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First Principles Study for Proton Transport and Diffusion Behavior in Hydrous Hexagonal WO3 CHI-PING LIU, FEI ZHOU, VIDVUDS OZOLINS, Materials Sciences Engineering, UCLA, QPAM TEAM — Proton transport is of great importance in biological species and energy storage and conversion systems. Previous studies have shown fast proton conduction in liquids and polymers but seldom in inorganic materials. In this work, first principles density functional theory (DFT) reveals that the formation of hydronium and water chains inside the hexagonal channels plays the key roles for the anomalously fast proton transport, by following modified Grotthuss mechanism. Our DFT study shows the detailed microscopic proton diffusion mechanism along the channel in hydrous WO3 with 50% water composition, which is proper for water chain formation. The water chain in the channel serves as a possible diffusion media for hydronium (H3O+). With the continuous formation and cleavage of hydrogen bonds in the channel, the hydronium diffuses by hydrogen bonds exchange between water molecules. This mechanism is very similar with Grotthuss relay mechanism for proton transport in liquid. The possible proton diffusion were studied for hydronium is either far away from the water chain bond defect or next to H2O defect at the end of water chain. The diffusion barriers for both conditions are around 150 meV to 200 meV, and water defects reorganization in the chain is the rate-limited step for proton diffusion. These small diffusion barriers could explain the fast 1-D proton transport in hydrous WO3 channel. Further studies about fast proton transport in other inorganic materials could be an important topic in not only biochemistry but also clean energy applications like fuel cell applications.

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