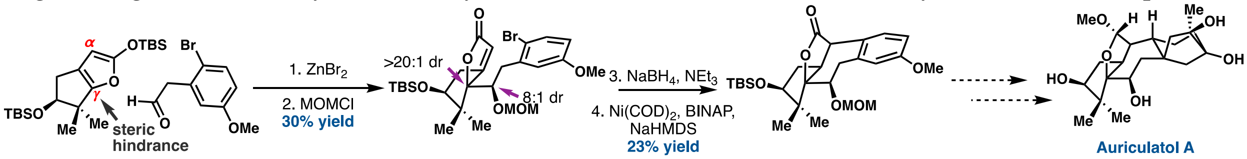


Figure 2. Preliminary results towards Auriculatol A utilizing a neat vinylogous Mukaiyama Aldol reaction.

During my time as an undergraduate, I worked through *Grossman's Art of Writing a Reasonable Mechanism* and Czako and Kurti's *Strategic Applications of Named Reactions in Organic Synthesis* in full. I took every graduate organic chemistry course available to me, including two organometallics courses from Professor John Hartwig, two physical organic chemistry courses from Professor Bob Bergman, and two synthetic organic chemistry courses from Professor Dean Toste. I was able to graduate UC Berkeley with a 3.80 GPA, achieving high honors in the major and receiving a departmental award, the *Koo-Liu Siok Han Award* for excellence in chemistry research while balancing being a student athlete all four years. After graduating from Berkeley and receiving an honorable mention from the NSF GRFP awards for the 2020 competition, at Caltech, I have achieved a 4.1 GPA. I have now worked on three total syntheses and made significant progress on each one since starting in the field three short years ago. Through my graduate training, I will continue to advance the field of total synthesis and chemistry more broadly by being an active member in the community as well as advanced researcher. I have an innate desire to continue to develop syntheses of medicinally relevant compounds, granting access for biologists to study them while highlighting novel chemistry in their making.

Broader Impacts: Outreach online has been a large part of my life since starting at Caltech, especially with COVID-19 preventing in-person interactions. To increase engagement in science, I started creating short science communication videos on *TikTok* and acquired over 20,000 followers in the span of 3 months. The videos I have been making most recently have been related to applying to graduate school and knowing if graduate school is right for you to gain interest from the younger generation in science and STEM fields. My most popular video has been viewed over 900,000 times and shared 6000 times. My videos also focus on science communication and scientific literacy, teaching fundamental concepts in organic chemistry or research going on in organic chemistry labs at Caltech or throughout the world. My overarching goal is to increase engagement with the younger generation in STEM. In line with these science communication efforts, I have served as an editor for *Caltech Letters*, a Caltech club focused on publishing articles written for the broader community on the science that graduate students conduct to increase scientific literacy and understanding. We are set to publish my first article as lead editor on the research being conducted in Caltech's psychology department about fear and overcoming fearfulness. I plan to stay very involved in science communication throughout my time at Caltech.

Part of my *TikTok* platform has been advocating for LGBTQ+ persons in STEM. This has been an ongoing passion of mine since helping organize student orientation all four years at Berkeley and leading first-hand

DEI initiatives. When I was a freshman in 2017, I had a unique opportunity: UC Berkeley was completely remodeling its new student orientation (which had followed the same format for the previous 100+ years). *New Student Services* wanted to adopt a 7-day welcome week model, with programming from 7 am to midnight each day; however, they did not have the workforce or funding to do so. As such, I was part of *New Student Services'* first volunteer cohort who developed many of the inner workings of the program. My involvement consisted of mentoring the next classes of orientation leaders, developing diversity, equity, and inclusion training, devising budget plans, and providing information to new students via cell phone and email. As part of a special project as an orientation mentor, I created a personal segment for our required DEI training where I shared my own personal experiences to 10,000 new students about homophobia on sports teams. The message of this presentation focused on being inclusive to others and creating spaces for kind dialogue about our different identities. This has translated to my life at Caltech, where I am currently working on an investigative journalism project to assess the sense of belonging for queer individuals in STEM academia at the doctoral or tenure-track faculty level. The goals of the project are to design a comprehensive questionnaire that assesses the sense of belonging of queer people at the doctoral or tenure-track faculty level in STEM and conduct a pilot data-driven study at MIT and Caltech using the same questionnaire. The questionnaire was completed back in January 2021, and we have gathered data from over 50 open LGBTQ+ faculty in STEM academia across the nation as well as 100 self-identifying students at MIT and Caltech. We are also collaborating with Professor Jon Freeman at NYU, a leader of an ongoing petition to the White House to add LGBTQ+ identities to the NSF census. From telling my story as an LGBTQ+ hockey player who experienced homophobia to 10,000 students at UC Berkeley, to promoting LGBTQ+ in STEM content to thousands of people on *TikTok* and my current investigative journalism project, I have realized that many members of my community look up to me. I am a proud member of the LGBTQ+ community and strive to pave the way for more members of my community to enter STEM.

