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Computational characterization of solid electrolyte membranes for polysulfide retention in Li-S batteries

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The increasing energy requirements of the current society trigger an important need of developing better energy- storage devices. The lithium-sulfur battery appears as a promising chemistry because of their component properties, such as low cost and high theoretical capacity. However their practical implementation has various challenges. Among them, a major issue is the migration from cathode to anode of the long-chain soluble lithium polysulfides (PS) causing instability and low capacity in the battery. Retention strategies include coating the cathode with special materials able to retain these molecules, or developing membranes that could be incorporated into the separator with the same purpose. The selection of the solid polymer electrolyte is a key for the performance of the battery, either the minimization of the shuttle process or PS retention mechanisms depend on it. In this work, we investigate polymer electrolyte systems that have a suitable chemical backbone in order to facilitate the lithium polysulfide retention. These materials will act as membranes in contact with the electrolyte solution including the PS species, solvents, and salts. We use density functional theory and classical molecular dynamics to evaluate the PS retention properties of these polymer electrolytes.

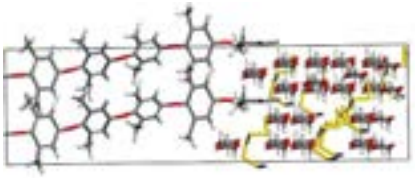

Figure 1: The solid electrolyte membrane surface. The vacuum area contains solvents and lithium polysulfide.

Recent Publications:

1. E López-Chavez and Y Pena-Castaneda (2017) Ti-decorated C120 nanotorus: A new molecular structure for hydrogen storage. International Journal of Hydrogen Energy DOI: 10.1016/j.ijhydene.2017.08.095.
2. E López-Chavez and Y Pena-Castaneda (2016) Ion conduction and chemical and physical properties of sulfonated polyetherimide as membrane: theoretical study. International Journal of Hydrogen Energy DOI: 10.1016/j.ijhydene.2016.09.035
3. E López-Chavez and Y Pena-Castaneda (2015) Behavior of ionic species in sulfonated PEI using DFT simulations: A study to determine ionic conductivity. Journal of Hydrogen Energy DOI: 10.1016/j.ijhydene.2015.07.096
4. E López-Chavez and Y Pena-Castaneda (2015) Theoretical methodology for calculating water uptake and ionic exchange capacity parameters of ionic exchange membranes with applications in fuel cells. International Journal of Hydrogen Energy DOI: 10.1016/j.ijhydene.2015.03.046
5. E López-Chavez and Y Pena-Castaneda (2014) Role of sulfonation in stability and selectivity of poly(ether-imide) to develop ionic exchange membranes: DFT study with applications in fuel cells. Journal of Molecular Modeling 20:2325.

Biography

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