SLATT UNDERGRADUATE RESEARCH FELLOWSHIP
FINAL REPORT

SCHOLAR NAME:	Daniel Palmer
FACULTY ADVISOR:	Dr. Jonathan Whitmer
PROJECT PERIOD:	5-20-2019 : 5:20:2021
PROJECT TITLE:	Discovering Properties of Ionic Liquid Crystals
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 (x) 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
Write Academic Journal Article	We have not written an article yet but will likely do so by the end of the year	80%
Attend and present at a professional Conference (Midwest Thermodynamic and Statistical Mechanics Conference)	This opportunity was unfortunately canceled due to Covid-19. We are looking for another conference to attend virtually hopefully.	n/a

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)
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 have been extremely happy and grateful for this research experience. I have learned so much under Dr. Whitmer and this research has been the most important thing I have done in my time as an undergraduate. Before starting this research, I did not think I wanted to go to graduate school. Now, I am applying to PhD programs in physics and materials science, and I cannot wait to pursue a career in research.

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.)

Comparing 4.4,20,1,1 system to Bates and Luckhurst

The gayberne potential is a common potential to describe liquid crystals in molecular dynamic simulations. Four numbers are needed to describe this potential, one for each possible orientation two elliptical molecules can interact. Bates and Luckhurst found that 4.4, 20, 1, 1 was a good approximation for realistic systems [1]. To match Bates and Luckhurst's results, the system must be found to be in equilibrium. Simulations were run in Lammps with 3375 molecules with a timestep of .0025. The simulation starts at a very low density and is very slowly compressed to a number density of .1756 over 500,000 timesteps using a fix deform and a fix nvt/ashpere. This initial step was done to randomize orientation at the given temperature, and to allow the liquid crystals to begin to align. Once the system is at the right density, the system is switched to a fix npt/asphere with a pressure of 2.0 and run for 1,000,000 timesteps to equilibrate.

Since the order parameter approaches a singular value and the fluctuations are decreasing, the system can be considered to be in equilibrium. Now that there is a simulation that can reach equilibrium for any given temperature, multiple simulations can be run for multiple temperatures. The order parameter can then be plotted vs. temperature which is shown in **figure 2.**

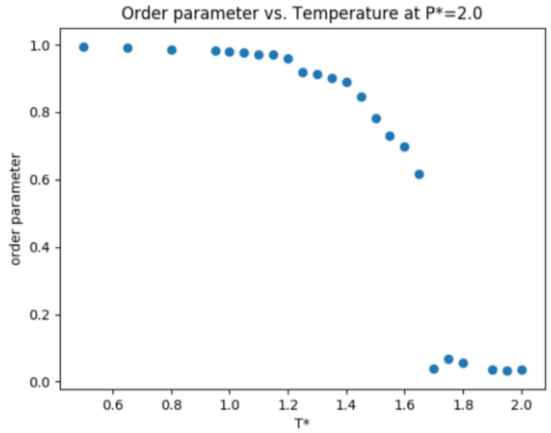


Figure 2. order parameter vs. temperature

In order to tell if the system is in the same state that Bates and Luckhurst found, Enthalpy of the molecular dynamics simulation and the monte carlo simulations run by Bates and Luckhurst were compared. These two results are shown in **figure 3.**

