Electronic Supplementary Information for

Non-Grotthuss proton diffusion mechanism in tungsten oxide dihydrate from first-principles calculations

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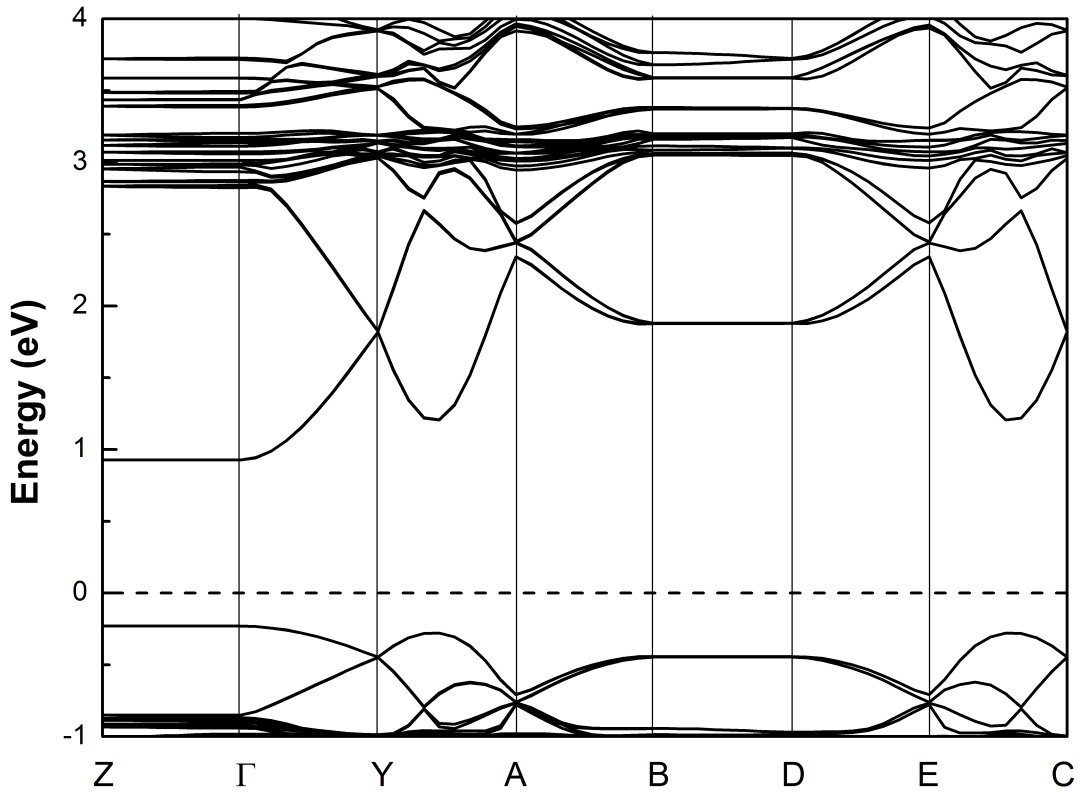

Fig. S1 Band structure of tungsten oxide dihydrate. The high symmetry points in the b direction are plotted in the range from Z (0, 1/2, 0) to Γ (0, 0, 0) and from B (0, 0, 1/2) to D (0, 1/2, 1/2).

