A COARSE GRAINED MODEL FOR ION TRANSPORT IN MICROSCALE BATTERIES

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Due to concerns over safety, reliability, and ease of processing, microscale batteries utilize solid membranes, rather than a liquid electrolyte, to facilitate ion transport between electrodes. However, unlike liquid electrolytes, which relax quickly under an applied potential to screen long range electrostatic interactions, ion-conducting polymers evolve under constrained, non-equilibrium dynamics due to chain entanglement. Furthermore, in contrast to liquid batteries, where safety considerations limit electrode separations to the macroscale, solid polymer membranes can be as thin as 10nm, which is on the same order as material heterogeneity. Taken together, these distinguishing characteristics make traditional mean-field models inappropriate to understand the driving forces of ion transport in solid membrane microscale batteries. We address this challenge using theory and numerical simulation. Here we present a coarse-grained model that takes into account long range electrostatic interactions and transport through a non-uniform membrane. We model the solid membrane as a set of slowly evolving kinetic constraints and electrodes as ideal conductors which obey Marcus criteria for electron transfer. Our novel methodology provides a full device-scale description without sacrificing molecular-scale heterogeneity and therefore enables a better understanding of the effect of material properties on overall device performance. In a preliminary study, we explore the consequences of ion-conducting polymers for which anions and cations diffuse along different physical pathways, as well as the role of polymer polarizability.