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Proton Diffusion in Tungsten Oxide Dihydrate: Hints from ab initio Calculations HAO LIN, University of California, Los Angeles, FEI ZHOU, Lawrence Livermore National Laboratory, CHI-PING LIU, VIDVUDS OZOLINS, University of California, Los Angeles — Knowledge of proton diffusion mechanisms in tungsten oxide (WO_3) and its hydrates ($WO_3{\cdot}H_2O$,$WO_3{\cdot}2H_2O$) is essential for designing fuel cell membranes, electrochromics, energy storage materials and gas sensors. It is generally believed that tungsten oxide dihydrate is a better proton conductor than anhydrous tungsten oxide and monohydrate, due to the existence of fast diffusion pathways through the interlayer structural water. Aiming to test this assumption, we performed density functional theory calculations and surprisingly found that the interlayer structural water in dihydrate does not contribute to proton diffusion and that proton diffusion mechanisms are similar in dihydrate and tungsten oxide.

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