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NDnano Summer Undergraduate Research
2017 Project Summary

1. Student name & university: Alisha Agrawal, Indian Institute of Technology Delhi, India

2. ND faculty name & department: Dr. Jennifer Schaefer & Dr. Jonathan Whitmer, Chemical Engineering

3. Project title: Synthesis and characterization of novel electrolytes for rechargeable batteries

4. Briefly describe new skills you acquired during your summer research:
I have learned a lot of computational work including how to do atomistic molecular dynamics simulations and also the specifics of working on an experimental project.
I on the outset experienced how to work in a research lab for the first time and learned how to approach problems in a lab setting. More specifically I learned how to synthesize small electrolytes and how to perform various characterization techniques (NMR, DSC, ICP etc.) on them.

5. Briefly share a practical application/end use of your research:
The small novel electrolytes which we have synthesized can be used in rechargeable batteries after stabilization them by means of polymerization

6. 50- to 75-word abstract of your project:
Polymer electrolytes have been in demand since solid state batteries were discovered. In addition to ease of processing, they have good mechanical properties and high chemical, electrochemical and photochemical stability. It is highly desirable to create high conductivity polymers which can be facilitated by engineering microstructures. This project includes the synthesis and study of small novel electrolytes such as lithium alkyl salts which can be used to study transport and phase transition(s) with an eye towards application in polymer electrolytes. After synthesis, elemental analysis, DSC and dielectric measurements were carried out for characterization. The effect of electrolyte composition on properties like conductivity and thermodynamics was studied. Simultaneously, changes in volume and enthalpy with respect to temperature were examined in atomistic molecular dynamics simulations to validate the phase transitions observed in experiments. Future work on these materials will involve stabilization by polymerization in order to lend mechanical stability to these phases.

7. References for papers, posters, or presentations of your research:
NA

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One-page project summary that describes problem, project goal and your activities / results:

The main reason for the synthesis of polymer electrolytes is that they have been in huge demand since they were discovered and also have a lot of applications in electrochemical industry due to their various properties and the ease of processing. This research mainly focuses on non-solvating ionomers. The objective was to synthesize small novel electrolytes and thus study their transport and characterization and finally creating high conductivity polymers by stabilizing these small electrolytes with polymerization in order to lend mechanical stability to these phases. In addition to the experimental work, atomistic molecular dynamics simulations were also done to validate the phase transitions observed in experiments and to get a better idea about the structure of the electrolyte during these transitions. After the synthesis of lithium alkyl salts, their characterization was being carried out using NMR, DSC (Differential Scanning Calorimetry), ICP (elemental analysis) and dielectric measurements of conductivity. The effect of electrolyte on properties like conductivity and thermodynamics (phase transitions) was studied. From the NMR data and the elemental analysis we were able to ensure that our novel electrolytes were pure and can be used for conductivity measurements and further tests. DSC curves gave an idea about the phase transitions of the product simultaneous to which changes in volume and enthalpy with respect to temperature were also examined in the molecular model so as to validate the data. The phase transitions obtained from the experimental results through DSC also matched with one of the reference papers which confirmed our synthesized electrolyte but the results were not being obtained from the molecular simulations and from this it was inferred that the force field used by us in the molecular simulations was quantitatively and qualitatively incorrect thus leading to these problems. This was also verified using the images of the molecular model which were not as ordered as we expected them to be. Finally on comparing the conductivity measurements of the corresponding lithium TFSI alkyl salts with the lithium sulfonate alkyl salts, it was found that the conductivity of TFSI lithium salts was much higher than the other one, thus leading us to think that these might be useful in the batteries upon further analysis. Future work includes more analysis of these conductivity results in addition to the SAXS data which will be instrumental in taking this research further and clear the remaining doubts.
It is highly desirable to create high conductivity polymers which can be facilitated by engineering microstructures. This project was mainly started with an eye towards application in polymer electrolytes.