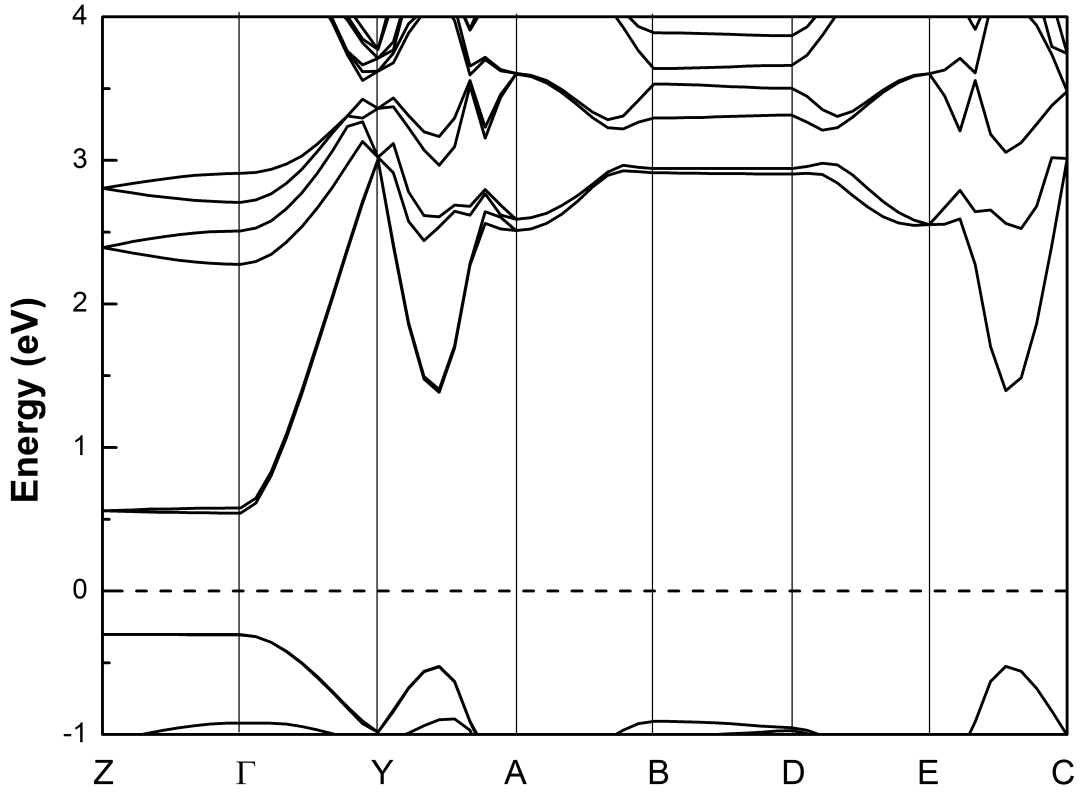

Fig. S2 Band structure of tungsten oxide monohydrate.

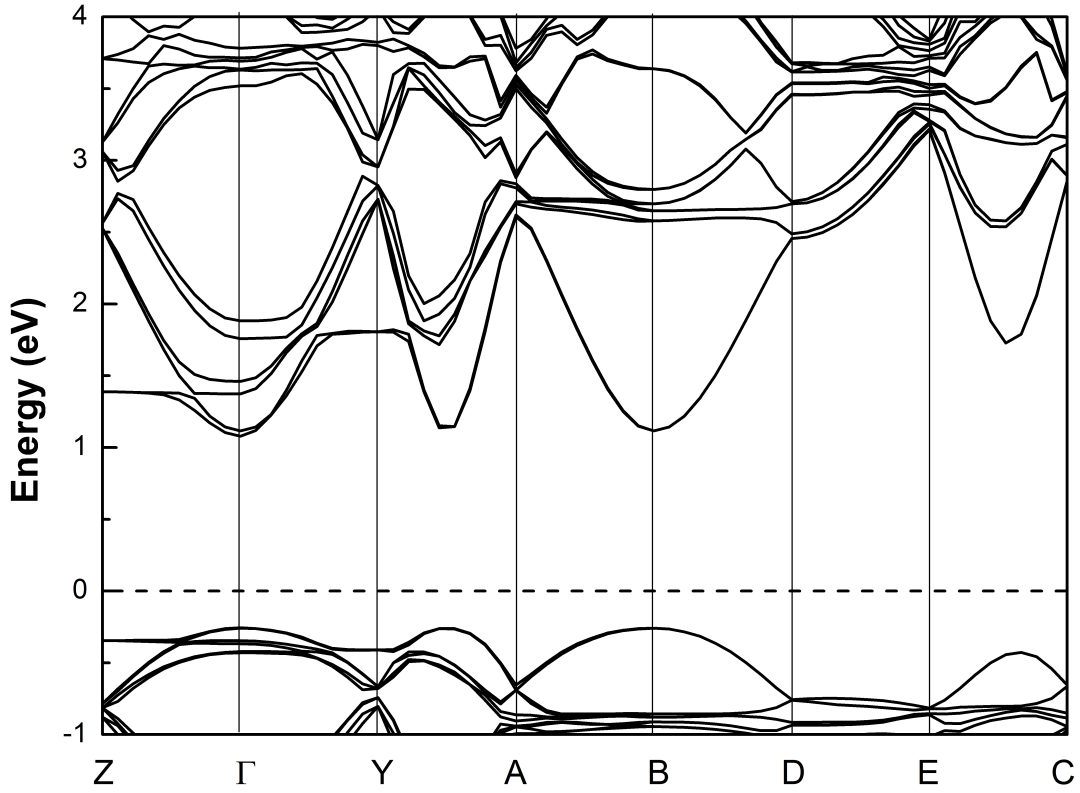

Fig. S3 Band structure of tungsten oxide.

