Discovering design principles for anion exchange membranes with high hydroxide conductivity: An ab initio molecular dynamics study

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It is clear that in the identification and development of clean energy sources, a range of technologies will need to be leveraged. Electrochemical devices are an important part of this mix of technologies, and among these, fuel cells constitute some of the cleanest and most sustainable. However, several key hurdles to harnessing the potential of fuel cells (as well as various other electrochemical technologies) remain to be surmounted. We have mounted a Materials Genome Initiative project that aims to address these challenges by designing, synthesizing, and testing new materials for use in alkaline fuel cells and to discover a set of rules for best practices in the development of future materials for fuel cell applications. An interdisciplinary team of investigators has been assembled and is focusing on *anion exchange membrane fuel cells,* which have advantages over other types of fuel cells in not requiring precious metals and being operable with a variety of fuels at low temperature [1]. The project will employ a cohesive strategy involving mathematical and computer modeling of specific materials components, which will, in turn, guide the synthesis of new materials, characterization and testing of these in actual fuel cells, and the determination of optimized key design principles that will govern future materials engineering for electrochemical applications. In this talk, I will outline the strategy of the proposed research and present results from work done to date employing density-functional theory based first-principles molecular dynamics calculations and dissipative-particle dynamics[2-5]. If time permits, I will also present a new scheme to employ machine learning techniques to bypass expensive density functional theory calculations while still generating energetics and molecular dynamics trajectories at full density-functional accuracy. Proof of concept examples will be presented.

References

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