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Computationally Guided Design of Polymer Electrolytes for Battery Applications ZHEN-GANG WANG, MICHAEL WEBB, BRETT SAVOIE, THOMAS MILLER, California Institute of Technology — We develop an efficient computational framework for guiding the design of polymer electrolytes for Li battery applications. Short-times molecular dynamics (MD) simulations are employed to identify key structural and dynamic features in the solvation and motion of Li ions, such as the structure of the solvation shells, the spatial distribution of solvation sites, and the polymer segmental mobility. Comparative studies on six polyester-based polymers and polyethylene oxide (PEO) yield good agreement with experimental data on the ion conductivities, and reveal significant differences in the ion diffusion mechanism between PEO and the polyesters. The molecular insights from the MD simulations are used to build a chemically specific coarse-grained model in the spirit of the dynamic bond percolation model of Druger, Ratner and Nitzan. We apply this coarse-grained model to characterize Li ion diffusion in several existing and yet-to-be synthesized polyethers that differ by oxygen content and backbone stiffness. Good agreement is obtained between the predictions of the coarse-grained model and long-timescale atomistic MD simulations, thus providing validation of the model. Our study predicts higher Li ion diffusivity in poly(trimethylene oxide-alt-ethylene oxide) than in PEO. These results demonstrate the potential of this computational framework for rapid screening of new polymer electrolytes based on ion diffusivity.

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