Throughout my time at Berkeley, I found my "why" in mentorship opportunities. I was involved in the *CalTeach* program all four years, which offered teaching support to middle school teachers in underserved areas. *CalTeach* was a consistent way I could give back to the community and work on my mentorship skills. I also TA'd for an introductory biology course, peer tutored for the Berkeley's *College of Chemistry*, and led weekly demonstrations in elementary schools through the *Bay Area Scientists in Schools Program*. The mentorship skills I acquired at Berkeley have translated very well since starting at Caltech. As an organic chemistry TA, I consistently scored over 4.8/5 on the *teacher quality feedback reports*. I also volunteered this summer for 10 hours a week at an underserved elementary school, leading science demos through Caltech's *Ready21* Program for students who struggled with online learning. Vital to these experiences has been good mentorship -- having courtesy, respect, and empathy.

In addition to these mentorship efforts, I am working to organize and promote an inclusive and supportive culture at Caltech. I joined the *Chemistry Graduate Student Council* (*CGSC*) the moment I arrived as a first year student. I am the only second year on the CGSC. On the *CGSC*, I helped organize the *CGSC Summer Seminar Series*, which hosts department-wide scientific talks from Caltech faculty aimed at building connections between Caltech faculty and graduate students. I am also one of four students organizing the division-wide Seminar Day, a day-long event with a $7000 budget that includes a poster session with prizes for best posters, short 20-minute student and post-doctoral talks, and a Division-wide dinner for presenters, faculty, and attendees. I have also taken on smaller tasks such as spear-heading the organization of our department-wide big-little sibling program and planning a first year social. Noticing my willingness to get involved, Professor Reisman asked me to be the only student representative helping to plan the *Merck SoCal Symposium*, a symposium bringing together Merck scientists and researchers from UCLA, UC Irvine, and Caltech. During this time, I independently constructed a virtual world on a website called *Gathertown* where attendees and presenters could logon, explore, and interact with other attendees and presenters. In this virtual world I added poster boards and uploaded everyone's poster for the poster presentation. I met with the Director of Chemistry at Merck San Francisco, Eric Ashley, and showed him the world and how it worked. I received very positive feedback on the world I built online. Internally in the Reisman lab, I have supported every outreach opportunity we have organized since arriving at Caltech. I plan to stay active in my group and in the community at large.

Graduate Research Plan Statement

Motivation and Background: According to the National Institute on Aging, Alzheimer's disease is the sixth leading cause of death in the US and third for the elderly.[1] Current medications function as cholinesterase inhibitors but are only beneficial in mild or moderate cases, and *there exists no cure*.[2] *Only one FDA-approved drug may change disease progression*, Aducanumab, but this drug costs $56,000/year and has severe side effects.[2] Neuroscientists have identified a new metric, long term potentiation (LTP), for identifying a medicinal target's efficacy instead of antiacetylcholinesterasae activity.[3,4] This new metric could revolutionize our understanding of Alzheimer's – LTP in the hippocampus has been linked to cognition and memory [3,4] and has *never* been targeted as an Alzheimer's therapeutic. By studying this new metric, a new and promising class of medicinal targets may arise. 14-hydroxylobscurinol (**1**) and Phlegmadine A **(2)** (Figure 1), isolated from *Phlegmariurus phlegmaria* in 2019, have been shown to exhibit *remarkable* preventative effects on LTP impairment.[5] Biologists, however, have not been able to thoroughly study and understand their unprecedented potency due to prohib ively low isolation yields (only 8 mg of **1** isolated from 20 kg of plant material), however, the isolation chemists demonstrated that **2** can be prepared from **1** via a [2+2] cycloaddition.[5] Chemical synthesis represents a promising route to **1** and **2**. *No syntheses have been completed to date*. An efficient, scalable synthesis of **1** and **2** will allow access to gram quantities of **1** and **2** to further the community's understanding of Alzheimer's and offer a lifesaving therapeutic to society.

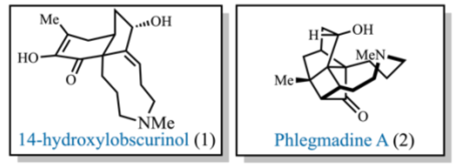


Figure 1: Structure of **1** and **2**.

