

Abstract Submitted  
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**Hydrogen diffusion and tunneling in  $\text{KTaO}_3$  from first principles**<sup>1</sup> HAZEM ABU FARSAKH, CHRIS G. VAN DE WALLE, Materials Department, University of California, Santa Barbara — The high proton conductivity in many perovskites has attracted interest for potential applications, such as in fuel cells. A promising approach to increase their conductivity at lower temperatures involves enhancing quantum-mechanical tunneling. In order to determine the role of tunneling for H in  $\text{KTaO}_3$  we employ first principles calculations for H interstitial atoms. We identify H binding sites and diffusion channels and calculate the associated activation energies. In addition, we analyze the effect of lattice relaxations on the diffusion barriers. Through calculating the 3D potential energy surface of H, we determine accurate H tunneling rates by numerically solving Schrödinger's equation for H in the 3D potential energy surface. Finally, we examine lattice vibrations and analyze their role in assisting proton tunneling.

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