

Impact of Cation-Ligand Interaction Strength on the Permselectivity of Ligand-Functionalized Polymer Membranes

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Polymer membranes are emerging as a cheap and scalable alternative for existing ionic separation processes. Functionalization of ligands onto the polymer chains can be used as a mechanism to incorporate host-guest interactions, which allows polymer membranes to be utilized for carrying out specific ion-ion separations. We conduct molecular dynamics (MD) simulations to probe the impact of cation-ligand interaction strength on salt transport in ligand-functionalized polymer membranes (LFPs). Our results indicate an enhancement in salt partitioning in conjunction with a reduction in salt diffusivity upon increase in the cation-ligand interaction strength. However, the enhancement in salt partitioning supersedes the decline in salt diffusivity, thereby resulting in an enhanced overall salt permeability at greater cation-ligand interaction strengths. It is observed that equimolar binary mixed salt systems (sharing a common anion) exhibit more selective salt partitioning within the membrane as compared to their single salt analogs. On the other hand, single salt systems exhibit higher salt diffusivity ratios relative to their mixed salt counterparts. The overall salt permeability selectivity is found to closely resemble the observed trends for partitioning selectivity in both single and mixed salt systems, which suggests that diffusivity selectivity plays a relatively weaker role in dictating permselectivity trends in LFPs, at least for the parameter space explored in the current study.