Aim 1: ***Develop a machine learning algorithm for predicting allylic oxidation conditions.*** While allylic oxidations are incredibly useful, applying them in synthesis may be challenging. A universal and robust set of conditions does not exist: new substrates often require extensive screening and optimization to identify the best catalyst, oxidant, acid/base, and solvent. The Reisman Lab has an ongoing focus on developing machine learning (ML) models to solve the "above the arrow" problem.[6] Building on our prior work, we will train multilabel classification models on known allylic oxidations to predict conditions given a substrate and product of interest.[6,7] A Reaxys® search revealed 2614 published allylic oxidation reactions on similar substrates containing two fused rings. This dataset would be used to train a variety of machine learning models (eg. random forest, neural network) for the condition prediction task. This work is part of an ongoing collaboration with Caltech's Computational and Mathematical Sciences department and will be expanding the use of ML technology in organic chemistry.

Aim 2: ***Develop a succinct synthesis of 1 and 2.*** Retrosynthetically, I propose **1** can be simplified to **7** via

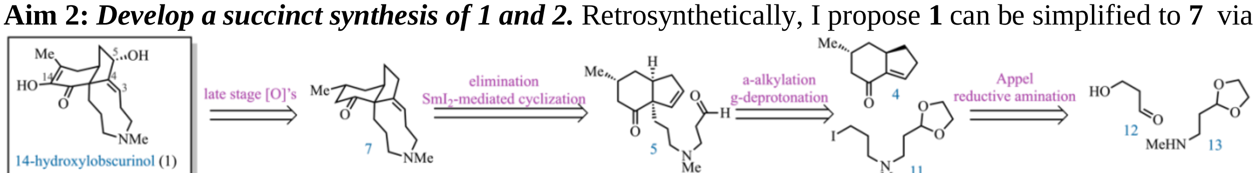


Figure 2: Retrosynthetic Analysis of **1**.

late stage oxidation at C-5. The C3-C4 olefin could arise from alcohol elimination under acidic conditions, noting that these conditions have been shown to form the more stable cis-olefin geometry in 9-membered rings.[8] Our lab has an ongoing focus on using SmI_2 cyclizations.[9] I believe the 9-membered ring could form from a novel SmI_2-mediated 9-*exo-trig* cyclization of aldehyde **5**. Next, I envision α-alkylation from γ-deprotonatated **4** with **11** would be possible. **11** should be available from an Appel reaction to install the primary iodide and the reductive amination of known fragments **13** and 3-hydroxypropanal (**12**). The proposed synthetic sequence of **1** is presented in Figure 3. I propose that conjugate addition into a,b-unsaturated ketone **3** will occur smoothly, and a subsequent acid-catalyzed aldol condensation would install the enone moiety to give **4** with high stereoselectivity. Next, screening kinetic bases such as LDA or more thermodynamic bases such as KO^{t}Bu could affect the gamma deprotonation of **4** and afford an intermolecular α-alkylation with **11**. If needed, soft enolization methods to give the silyl enol ether could also be pursued (Figure 4A).[10] The stereochemistry of the alkylation is predicted as shown based on the *Furst Plattner Rule*, which states that nucleophilic addition favors the axial position. Conformational analysis is provided in Figure 4B. Formation of key intermediate **5** will segue nicely to a novel intramolecular SmI_2-mediated cyclization to afford **6**. While 9-membered ring formation from Sm ketyl addition into alkenes is anticipated to be challenging – to our knowledge, such a reaction has *not* been reported – we believe this reaction has promise based on precedent for 9-membered ring Reformatsky-type SmI_2-mediated cyclizations, as well as Barbier-type reactions.[11] Aldehyde in **5** should be easier to reduce than the ketone,[12] and cyclization of ketyl radicals onto ketones over alkenes is rare.[11,12]

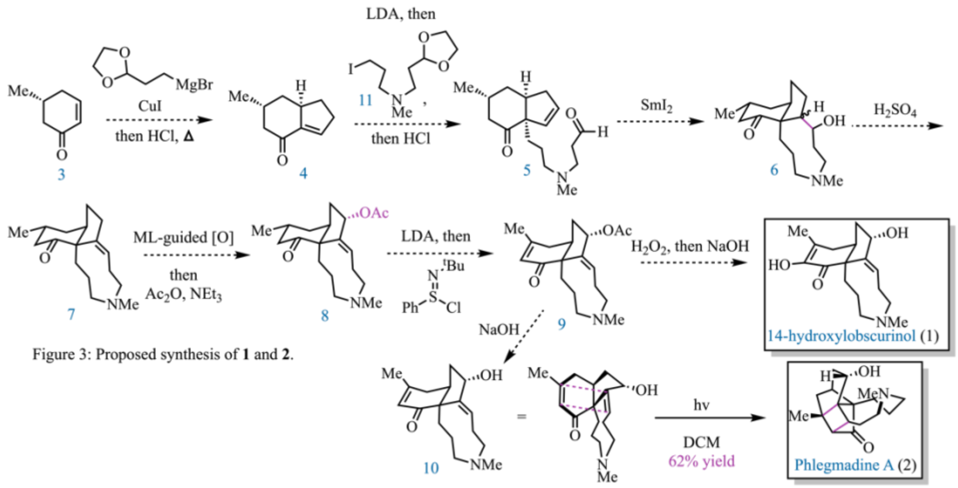


Figure 3: Proposed synthesis of **1** and **2**.

