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Systematic Experimental and Computational Investigation of Ion Transport in Novel Polyether Electrolytes DANIELLE PESKO, University of California, Berkeley, MICHAEL WEBB, California Institute of Technology, YUKYUNG JUNG, QI ZHENG, Cornell University, THOMAS MILLER III, California Institute of Technology, GEOFFREY COATES, Cornell University, NITASH BALSARA, University of California, Berkeley — Polyethers, such as poly(ethylene oxide) (PEO), are considered to be the most promising polymer electrolyte materials due to their high ionic conductivity and electrochemical stability, both essential for battery applications. To gain a fundamental understanding of the transport properties of polyether systems, we design a systematic set of linear PEO-like polymers to explore the effect of adding carbon spacers to the backbone of the chain. Ac impedance spectroscopy is employed to measure the ionic conductivity of polyether/lithium salt electrolytes; the results elucidate tradeoffs between lowering the glass transition temperature and diluting the polar groups on the polymer chain. Molecular-level insight is provided by molecular dynamics simulations of the polyether electrolytes. We define the useful and intuitive metric of "connectivity", a parameter calculated from simulations which describes the physical arrangements of solvation sites in a polymer melt. Direct comparison of experiment and theory allows us to determine the relationship between connectivity and conductivity. The comparison provides insight regarding the factors that control conductivity, and highlights considerations that must be taken when designing new ion-conducting polymers.

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