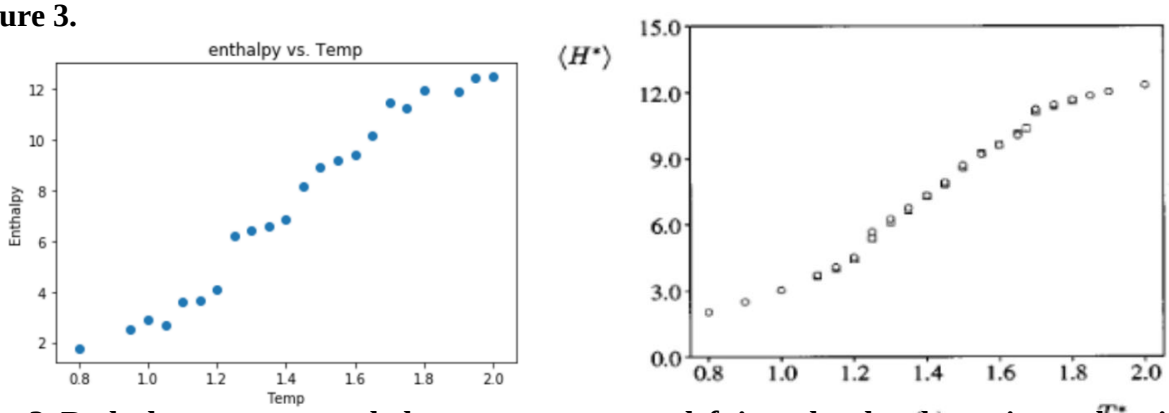


Figure 3. Both show average enthalpy vs. temperature, left is molecular dynamic results, right is Bates and Luckhurst monte carlo results.

Here the transition temperatures occur at all of the same temperatures, about 1.2 and 1.7, and the graphs seem to match well. It is important to note that in order to account for all degrees of freedom of the ellipsoid, a fix_modify must be used with a compute keyword in Lammps.

Matching Saielli

In Tommaso Margola, Katsuhiko Satoh, and Giacomo Saielli's paper "Comparison of the Mesomorphic Behaviour of 1:1 and1:2 Mixtures of Charged Gay-Berne GB(4.4,20.0,1,1) and Lennard-Jones Particles" they look at how charged ions affects the 4.4, 20, 1, 1 system [2]. The first step was to replicate the system with a 1:1 stoichiometry of Lennard

Jones ions to Liquid Crystals. A fix_nvt/asphere and fix_deform were used to initialize the system and get it to the right density over 700,000 timesteps with a timestep of .0025. Next, a fix nvt/asphere was run for 1,800,000 timesteps to equilibrate the system. To see if the correct systems were created, the order parameter vs. temperature was compared which is shown in **figure 4.**

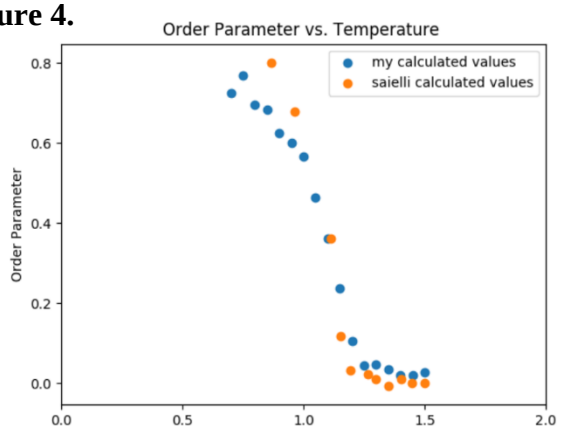
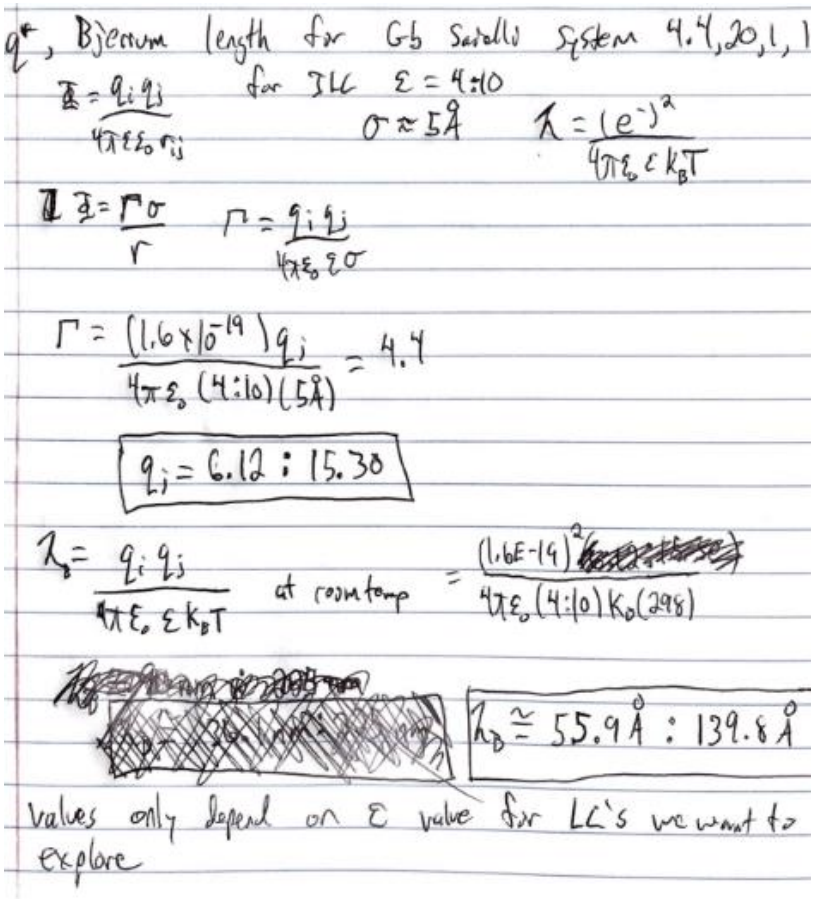


