SLATT UNDERGRADUATE RESEARCH FELLOWSHIP
FINAL REPORT

SCHOLAR NAME:	Andrew Scott Manning
FACULTY ADVISOR:	Jennifer Schaefer, Jonathan Whitmer
PROJECT PERIOD:	December 2020 – Present
PROJECT TITLE:	Using Molecular Simulations to Characterize Phase Behavior of Liquid Electrolyte Systems
CONNECTION TO ONE OR MORE ENERGY-RELATED RESEARCH AREAS (CHECK ALL THAT APPLY):	**( ) Energy Conversion and Efficiency** **( ) Sustainable and Secure Nuclear** **(X) Smart Storage and Distribution** **( ) Transformation Solar** **( ) Sustainable Bio/Fossil Fuels** **( ) Transformative Wind**

MAJOR GOALS AND ACCOMPLISHMENTS

Summarize your research goals and provide a brief statement of your accomplishments (no more than 1-2 sentences). Indicate whether you were able to accomplish your goals by estimating the percentage completed for each one. Use the next page for your written report.

RESEARCH GOALS	ACTUAL PERFORMANCE AND ACCOMPLISHMENTS	% OF GOAL COMPLETED
Learn to Conduct Molecular Simulations	I had to learn the foundations of molecular simulations to begin the research project. I have learned how to use Linux, build basic molecular simulations, run molecular simulations (energy minimization runs, standard production runs, and temperature ramp runs), and analyze and display data using Python. I now plan to understand the mechanics of building force field and of developing parameters for molecules so that I can eventually design molecular simulations from scratch.	60%
Analyze Liquid Crystalline Electrolytes using Molecular Simulations	The stated purpose of this research project was to analyze the phase and ion transport behavior of liquid crystalline electrolytes that Professor Schaefer uses in her research on new battery technologies. These liquid electrolytes contain complex molecular structures, however, so Professor Whitmer and I agreed that I should learn how to run molecular simulations on simpler systems first so that I understand the theory and mechanics of molecular simulations. I have conducted runs on simple Argon systems, and I have worked on simulating more complex systems like OMIM-BF4. I am now ready to begin modeling the liquid electrolyte systems that Professor Schaefer works with. This project is ongoing, and I plan to continue with this research in the future.	30%

RESEARCH OUTPUT

Please provide any output that may have resulted from your research project. You may leave any and all categories blank or check with your faculty advisor if you are unsure how to respond.

CATEGORY	INFORMATION
EXTERNAL PROPOSALS SUBMITTED	(Sponsor, Project Title, PIs, Submission Date, Proposal Amount)
EXTERNAL AWARDS RECEIVED	(Sponsor, Project Title, PIs, Award Date, Award Amount)
JOURNAL ARTICLES IN PROCESS OR PUBLISHED	(Journal Name, Title, Authors, Submission Date, Publication Date, Volume #, Page #s)
BOOKS AND CHAPTERS RELATED TO YOUR RESEARCH	(Book Title, Chapter Title, Authors, Submission Date, Publication Date, Volume #, Page #s)
PUBLIC PRESENTATIONS YOU MADE ABOUT YOUR RESEARCH	(Event, Presentation Title, Presentation Date, Location)
AWARDS OR RECOGNITIONS YOU RECEIVED FOR YOUR RESEARCH PROJECT	(Purpose, Title, Date Received)
INTERNAL COLLABORATIONS FOSTERED	(Name, Organization, Purpose of Affiliation, and Frequency of Interactions) Work with Professor Whitmer to develop the skills necessary to assist Professor Schaefer.

EXTERNAL COLLABORATIONS FOSTERED	(Name, Organization, Purpose of Affiliation, and Frequency of Interactions)
WEBSITE(S) FEATURING RESEARCH PROJECT	(URL)
OTHER PRODUCTS AND SERVICES (e.g., media reports, databases, software, models, curricula, instruments, education programs, outreach for ND Energy and other groups)	(Please describe each item in detail)

RESEARCH EXPERIENCE

Please let us know what you thought of your research experience: Did this experience meet your expectations? Were lab personnel helpful and responsive to your needs? What else could have been done to improve your experience or achieve additional results?

I had an excellent if unexpected research experience through the Slatt Undergraduate Research Fellowship. My original research project to work with Professor Schaefer in the lab did not materialize because of COVID-19. Instead, I began working with Professor Whitmer on a different project in December 2020. Professor Whitmer, Professor Schaefer, and I agreed that I would learn about molecular simulations to remotely evaluate the behavior of molecules that Professor Scheafer works with in lab. Over the course of the two-month research project I have learned a lot about computers, programming, and molecular simulations. The project, though unexpected, has been incredibly rewarding because I have had the opportunity to learn about an entirely new field within engineering. I am incredibly excited to continue conducting research with molecular simulations.

