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Ionomers for Ion-Conducting Energy Materials RALPH COLBY, Materials Science and Engineering, Penn State University — For ionic actuators and battery separators, it is vital to utilize single-ion conducting ionomers that avoid the detrimental polarization of other ions. Single-ion conducting ionomers are synthesized based on DFT calculations, with low glass transition temperatures (facile dynamics) to prepare ion-conducting membranes for battery separators that conduct Li^+ or Na^+. Characterization by X-ray scattering, dielectric spectroscopy, FTIR, NMR and linear viscoelasticity collectively develop a coherent picture of ionic aggregation and both counterion and polymer dynamics. ^{7}Li NMR diffusion measurements find that diffusion is *faster* than expected by conductivity using the Nernst-Einstein equation, which means that the majority of Li diffusion occurs by ion pairs moving with the polymer segmental motion. Segmental motion only contributes to ionic conduction in the rare event that one of these ion pairs has an extra Li (a positive triple ion). This leads us to a new metric for ion-conducting soft materials, the product of the cation number density p_0 and their diffusion coefficient D; p_0D is the diffusive flux of lithium ions. This new metric has a maximum at intermediate ion content that corresponds to the overlap of ion pair polarizability volumes. At higher ion contents, the ion pairs interact strongly and form larger aggregation states that retard segmental motion of both mobile ion pairs and triple ions.

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