

Proton transport in aqueous and non-aqueous media  
studied by first-principles molecular dynamics  
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Proton transport in aqueous and non-aqueous hydrogen-bonded media has long been an area of intense study due to its fundamental importance in emerging energy technologies such as hydrogen fuel cells and in biological problems such as proton pumping. Our understanding of proton transport phenomena is based on the concept structural diffusion of a topological defect in the hydrogen bond network originally proposed by C. J. T. von Grothuss in 1806. Within this picture, long-range proton transport is driven by specific structural rearrangements in the local hydrogen bonding environment, however, pinning down the specific microscopic mechanisms in different media remains an immense challenge that has an immediate impact on the problem of designing novel materials for enhancing the proton transport process. In this talk, I will show how first-principles molecular dynamics, employing a density functional theory description of the electronic structure, has contributed to our understanding of proton transport phenomena in a variety of systems including acidic and basic solutions, acid hydrates, and phosphoric acid. It will be shown that proton transport in aqueous systems relies largely on local fluctuations in the hydrogen bond network while phosphates, by contrast, transport protons along extended, polarized chains in a manner much closer to the original picture suggested by von Grothuss.