SLATT UNDERGRADUATE RESEARCH FELLOWSHIP
FINAL REPORT

SCHOLAR NAME:	Chloe Behringer
FACULTY ADVISOR:	Jonathan Whitmer
PROJECT PERIOD:	Fall Semester 2023
PROJECT TITLE:	Coarse-Grained Modeling of Ionic Liquid Crystals: Understanding Phase Transitions and Ionic Conductivity
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
We hypothesized the ionic liquid crystals can be leveraged in energy storage devices due to its high energy density and ionic conductivity. As a result, our primary research goal was to understand the phase behavior and ionic conductivity of Ionic Liquid Crystals (ILCs) through coarse-grain molecular simulations with varying concentrations of solvent and under various pressures and temperatures.	In our simulations, we uncovered a great deal of valuable information about Ionic Liquid Crystals; we can describe its phase behavior with varying solvent concentrations by closely investigating results of the radial distribution analyses. Furthermore, we calculated ion mobility by finding the mean square displacement (MSD) of the molecule, finding the diffusion constant, and relating it to ionic conductivity; this allowed us to observe that the liquid-like phase of the ILC has the best ion mobility, followed by the smectic and crystalline phases.	85%

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	
EXTERNAL AWARDS RECEIVED	
JOURNAL ARTICLES IN PROCESS OR PUBLISHED	A journal article for this research is in progress. We plan to submit it to the scientific journal, *Physical Review Letters.*
BOOKS AND CHAPTERS RELATED TO YOUR RESEARCH	
PUBLIC PRESENTATIONS YOU MADE ABOUT YOUR RESEARCH	
AWARDS OR RECOGNITIONS YOU RECEIVED FOR YOUR RESEARCH PROJECT	
INTERNAL COLLABORATIONS FOSTERED	
EXTERNAL COLLABORATIONS FOSTERED	
WEBSITE(S) FEATURING RESEARCH PROJECT	
OTHER PRODUCTS AND SERVICES (e.g., media reports, databases, software, models, curricula, instruments, education programs, outreach for ND Energy and other groups)	

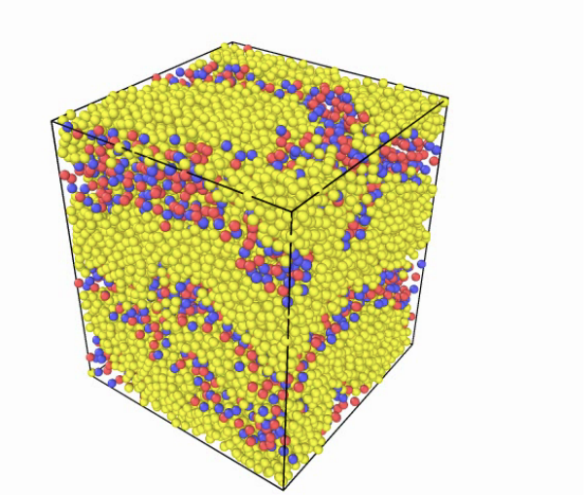
RESEARCH EXPERIENCE
Please let us know what you thought of your research experience: Did this experience meet your expectations? Were lab personnel helpful and responsive to your needs? What else could have been done to improve your experience or achieve additional results?
This experience certainly met my expectations; this was my second semester working with Dr. Whitmer on ILCs, so I had familiarity with the topic and molecular simulations as a whole and was able to jump directly in with the graduate student I had been working with. All lab personnel were very helpful, and I very much enjoyed my time with the Whitmer lab.

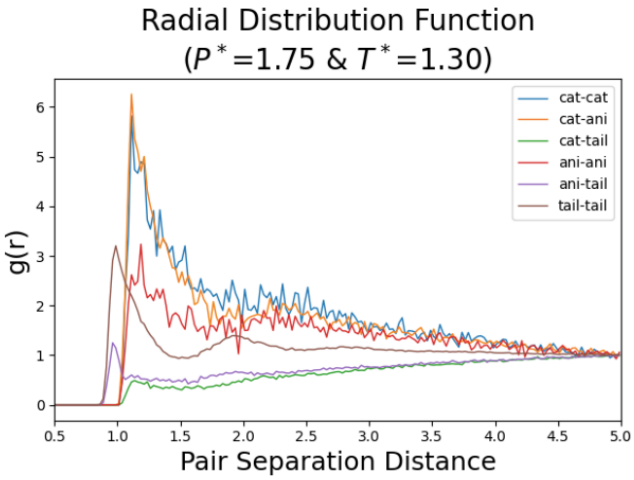
FINAL WRITTEN REPORT

(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.)

