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Abstract for an Invited Paper for the MAR05 Meeting of the American Physical Society

## Proton Solvation and Transport in Aqueous Environments

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The solvation and transport of excess protons in several important systems will be described using the multi-state empirical valence (MS-EVB) approach combined with large scale molecular dynamics (MD) simulation. The MS-EVB approach allows for the treatment of explicit proton shuttling (dynamical bond-breaking), which, in turn, strongly influences the properties of excess protons in various aqueous environments. Proton solvation and transport in bulk water, water clusters, the water liquid-vacuum interface, and water-filled channels will be discussed.