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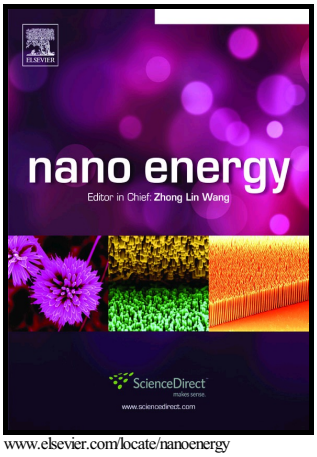

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How Theory and Simulation Can Drive Fuel Cell Electrocatalysis

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Abstract

Over the last decade, theory and modeling have become essential tools to navigate the parameter space that governs activity and stability of electrocatalyst systems for polymer electrolyte fuel cells. This perspective covers essential phenomena from atomic to nanoscale and discusses the impact of the key parameters at play. It is centered around the development of first-principles electrochemical methods as a foremost goal in the field. The general modeling framework entails at its core a self-consistency problem that must be solved to relate the metal phase potential to descriptors of catalyst activity and stability. Density functional theory has captured a central role in this rapidly evolving field. The article puts more than usual emphasis on aspects of the multifaceted challenges in fuel cell electrocatalysis that at present lie beyond the capabilities of density functional theory; they include metal charging and solvent effects. Following the general discussion of the theoretical-computational framework, an approach for "deciphering" the oxygen reduction reaction is demonstrated; it reconciles reaction pathways and free energy profiles obtained from density functional theory simulations with kinetic modeling of surface reactions and effective kinetic parameters. Another section dwells on the importance of metal charging phenomena that are especially important for the catalytic function of nanoporous media. The penultimate section exposes the ambivalent role of Pt oxide formation in modulating catalytic properties for the oxygen reduction reaction as well as

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