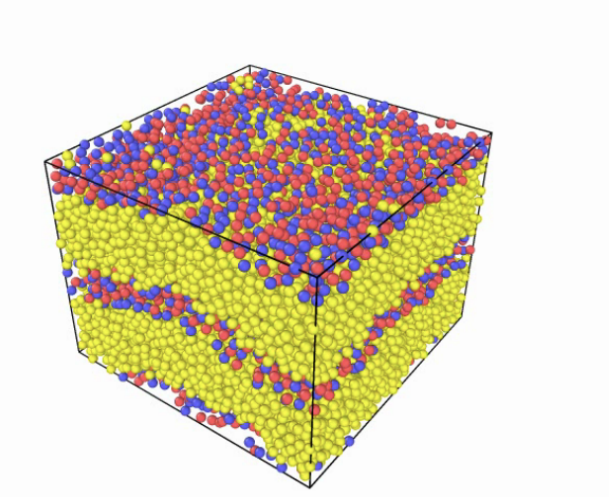
This project seeks to understand the behavior of Ionic Liquid Crystals (ILCs) under varying pressures, temperatures, and concentrations of solvent. ILCs are hypothesized to be a potential technology for energy storage applications due to its high energy density and ionic conductivity. Furthermore, ILCs are customizable by modifying its cations and anions, controlling its thermal stability, mesophase behavior, conductivity, and other notable properties. As a result, this research project included building out a molecular simulation model that allows for flexibility in the molecular structure to optimize the performance of the ILCs. Furthermore, it has been observed in physical lab research that the inclusion of a solvent such as ethylene carbonate increases ion mobility in ILCs; as a result, the computational model of ILCs is also observed under varying degrees of solvent to quantify conductivity.

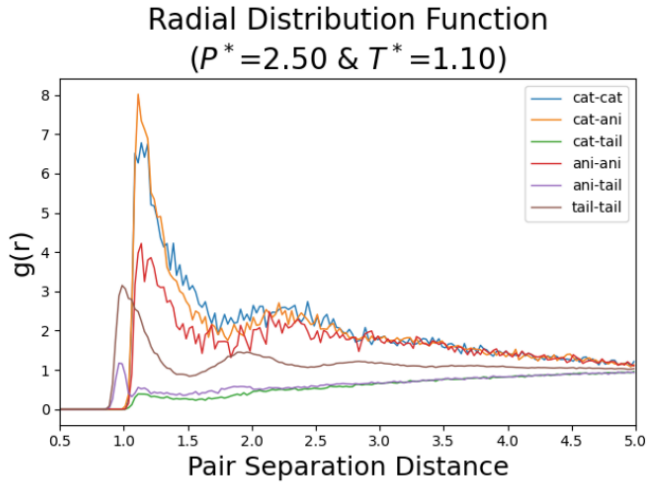
This research implements a coarse-grained model, utilizing the unitless quantities of mass, σ, ϵ, and the Boltzmann constant k_B, set to be 1. After equilibrating and initializing the crystalline structure to be in a bi-layer formation, we investigate phase behavior using both a visual analysis using Visual Molecular Dynamics (VMD) and radial distribution analysis. The system without solvent forms three distinct mesophases that are dependent on both pressure and temperature; Figure 1 below demonstrates these results with both the VMD and radial distribution results. When we add solvent to the system, we observe the modified phase behavior within the ILC structure; these results are visible in Figure 2. These results indicates that solvent contributes to stabilizing the smectic phase, but the crystalline region is generally unaffected by the solvent.