Figure 4. Order Parameter vs. temperature, comparing my data to Saielli's data for 2467 neutral Lennard Jones molecules and 2467 Liquid Cyrstals at a density of .261

Here the transition occurs at a similar point for both sets of data, and the values match somewhat well.

In order to relate this system with charge to a realistic system such as p-terphenyl, the reduced charge and Bjerrum length were calculated and shown below. A realistic dielectric constant for an Ionic Liquid crystal is from 4-10 and a contact parameter, σ, of about 5 angstrom.



Now several similar simulations were run at different temperatures with the charge of the liquid crystal at 6.12, the Lennard Jones ions at -1 and a dielectric constant of 4. Order Parameter vs. temperature is shown in **figure 5** however there are still bugs in the simulation script that need to be sorted out as to why there is no ordering at any temperature.

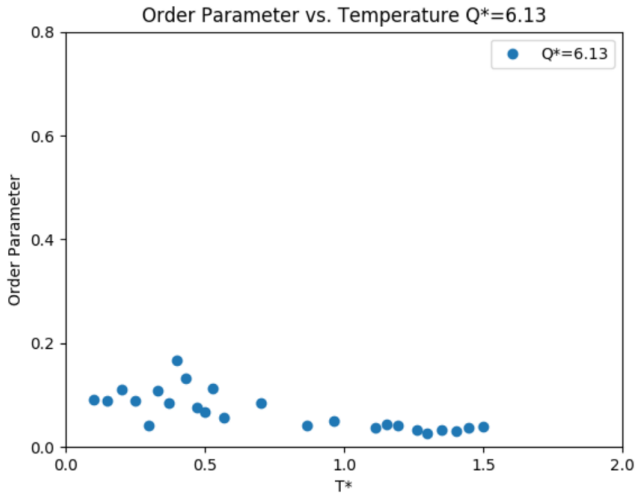


Figure 5. Order parameter vs. temperature for charge of 6.13 system

Key Outcomes

We have found some important bugs in the Lammps molecular dynamics software package and I have learned about many of the intricacies and oddities of Lammps. When calculating the Enthalpy of a gayberne molecule with 5 degrees of freedom, we found that Lammps calculates the enthalpy as if the molecules had six degrees of freedom. This was an important realization as it allowed us to match previous results from other research groups as well as alert the owners of Lammps to the problem. Another key outcome was matching results from Monte Carlo simulations and Molecular dynamics simulations of multiple research groups with similar systems. The simulation results were verified by looking at thermodynamic variables and order parameters and seeing if the published results fit into our simulations within a given error. The error was calculated by running many simulations at many temperatures and finding the standard deviation of a thermodynamic variable at a given temperature. The problems we have found in regards to the charged ion simulations may be a systematic problem with Lammps that needs fixing. Once those problems have been fixed, we can look at the properties of the system such as the ionic conduction, which is crucial to understand its importance in how batteries or solar cells can behave.

1. https://aip.scitation.org/doi/pdf/10.1063/1.478563?class=pdf
2. Margola, T.; Satoh K.; Saielli, G.; Comparison of the Mesomorphic Behaviour of 1:1 and1:2 Mixtures of Charged Gay-Berne GB(4.4,20.0,1,1) and Lennard-Jones Particles. *Crystals.* **2018,** *8, 371*.