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Insights on Li-TFSI diffusion in polyethylene oxide for battery applications[1] NICOLA MOLINARI, Imperial College London, JONATHAN MAILOA, BORIS KOZINSKY, Robert Bosch LLC, ROBERT BOSCH LLC COLLABORATION — Improving the energy density, safety and efficiency of lithium-ion (Li-ion) batteries is crucial for the future of energy storage and applications such as electric cars. A key step in the research of next-generation solid polymeric electrolyte materials is understanding the diffusion mechanism of Li-ion in polyethylene oxide (PEO) in order to guide the design of electrolytes materials with high Li-ion diffusion while, ideally, suppress counter-anion movement. In this work we use computer simulations to investigate this long-standing problem at a fundamental level. The system under study has Li-TFSI concentration and PEO chain length that are representative of practical application specifications; the interactions of the molecular model are described via the PCFF+ all-atom force-field. Validation of the model is performed by comparing trends against experiments for diffusivity and conductivity as a function of salt concentration. The analysis of Li-TFSI molecular dynamics trajectories reveals that 1. for high Li-TFSI concentration a significant fraction of Li-ion is coordinated by only TFSI and consistently move less than PEO-coordinated Li-ion, 2. PEO chain motion is key in enabling Li-ion movement.

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