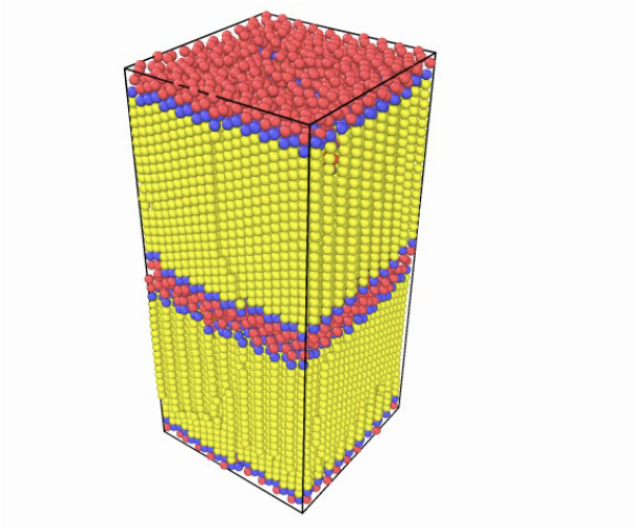


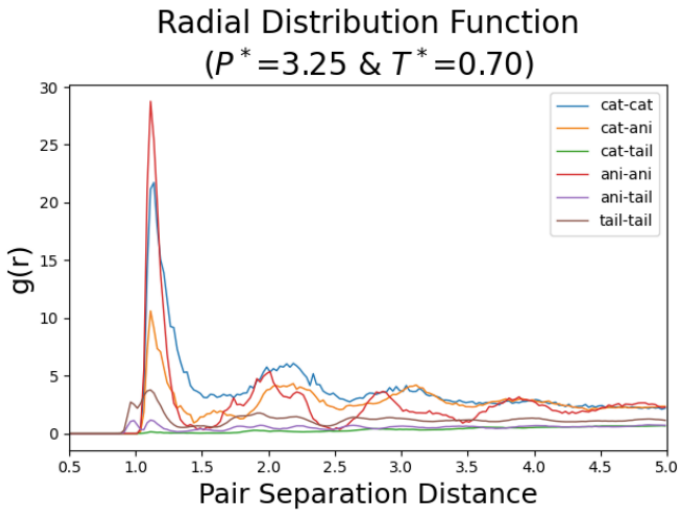
a) Liquid-like Mesophase





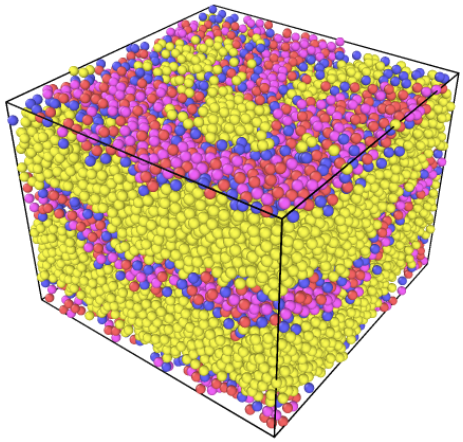
b) Smectic Mesophase

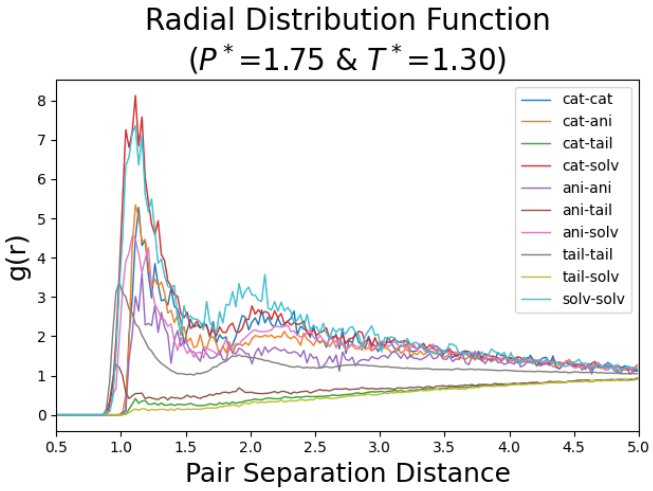




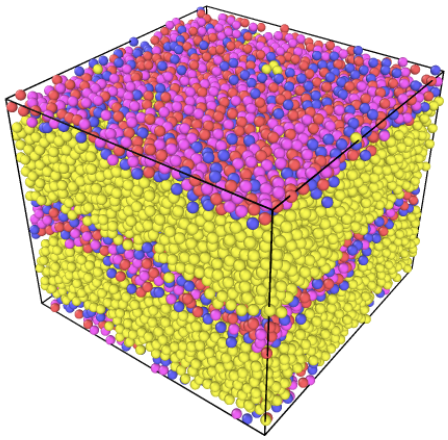
c) Crystalline Mesophase

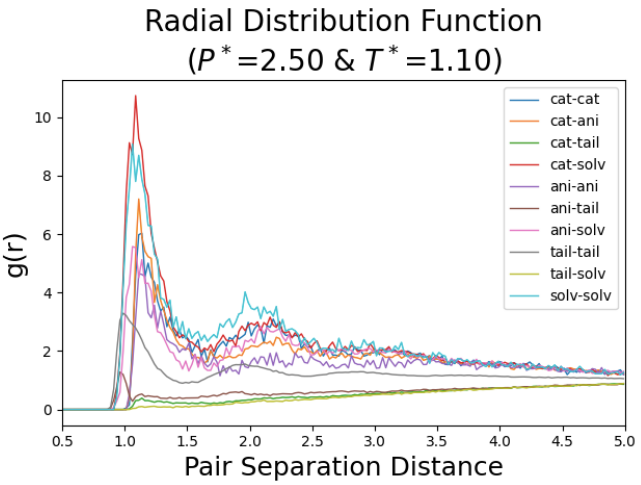
Figure 1 (a, b, and c): The VMD and Radial Distribution Function results of the system under three different temperature and pressure conditions without solvent.



