First-Principles Discovery of Design Rules for Anion Exchange Membranes with High Hydroxide Transport

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The understanding and design of cost-effective and reliable polymer architectures for use as anion-conducting membranes is an important challenge facing emerging electrochemical device technologies. A key ingredient for characterizing the main design principles is embedded in the fundamental understanding of the hydroxide diffusion mechanisms. Recently, nano-confined structures have become a popular tool for exploring the functionalities of anion exchange membranes. As the water structure in nano-confined structures is diverse and controlled by the shape and size of the confined structures, it is suggestive that the hydroxide diffusion mechanism would change dramatically and therefore should be distinct and studied for variant kinds of AEM cells. To this end, we are using the full-atomic scale ab initio molecular dynamics calculations to obtain a molecular level understanding of the mechanisms of hydroxide solvation and transport in different chemical environments to guide the synthesis and experimental materials design. To mimic the complicated AEM environment, our theoretical model contains graphane sandwich structures to which the cationic groups are attached. The cation groups are then surrounded by water up to experimentally relevant ratios and hydroxide ions. Parameters to be varied include the chemical composition of the cation, the number of water molecules solvating the system, the cell geometry and the system temperature.