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Polymer/ Lithium Batteries Studied with MD Simulations and Dynamic Neutron Scattering

Li-ion batteries (LIBs) play a key role in our everyday lives as a component of electronic devices such as mobile phones and electric vehicles [1, 2]. They are also employed as high-density energy storage source in various industries, such as power plants, military equipment, and aerospace. In spite of their wide use, LIBs suffer from some shortcomings, such as the low boiling point of the commercial liquid electrolyte, which poses safety risks, including leaks, burning, and explosions [3, 4]. To this day a lot of money had been put in research to develop high-performance and especially safe batteries for which solid polymer electrolytes (SPE) are excellent candidates. To find the right electrolyte and to avoid any trial and error, innovative studies intend to develop a microscopic picture of the Li –ion conductivity process which is difficult to obtain from standard in-house laboratory techniques. However, Neutron scattering in combination with MD simulation form a suitable basis for this. Also, Poly-ethylene oxide (PEO) is the most commonly used polymer electrolyte due to its high conductivity up to to 10-3 S/cm even in its pure occurrence. In PEO based Lithium batteries, it is generally accepted that the charge transportation mechanism of the Li+ ion is directly depending on the segmental and backbone motions of the polymer. If optimized, these processes can make the conductivity process of Li - ion faster which directly results in faster charging and discharging of the battery. Once confirmed with Quasi elastic Neutron Scattering and dielectric measurements with MD simulation we can access and enlighten the microscopic picture of Li –ion transport process through the polymer matrix. Here we report on the results of a study of a comb PEO polymer which leads to the development of 4-arm star PEO polymers. While all of them offer their own specific conductivity mechanism, the technique of tailoring towards better and higher performing polymers especially studying the conductivity mechanism is reported. A variety of Li-salt/ polymer candidates will be simulated alongside with the study via QENS measurements.
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Topic

Energy Storage

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