Control of Ionic Mobility via Charge Size Asymmetry in Random Ionomers

Boran Ma, Trung Dac Nguyen, Monica Olvera de la Cruz

Here we demonstrate that size asymmetry, $\lambda$, represented by the ratio of counterion to charged monomer size, plays a key role in both the nanostructure and in the ionic dynamics. The ionic mobility increases as $\lambda$ decreases (small counterions) in the weak electrostatics (high dielectric constant) regime. Whereas in systems with strong electrostatic interactions, ionomers with higher size symmetry ($\lambda \approx 1$) display higher ionic mobility. Moreover, ion transport is found to be dominated by the hopping of the ions and not by moving ionic clusters (also known as “vehicular” charge transport). As for discharging process, introducing some degree of size asymmetry between counterions and monomers can improve ion transport in random ionomers with high dielectric constant. These results serve as a guide for designing ion-containing polymers for ion transport related applications.