CALIFORNIA STATE SCIENCE FAIR
2016 PROJECT SUMMARY

Name(s)

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Project Number

S0623

Project Title

Diffusivity and Solvation of Alkali and Halogen Ions in Solid and Aqueous Battery Electrolytes

Abstract

Objectives/Goals

Although lithium-ion batteries are effective for current small-scale applications, wider adoption of Li-ion batteries is hindered by their limited energy density, gradual rate of decomposition, and dangerous risk of flammability. The objective of this project is to employ molecular dynamics simulations in order to determine (a) whether there are alkali, alkaline earth, and halogen metals that outperform lithium in various battery electrolytes and (b) whether solid polymer electrolytes offer significant benefits over liquid electrolytes.

Methods/Materials

The molecular dynamics simulator LAMMPS along with Visual Molecular Dynamics (VMD), Python, TCL, and Matlab were used to generate and process all simulations. Simulations were performed on several test environments consisting of various alkali, alkaline earth, and halogen ions submerged in either a solid PEO (polyethylene oxide) electrolyte or liquid DME (dimethyl ether) electrolyte.

Results

The simulations revealed that, in terms of their relative rates of ionic diffusivity, solid electrolytes were generally outclassed by their liquid counterparts. Lithium in particular performed poorly in both the solid and liquid electrolytes, while other ions (especially the halogens) experienced high rates of diffusivity and encountered less dense solvation shells.

Conclusions/Discussion

Given the fact that solid polymer electrolytes will eliminate the intrinsic drawbacks of liquid electrolytes, these results point to the possibility of solid polymer electrolyte (SPE) batteries featuring ions other than lithium. Not only that, but the data generated suggests that synthetic polymers designed to maximize ionic diffusivity by minimizing the density of solvation shells within electrolytes could be the future of next-generation rechargeable batteries.

Summary Statement

Molecular dynamics simulations were used to analyze the performance of various alkali, alkaline earth, and halogen ions in solid and aqueous electrolytes with the goal of finding better materials for future batteries.

Help Received

Mentored and supervised by the Miller research group at Caltech.