FINAL WRITTEN REPORT

(Please use the space below to describe your research project and objectives, any findings and results you can share, and graphs, charts, and other visuals to help us understand what you achieved as a result of this research experience.)

I used my Slatt Undergraduate Research Fellowship to conduct molecular simulation research with Professor Jonathan Whitmer in the chemical and biomolecular engineering department. As I finish up my fellowship, I am prepared to continue with research and to produce useable results over the next year. I do not currently have results or findings to share, but I made good use of my research fellowship by developing the technical foundation and theoretical understanding of molecular simulations that I will need to simulate more complex molecules that are of particular importance to energy storage technological development.

For my original research project, I intended to conduct lab work in Professor Jennifer Schaefer's lab group to assist in their efforts to create alternative materials for next generation energy storage devices. In this project, I intended to focus on developing polymer layers that separate the anode and cathode in batteries to limit destructive ion transfer, facilitate beneficial ion transfer, and maximize battery conductivity. To achieve these improvements to battery technologies, researchers must continue to study the transport of ions in polymer layers. This inquiry leads to considerations of polymer matrix composition, and my intended project focused on engineering porous polymers that regulated ion transport.

I intended to begin this research with Professor Jennifer Schaefer in Summer 2020 by working 40 hours each weak for ten to twelve weeks. Unfortunately, with the COVID-19 situation I had to reschedule the research for Fall 2020.

I intended to return to in-person classes for the Fall semester, but with the spike of cases on campus I received an accommodation to work remotely from home for the remainder of the semester. Without access to the on-campus lab, I again postponed the start of my research project.

I finally began conducting research in late November and early December of 2020 when I worked with Professor Schaefer and with Professor Whitmer to create a remote research project for the Winter Session. Professor Schaefer needed the materials used in battery technologies to be better understood so that the materials could be adjusted for optimal battery performance. Schaefer's lab group works with liquid crystal electrolytes which are ionic solutions that fill the space between the anode and cathode of the battery. With these electrolytes the Schaefer group hopes to improve ion transport and conductivity in batteries. The liquid crystal electrolytes are difficult to work with, however, because they are composed of complex ionic species that form a variety of phases depending on the conditions of the system. To add even more complexity to the problem, previous research efforts confirm that different phases for these electrolytes impact the degree of ion mobility. For effective and optimized energy storage development, it is imperative that researchers learn more about the different phases and the phase behaviors that liquid crystal electrolytes experience.

Molecular simulations are a promising technology that allows researchers to understand the behavior of complex, bulk systems like liquid crystal electrolytes. Molecular simulations involve the application of a set of molecular parameters and forces (in a "force field") to a set of hundreds of ions. A computer runs through millions of calculations using the force field to calculate the

interaction between molecules in the system. In a well-described system, a molecular simulation offers a plausible progression of molecular interactions. By subjecting the system to various inputs, including temperature, pressure, and the presence of a solvent, researchers can better understand the phase behavior and transport phenomena in complex systems.

Professor Shaefer, Professor Whitmer, and I agreed that I would conduct a remote research project using molecular simulations to simulate complex liquid electrolyte systems. Over the winter session, Professor Whitmer became the primary advisor for the project because he uses molecular simulations in his research efforts. Molecular simulations are complex and require an understanding of computing, computer programming, and molecular theory. By meeting with Professor Whitmer once a week and by setting learning goals every week, I progressed in my understanding of and in my ability to conduct molecular simulations. In the course of two months, I have learned how to navigate a remote desktop using Linux, operate Bash scripting, develop simulation input files, run simulations, conduct energy and temperature analyses on the data, and manipulate the data using Python. Through my efforts I have developed a solid foundation to begin working on more complex molecular simulations.

Given my progress I will begin simulating the liquid crystal electrolyte systems that Professor Scheafer uses in the next few months. The liquid crystal electrolytes may require additional parametrization to fully capture the electric interactions of the atoms in each molecule, so the project will give me the opportunity to explore molecular simulation forcefields and parameter files in more depth.

The Slatt Undergraduate Research Fellowship has provided me with the opportunity to explore the rapidly developing and promising world of molecular simulations. Given COVID-19 challenges, I only started my research project in December 2020, and the remote project was very different from what I anticipated. But I now intend to continue the research with molecular simulations. Now that I have a solid foundation in molecular simulation work, I am prepared to begin running simulations and generating data for the liquid electrolyte systems that Professor Schaefer uses in her next generation battery research.