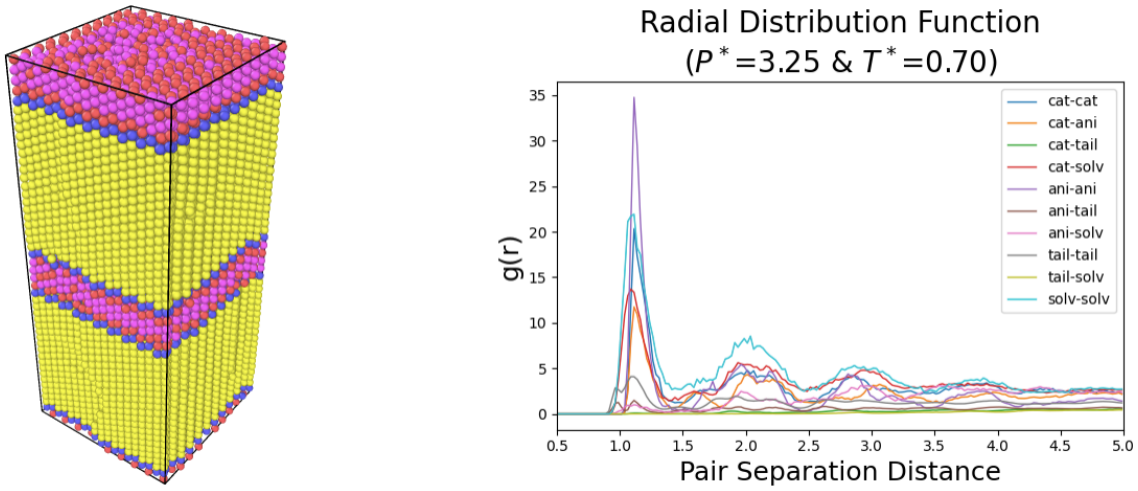


a) Smectic Mesophase





b) Smectic Mesophase



c) Crystalline Mesophase

Figure 2 (a, b, and c): The VMD and Radial Distribution Function results of the system under three different temperature and pressure conditions with solvent.

This system also reveals important information on the cation mobility of ILCs. By using an isothermal (NVT) production run, we can calculate the mean squared displacement (MSD) of all molecules. The MSD can be directly related to the diffusion coefficient, which then relates to ionic conductivity through the Nernst Einstein equation,

$$\sigma = \frac{N|q|^2 D}{V k_B T}, \qquad (1)$$

where σ is the ionic conductivity, N is the number of molecules, q is the absolute charge, D is the diffusion coefficient, V is the volume of the system, k_B is the Boltzmann constant, and T is the temperature. This analysis leads to a direct quantification of the mobility. To wholly understand the effect of solvent, the simulation was run under a control condition and under varying degrees of solvent layering. This result is visible in Figure 3 below.

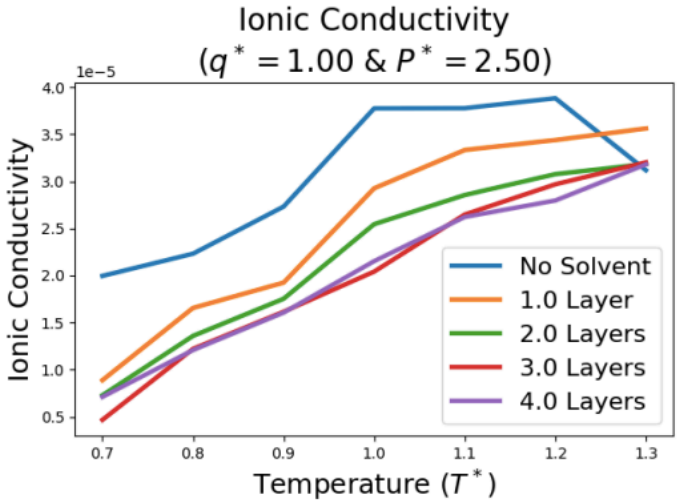


Figure 3: The ionic conductivity of the system with varying amounts of solvent added to the system.

These results indicate that cation mobility is inversely related to the addition of solvent, which is contrary to experimental evidence. This leaves room for further investigation and perfecting of the system modeling the ILCs. We hypothesize moving forward that an increased charge in the ILCs will more accurately reflect the experimental condition and result in stronger coulombic attractive forces between cations and anions. This leaves a great deal of room for further investigation and understanding of this model and of ILCs.

This research makes me extremely optimistic about the future of energy storage devices; although understanding ILCs in energy storage applications is still in its infancy, this research has indicated that there is great promise for its growth in industry.