Alternate: 1.1.4 Polymers in Batteries and Electrochemical Capacitors for the MAR16 Meeting of The American Physical Society

> Aggregate-mediated charge transport in ionomeric electrolytes KERAN LU, JANNA MARANAS, SCOTT MILNER, Pennsylvania State University — Polymers such PEO can conduct ions, and have been studied as possible replacements for organic liquid electrolytes in rechargeable metal-ion batteries. More generally, fast room-temperature ionic conduction has been reported for a variety of materials, from liquids to crystalline solids. Unfortunately, polymer electrolytes generally have limited conductivity; these polymers are too viscous to have fast ion diffusion like liquids, and too unstructured to promote cooperative transport like crystalline solids. Ionomers are polymer electrolytes in which ionic groups are covalently bound to the polymer backbone, neutralized by free counterions. These materials also conduct ions, and can exhibit strong ionic aggregation. Using coarsegrained molecular dynamics, we explore the forces driving ionic aggregation, and describe the role ion aggregates have in mediating charge transport. The aggregates are string-like such that ions typically have two neighbors. We find ion aggregates self-assemble like worm-like micelles. Excess charge, or free ions, occasionally coordinate with aggregates and are transported along the chain in a Grotthuss-like mechanism. We propose that controlling ionomer aggregate structure through materials design can enhance cooperative ion transport.

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