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Multiscale Simulation of Electrochemical Phenomena: Fuel Cells and Batteries

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Results will be presented from multiscale simulations of two important systems from renewable energy technology, fuel cell proton membranes and electrochemical cells. In the first case, the solvation and transport of hydrated protons in proton exchange membranes (PEMs) such as NafionTM will be described using a novel multi-state reactive molecular dynamics (MD) approach. The multi-state MD methodology allows for the treatment of explicit (Grotthuss) proton shuttling and charge defect delocalization which, in turn, can strongly influence the properties of the hydrated protons in various aqueous and complex environments. The role of PEM hydration level and morphology on these properties will be further described. A new multiscale computational methodology for describing the mesoscopic features of the proton transport will also be described, which can be coupled to the results from the molecular-scale simulations. On the second topic, a computationally efficient method will be presented for the treatment of electrostatic interactions between polarizable metallic electrodes held at a constant potential and separated by an electrolyte. The method combines a fluctuating uniform electrode charge with explicit image charges to account for the polarization of the electrode by the electrolyte, and a constant uniform charge added to the fluctuating uniform electrode charge to account for the constant potential condition. The method is used to calculate electron transport rates using electron transfer theory; these rates are incorporated in a multiscale approach to model oxidation/reduction reactions in an electrochemical cell efficiently.