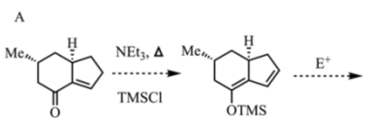


Figure 4A: A promising backup strategy.

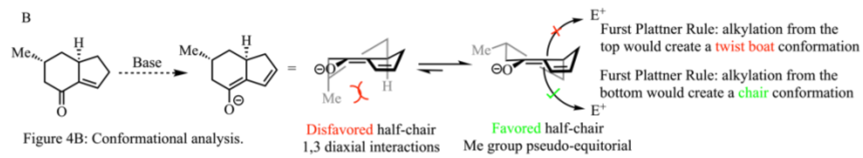


Figure 4B: Conformational analysis.

After acid-catalyzed elimination to form **7**, an allylic oxidation with conditions selected by ML, followed by acetylation would deliver **8**. A Mukaiyama dehydration of **8** should occur smoothly,[13] followed by an H_2O_2-mediated epoxidation and elimination[14] with concomitant deacetylation to afford **1**. Upon completion of the first synthesis of **1**, deacetylation of **9** should form **10**, which will give **2** from a known [2+2] cycloaddition. Our greatest anticipated challenge is the α-alkylation step to form the quaternary center. A backup route is detailed in Figure 4, where substitution at the alpha position of known compound **14** forms the challenging quaternary center early through a similar acid catalyzed aldol reaction to form **15.** Mesylation and elimination would form **16**, which contains a terminal alkene as a functional group handle to install the amine unit.

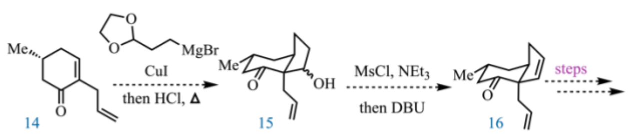


Figure 5: A promising backup route.

Intellectual Merit: This project describes the first synthesis of **1** and **2** and highlights the efficiency of late stage oxidations for synthetic planning. A novel SmI_2 cyclization is described and has promising literature precedent. Development of machine learning models will advance our understanding of ML methods.

Broader Impacts: This work details a promising Alzheimer's therapeutic to save lives. Given the prohibitively low isolation yields (<0.0008%), synthesis offers a compelling method to providing gram-quantities of compound **1** and **2** to biologists. Given the remarkable and unprecedented efficacy of **1** on LTP impairment, the project will allow biologists to further study and understand LTP impairment, an important new metric for understanding Alzheimer's. This proposal outlines the use of ML in synthesis, an area of synthesis that is particularly underdeveloped and requires collaboration as interdisciplinary research.

References: (1) Alzheimer's disease fact sheet. *NIH National Institute on Aging*. (2) Medications for memory, cognition, and dementia-related behaviors. *Alzheimer's Association*. (3) Bliss, T. V.; Tomo, V. *J. Physiol.* **1973**, 232, 331. (4) Whitlock, J. R. et al. *Science* **2006**, 313, 1093. (5) Zhang, Z. et al. *J. Org. Chem.* **2019**, 84, 11301. (6) Li, J.; Eastgate, M. D. *React. Chem. Eng.* **2019**, 4, 1595. (7) Maser, M. R. et al. *J. Chem. Inf. Model.* **2021**, 61, 156. (8) Ito, S. et al. *J. Org. Chem.* **1986**, 51, 1130. (9) Farney, E. P. et al. *J. Am. Chem. Soc.* **2018**, 140, 1267. (10) Wan, C. S. K. et al. *J. Org. Chem.* **1985**, 51, 3335. (11) Szostak, M. et al. *Chem. Rev.* **2014**, 114, 5959. (12) Edmonds, D. J. et al. *Chem. Rev.* **2004**, 104, 3371. (13) Mukaiyama, T. et al. *Chem. Lett.* **2000**, 29, 1250. (14) Klix, R. C.; Bach, R. D. *J. Org. Chem.* **1986**, 52, 580.

