

Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

A First-principles Investigation of Superprotonic Activity in CsHSO₄ BRANDON WOOD, MIT, NICOLA MARZARI — With the recent push to realize the hydrogen economy, there has been a surge of interest in viable solid-state materials for use as fuel cell electrolytes. Among the candidates are various derivatives of the anhydrous superprotonic conductor CsHSO₄, which exhibits reasonably high ionic conductivity at relevant operating temperatures while remaining electronically insulating. However, despite being widely characterized experimentally, a truly atomistic picture of the diffusion pathways and mechanisms in the material is missing. To this end, we have characterized this material with extensive first-principles static and dynamical calculations on 112-atom supercells of CsHSO₄. We isolate the dominant atomistic mechanisms involved in the superprotonic behavior and discuss the effect of correlated diffusive events in enhancing proton transport. We also offer a detailed description of the dynamics of the hydrogen bond network topology as the diffusing protons propagate through the lattice structure. The role of our findings in understanding superionic behavior are discussed.

Brandon Wood
MIT

Date submitted: 22 Nov 2005

Electronic form version 1.4