Thermodynamically consistent modeling of ion exchange membranes in multi-ionic environments

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Ion exchange membranes (IEMs) have enormous potential to improve a range of electrochemical technologies, including water desalination, fuel cells and batteries. E.g., in zinc-manganese batteries, the crossover of zincate degrades the manganese electrode by formation of poorly soluble phases such as hetaerolite; in zinc-air batteries the zincate can clog the air electrode through precipitation. Thus, suppressing parasitic crossover while imposing minimal hindrance towards functionally relevant transport can significantly extend battery lifetime. [1,2]
Since common membrane models are usually limited in their applicability or predictive value for highly concentrated multi-ionic environments, we formulate a more broadly applicable, thermodynamically consistent multiscale framework. This framework combines exclusion, single-site occupation and mean-field interactions along the polymer chain, consolidating central ideas of established membrane models into a unified free-energy description. [3,4,5]
The resulting model not only matches the experimental data well even at high ion concentrations, but also provides detailed insight into the underlying mechanisms and recovers key findings of several common membrane models as limiting cases. Incorporation of this model into a cell-scale battery simulation enables theory-guided membrane optimization for enhanced aqueous battery lifetime and efficiency.

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