<u>Personal Overview:</u> *"Dear NASA",* I wrote in barely legible handwriting, shaky from excitement. "*I think I can help you solve your black hole problem."* I was five years old.
Unsurprisingly, my "solution"—whipped up in a frenzy of scrutinizing various age-appropriate scientific encyclopedias—did not survive a more thoughtful analysis, their reply congratulating my less-than-brilliant idea and reminding me to "study hard in school". Nevertheless, this letter pinpoints my humble beginnings, the start of my desire to engage with, participate in, and lead in scientific investigation.

While amusing in retrospect, my first-ever "proposal" underscores my passion for science and research, and hints at the mechanisms that continue to drive my endeavors today. Chief among them is a sense of duty and service: **I am driven toward a problem if I believe working on it will better the community**, whether that means enhancing the experiences of my peers or contributing to the scientific body of knowledge. In the same vein, **I associate curiosity with a call to action**: A curious inconsistency or interesting idea can equivalently be interpreted as an appeal for investigation, that interest alone is sufficient to warrant the required unrelenting efforts towards resolution. And finally, permeating these beliefs is **a *modus operandi* rooted in multidisciplinary thinking, sharing, and distribution**: the open exchange between disciplines provides new ways to look at old and new problems alike. I am convinced the solutions to our most vexing challenges will be pioneered by interdisciplinary thinkers that can integrate and leverage the tools and mindsets of many different disciplines across STEM.

These core values have influenced my research and extracurricular activities, and inspired me to pursue a professional career in research, starting with a PhD at Caltech (which I chose for its similar mission to "benefit society through research integrated with education"). **I am especially fascinated by the intersection of optimization and physics**, as it holds the potential for progression in what initially seem intractable systems to physics alone and permits investigation of fundamental insights while still yielding tangible impacts for industry or community. The path to my current interest is a deliberately diverse route through many disciplines allowing me to learn and apply skills from multiple fields. As a result of following this inspiration, my experiences are broad, but not lacking in depth, instead driving originality, and promoting self-autonomy where others require close supervision. My diverse background provides a unique perspective that can bridge the gaps between specialized communities, enabling effective communication between theorists, analysts, and directors alike. I thrive in this integration, and that is why I am pursuing this fellowship—**I intend to take the necessary steps to become a multi-faceted leader, communicator, and collaborator within my field**, and I know your program is aligned with my background and interests, forming the next leg on my journey to achieving my long-term goals.

<u>Intellectual Merit – Background and Experience:</u> When I started college at Princeton, the physics department was an obvious choice given my interests, but upon mentioning my desire to combine a theoretical basis with more applied/computational methods, my late adviser, Dr. Steven Gubser, suggested I attempt stochastics and optimization courses within the Operations Research department. I was struck by the subtleties relating data, random events, and the natural processes familiar from physics, and pivoted towards a captivating realm of problem-solving, combining physics theory with the insight of computational models and methods. Since then, I have pursued these interests in parallel. From iterative algorithms in quantum chemistry to machine learning in metamaterials, **I have gained experience from a myriad of physics and computational subfields, each project better preparing me for the next**:

The primary projects following this pivot were my first introduction to collaborative projects in a professional setting. My freshmen summer, I was selected for summer research in material properties at Catholic University of America (CUA). The program allowed students to shadow ongoing PhD projects and assist researchers to gain research experience, but when I saw most of the researchers lacked a computational background, I volunteered to self-study quantum chemistry and create computational simulations of the ongoing projects to provide CUA with theoretical benchmarks to compare with their experiments. As a result, **I accomplished the first-ever computational prediction of the Anomalous Hall Conductivity of Co_2TiGe**. Furthermore, I modified my code so the other researchers could continue to use my models for new materials after I left the internship, even if they were unfamiliar with coding and simulation. It was invigorating to take ownership in a project and go beyond the internship requirements to offer a larger contribution to the team. I learned the value of being proactive, as well as how to recognize and maximize different team members' strengths in a collaborative project.

These lessons proved useful the following summer when I worked as an Operations Research Intern for Applied Research Associates to help in the development of a virtual environment for analytics for the Department of Homeland Security (DHS). Instead of waiting for an assignment, I volunteered to help spearhead the machine learning section of the environment. Over the next 8 weeks, I wrote a machine learning toolkit to predict violative shipments before they entered the United States, **drastically reducing the existing analysis time from days to minutes**, and I also automated the process so others without my background could make use of my toolkit. I was asked to present the project to DHS leadership, and, recalling what I learned the previous summer, I also modularized the toolkit for general application of supervised learning for DHS analysts, enabling a powerful tool for those not familiar with the complexities of machine learning. Our work **received recognition and accolades from the DHS Science and Technology Directorate**. It was energizing to create a tangible product that had impact for such a large organization, and it piqued my interest in government-oriented applications of STEM.

