NDnano
Notre Dame Nanoscience and Technology

NDnano Summer Undergraduate Research
2023 Project Summary

1. Student name & home university:
   Peter Schimpf, University of Notre Dame
2. ND faculty name & department:
   Dr. Jennifer L. Schaefer, Dept. of Chemical and Biomolecular Engineering
3. Summer project title:
   Polymers in next-generation rechargeable batteries
4. Briefly describe new skills you acquired during your summer research:

   COMSOL, adapting existing research for use on this project, communicating technical research to a wide range of audiences during poster presentation, 3MT, and final NURF presentation.

5. Briefly share a practical application/end use of your research:

   The use of gel polymer electrolytes can decrease the risk of thermal runaway in lithium-ion batteries. This research will allow for safer lithium-ion batteries to be produced for use in many portable electronic systems.

6. 50- to 75-word abstract of your project:

   Typical lithium-ion batteries use organic liquid electrolytes, which are highly volatile. The use of gel polymer electrolytes has been studied to increase the safety of lithium-ion batteries by decreasing the propensity of thermal runaway. COMSOL Multiphysics was used to create a simplified model of thermal runaway in a lithium-ion coin cell. The simplified model will be used to understand the effect of using a gel polymer electrolyte in place of a conventional liquid electrolyte.

7. References for papers, posters, or presentations of your research:
   Schimpf, Peter. Increasing Safety in Lithium-Ion Batteries with Gel Polymer Electrolytes by Modeling Thermal Runaway. Poster presented at: 2023 Summer Undergraduate Research Symposium; 26 July 2023; University of Notre Dame, Notre Dame, IN.

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

As the climate continues to be affected by anthropogenic greenhouse gas emissions, it is necessary to design power systems with low emissions in mind. Rechargeable battery systems are desirable due to low emissions when charged with low-carbon generated electricity, but they sacrifice the high energy density offered by fossil fuels. High energy density is a critical factor in designing viable systems that produce significant power without being too large for portable use. Lithium-ion batteries are favorable due to their high energy density when compared to other rechargeable batteries. However, the common use of organic liquid electrolytes in lithium-ion batteries puts these systems at risk of undergoing thermal runaway triggered by overuse, external heating, short circuits, or other factors. Thermal runaway is the cause for many safety concerns, which may shift public opinion away from widespread use of rechargeable battery systems as power sources. The use of gel polymer electrolytes has been studied to increase the safety of lithium-ion batteries by decreasing the risk of triggering thermal runaway. To understand this process and qualify how gel polymer electrolytes contribute to the safety of lithium-ion batteries, COMSOL Multiphysics was used to create a simplified model of thermal runaway in lithium-ion batteries. The model uses Arrhenius-type equations factoring in heat generated from the degradation of the separator, electrolyte, anode, and cathode. The model was initially made to be two-dimensional axisymmetric and based solely on thermal equations. The simplified model will be used to study the effect of gel polymer electrolytes on thermal runaway when the system is subjected to extreme external heating. The study will focus on a lithium-ion battery with a gel polymer electrolyte composed of polymerized polyethylene glycol diacrylate (PEGDA) suspended in a liquid electrolyte comprised of $LiPF_6$ in ethylene carbonate, dimethyl carbonate, and ethyl methyl carbonate (EC:DMC:EMC). Once the simplified model is validated against lab experiments, it can be expanded to compare many polymer and electrolyte compositions. The expanded model will include coupled electrochemical and thermal reactions. This will allow for thermal runaway to be triggered by internal short circuit (ISC) as well as external heating.