My junior year, I independently arranged study with the MITRE Corporation under Dr. Stephen Pappas to characterize the risks of "unhackable" quantum cryptographic systems implementing realistic electronics. Existing thought experiments suggested photon detectors in BB84/B92 protocols create "backflash" photons correlated to transmitted information, measurable by eavesdroppers without detection. I analyzed a real B92 setup and provided an inaugural quantification of this vulnerability, which reduced an intruder's detection chances by 2.5x and increased information interception by up to 31%, **a result which contradicted the random guessing proposed by established theories and resulted in my conferral of the Allen G. Shenstone Prize in Physics** by Princeton. From this revelation I learned the direct impacts theory and application can have on industry and society; an inspiration to adapt my research skills towards impacts in our experiences and challenges.

That summer, I was selected among dozens of Princeton students for research abroad on galactic evolution at Oxford University under Dr. Ralph Schönrich, to determine a stellar population synthesis method matching analytical isochrone models to the GAIA mission's data from the local Milky Way via Poisson statistics. The expansive search space was high-dimensional with many local minima, a challenge in many numerical physics problems. I contributed by recasting the fit as an optimization problem, introducing the team to meta-heuristics like simulated annealing (an adaptation of Markov Chain Monte Carlo modeling based upon cooling thermodynamic systems), coalescing and applying seemingly unrelated fields towards an overarching goal. **My method processed the largest available stellar data set faster and more accurately than the existing model**, and I again modularized it for the team to use in future research. I enjoyed the challenge of synthesizing the methodologies of physics and operations research in fields previously unfamiliar to me, and it furthermore reinforced my belief in the utility and merit of sharing techniques and capabilities, even internationally as well as at home.

By this point my interest in applying optimization methods in physics was set, so I chose to continue this trajectory for my senior thesis in quantum computing under Dr. Andrew Houck. A large issue faced by quantum computers is *decoherence*, the disassociation of properties of "qubits" that gives them their computational power. Even ideal theoretical qubits will decohere, but physical realizations of quantum computational architectures introduce mechanical imperfections and thermal noise which amplify this effect and cause applied operations (known as "gates") to have unintended effects. This throttles success in qubit gate creation to mostly single-qubit gates. Instead of the established paths of cryogenically limiting background noise and applying ideal gates to qubits, I implemented a black-box optimization approach to adjust ideal gates to *counter* inherent environmental noise and create generalizable "noise-cancelling headphones" for quantum computers that enabled investigation of multi-qubit gates. **I showed a 30% improvement in two-qubit gate fidelity was possible under my proposed alternative technique**. It was exciting to discover an alternative to established norms via out-of-the box thinking, for which I was **recognized via a second Allen G. Shenstone Prize** in Physics by Princeton.

Currently, I have been working in computational materials sciences in Caltech's PhD program. Under the guidance of Dr. Chiara Daraio, I am using generative adversarial networks (two competing neural networks) to generate novel, disordered material structures that would not be generalizable by humans alone, to create an efficient way to indirectly map how mechanical properties are impacted by the hierarchical form and structure of materials, even when not in a periodic or simplified unit-cell structure. This offers an intriguing new perspective from which to examine mechanical metamaterials, and can also be easily adapted to *optical* metamaterials, which drives my accompanying proposal in this application to combine my experience and the computational tools from this work with the optical expertise and photonic research of Dr. Andrei Faraon (also at Caltech). I am excited to learn and contribute to my interests—this connection between theory, experiment, and application through applied mathematics and computation offers much to society's goals, and I am driven to execute and promote this system.

Broader Impacts – Outreach and Career Goals: My contributions through my diverse research accomplishments confirm my desire and preparation for a well-rounded career in professional research, and my choices within them reflect my belief in the sharing, dissemination, and enabling wider application of my efforts. However, modularizing my projects and generating accessibility represents only half of my outreach—**not only should scientists have the responsibility to make their field more accessible, but they should also *actively* communicate their endeavors to a broader and general (even non-scientific) field**. This creed has inspired most of my extracurricular activities and offered fulfilling chances to take ownership and leadership in community outreach.

My sophomore and junior years, I was selected to be the Logistics Officer of Princeton's STEM outreach organization IgniteSTEM, which organizes national conferences to empower educators and provide cutting edge ideas to enhance STEM education with technology, design-thinking, and project-based learning like hackathons and maker-fairs. My STEM experiences have shown me the power of a hands-on and integrative curriculum and **I strive to help pass on the engagement and empowerment of these experiences to communities, educators, and students who have not yet had the opportunity**. As the Logistics Officer, I negotiated venue contracts and managed the conference logistics and other club members, successfully partnering with industry leaders like Google Education, Major League Hacking, and She++ for outreach to over 200 CEOs, principals, and educators through the annual flagship conference. The following year, I was recruited to be the Chapter President of the Ivy Space Coalition due to my IgniteSTEM success and used the same principles to organize space science conferences and networking opportunities in the space sector throughout the northeast. I have always cherished these memories and plan to pursue similar opportunities to train the next generation of STEM advocates and leaders both as a graduate student and a potential NSF Fellow.

However, on top of organization and presentation **I believe we also hold a responsibility to directly teach and mentor those in our community**, not only for the diffusion of skills and ideas, but to **immerse ourselves in the diverse range of experiences and build an empathy and understanding that surpasses cultural, political, and socio-economic divides**. It is because of this attitude that I was selected to become a Residential Adviser at Princeton and guide over 50 students from all over the world through their academic and social development and mediate interpersonal conflict, as well as tutor these students with different backgrounds and viewpoints. This has been one of my favorite and most fulfilling experiences in outreach and service to date, and has inspired me to continue teaching others.

Even today I continue to tutor, mentor and advise my Princeton advisees through their upperclassmen years, and currently at Caltech I have likewise pursued this objective by volunteering to be a Teaching Assistant, organizing meetings with students to help them grow their skills and teach them different approaches to problem-solving. Moving forward, I also aim to get involved in further outreach and education programs for the underrepresented communities in Pasadena, creating experiments to engage students seeking enrichment in STEM that would not have this opportunity otherwise.

My intersection of experiences in intellectual inquiry and community outreach makes me uniquely qualified not only for this NSF GRFP opportunity, but for a lifelong career as a professor and/or researcher in a government lab, in order to pursue my passions and leave a tangible impact in my community. Your fellowship will support me through this PhD, enable further empowerment and engagement in STEM mentorship, and catalyze my journey in these ambitions for many years to come.

Graduate Research Plan Statement: "AI Designers" of Photonic Metamaterials

Background/Motivation: The advent of contemporary nanofabrication methods in the mid-2010s has spurred a renaissance of "metamaterials", referring to devices and elements engineered from the ground-up for a desirable set of properties, i.e. "designer" materials whose structural form is driven by their preferred function [1]. Due to the power of modern computation, designs have evolved from simpler heuristic-based geometries to complex optimization-based geometries that can encode multiple functions into a single volume [2]. Optimizable metamaterial geometry is an exciting subfield with myriad applications that hold the potential to revolutionize medicine, defense, and scientific instrumentation at large [3], which begs the question of what will define the next advancement of present capabilities.

Most state-of-the-art *photonic* metamaterials (functions related to interactions with light) methods are limited to 3D *voxel-based topology optimization*, a direct gradient-based method for iteratively choosing the refractive index at every sublocation (voxel) in the output volume [1-3]. Most current photonics research and results employing these voxel-based methods share a common set of features, namely:

- *Binary*: The studies use a single material to design the structure (each voxel is material or free space), which requires additional continuity constraints in the optimization (no free-floating material).
- *Complexity*: The optimized structures are often complex; disordered or even "organic" in appearance. This in itself is not bad (restricting to *only* periodic options neglects many higher-performing geometries), but very irregular designs can create additional difficulty and bottlenecks in device fabrication, which already requires sub-wavelength resolution and accuracy in printing.
- *Scaling*: The number of optimizable parameters grows with both total design size and design resolution (the number of voxels). This is tractable for designs on the order of a few hundred wavelengths (miniaturized sensors, etc.), but is intractable for large systems (centimeters-scale, like LIDAR-blocking tiles for military aircraft, etc.) that are not microscopically periodic (reduced complexity).

These models offer advantages in functionality through their complexity capabilities, but also shun the full potential of an unconstrained parameter space with multiple material types, do not offer the same capabilities at large scale, and are sensitive to starting conditions. Furthermore, the current complexity precludes further analytical or human learning of how particular structures influence photonic properties.

We could benefit from complementary methods of generation/analysis that preserve complexity, permit further investigation/utilization of complex structures, and are scalable to a wider array of applications with less constraints. Can we extend and employ current results to a robust, widespread, and scalable architecture for photonic metamaterial generation?

<u>Artificial Intelligence (AI) offers many different resolutions to this question, forming the basis of this proposal and offering an exciting chance to employ successful tools from several disciplines.</u>

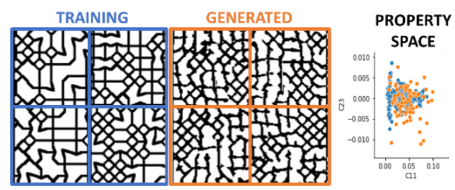
For example, Generative Adversarial Networks (GANs) were invented in 2014 and consist of two competing neural networks that learn and generate samples from a *probabilistic distribution* over supplied training data [4]. They have outpaced other models in creating realistic pictures and paintings that can fool humans, and even have "creative capabilities"; generating novel samples that humans cannot, samples that match the data distribution but are ambiguous with respect to predefined types of training data [5]. GANs have also shown success for complex regular and irregular texture generation/analysis for computer graphics and fashion research [6], suggesting their capabilities in geometry generation for metamaterials are already robust. GANs could thus generate (even "creatively") complex structures that humans could not for photonic metamaterials, and the resulting distribution could offer an investigative means to furthermore *relate* and analyze structures against their resulting properties. Additionally, biomechanics research has found recent success in generating voxel-based robotic geometries via Compositional Pattern Producing Networks (CPPNs), whose network structures are iteratively tuned via genetic algorithms (CPPN-NEAT) [7]. These networks smoothly "pattern" the output space as the output of composed functions. This approach dramatically reduces the dimensionality of the system to *only* the parameters of the network and results in infinite scalability, as voxels are decided by discretizing the functional output of the network at any desirable resolution. CPPNs can handle multiple material types and result in arbitrarily complex but regular patterns that can be optimized for multifunctional purposes [8]. The features of this model thus suggest a scalable, non-binary architecture by which to generate metamaterial structures that preserve output complexity, but in a more-regular manner that is more conducive to fabrication under modern printing and lithography capabilities. Furthermore, the intermediate models during the training of CPPNs also offer viable structures to analyze, compared to direct-optimization approaches where intermediate forms are often unrealistic or limited in function.

Aims/Methods/Measures: The goal of this proposal is to create "AI Designers" of photonic metamaterials—efficient tools to expand functionalities and augment current approaches in generating novel optimal structures, as well as investigate relationships between structures and overall function. Creating/analyzing the models as well as testing/measuring designs scale well to a three-year timeline:

-Aim 1: GAN for Data-Driven design/investigation (1 yr): Existing optimized structures from research offer training data for a GAN to learn the distribution of structures for a given photonic functionality, and generate novel ("creative", matching the distribution but remaining sufficiently different from human-generated and optimized designs) geometries from this distribution. Sampling from distributions is low-cost and provides a first-time statistical inference of relating complex geometrical forms to photonic function by comparing functionality distributions and their frequencies of different hierarchical structures. Samples can also be assessed and fabricated as a direct measure of GANs against current approaches.

-Aim 2: CPPN-NEAT for optimal design/fabrication (2 yr): Additional structures can be designed ground-up by CPPNs that are evolved to maximize the target function of a given photonic property (target spectrum, etc.), with the expanded capabilities of handling multiple material types and scaling to arbitrary structural sizes with significantly smaller dimensionality, as well as preserving complexity but in a manner more conducive to fabrication. Network dimensionality and training time can be benchmarked against current optimization techniques, as well as ease-of-fabrication and resulting performance of the subsequent geometries. These designs and their intermediate forms can also be fed back to the GAN as additional training data, to deliver further learning on how structural form influences photonic properties.

Feasibility/Resources: The success of GANs and CPPNs in their respective fields already offers promise to their extension into geometry creation for metamaterials, but even more so stems from the present research of the author which offers promising results for the capability of GANs to learn, generate, and interpret 2D metastructures relative to their *mechanical* properties, since swapping from mechanical to optical evaluation merely requires changing the post-processing, independent from the GAN. The author is well-versed in optimization and GANs, and the models to evaluate properties as well as the evaluation and fabrication hardware are either already used by the author or already exist at the author's institution under the sponsorship of the author's advisers, offering an investigation with ample experience, little overhead, and large ramifications.



GAN creates new 2D metastructures

Intellectual Merit: This project serves to advance both in-field and cross-field knowledge through the extension of known techniques from non-photonic disciplines in a previously unused way to photonic metamaterials. Furthermore, it offers an avenue to link structural forms to optical properties where current learning is precluded, and insights could be passed back to the fields inspiring this hybrid approach.

Broader Impacts: The ramifications for successful scalable photonic metamaterials are staggering, from sensitive single-substance sensors in chemistry, to miniaturized sensors and disease detectors in wearable medicine, more efficient solar cells, more passive and robust space instrumentation, and a revolution in defense capabilities. With these wide-spread applications in reach, I would also expect a long-term increase interest in the fields of metamaterials and optimization among a new generation of scientists. Near-term, I would distribute my work open-source and modularize the network creation tool to create an amateur-friendly and widely applicable tool in AI-generated/analyzed geometries utilizable for knowledge creation in fields even beyond metamaterials, such as computer graphics or robotics.

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