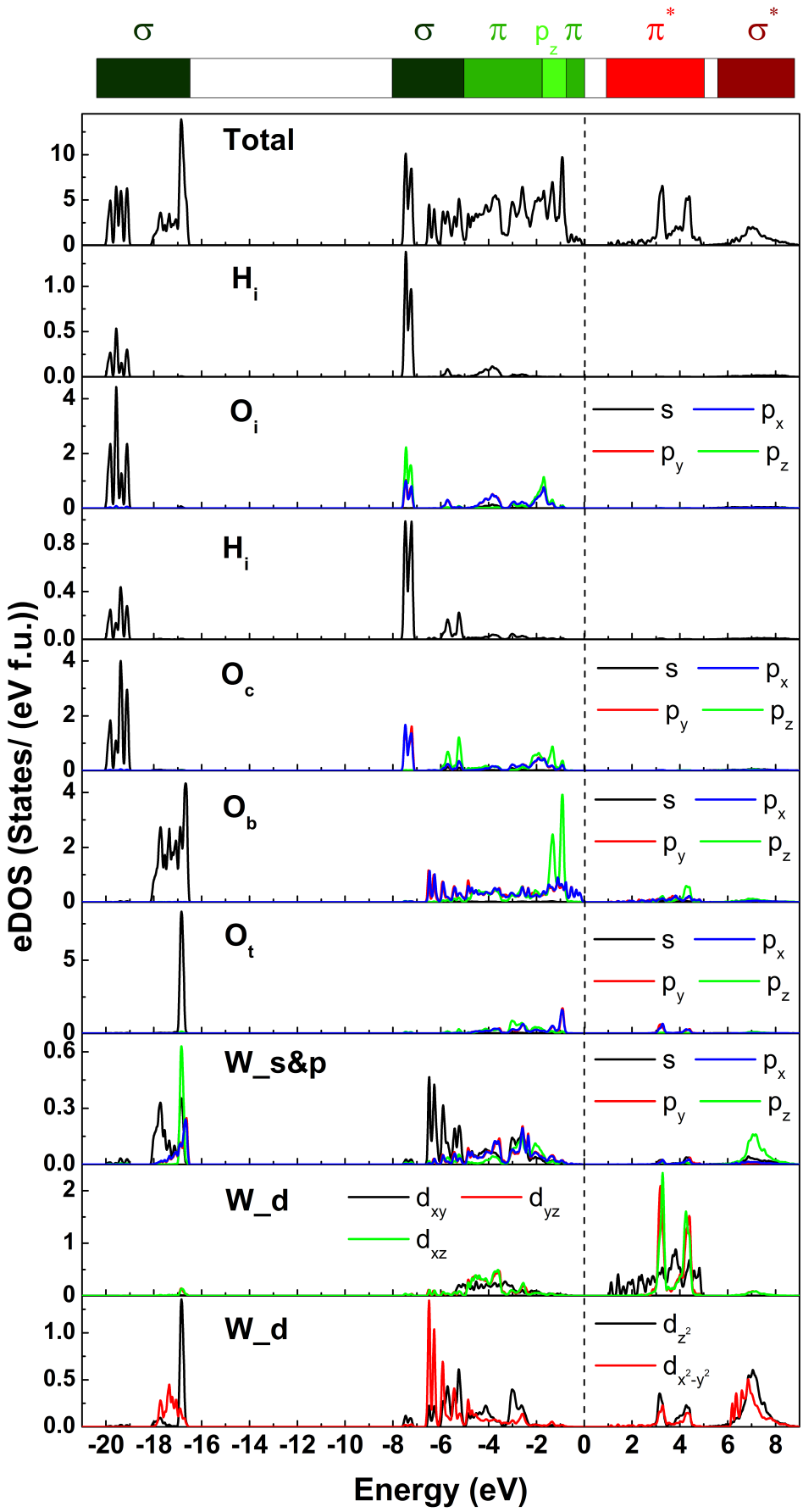

Fig. 4S The atom- and angular momentum-decomposed electronic density of states.

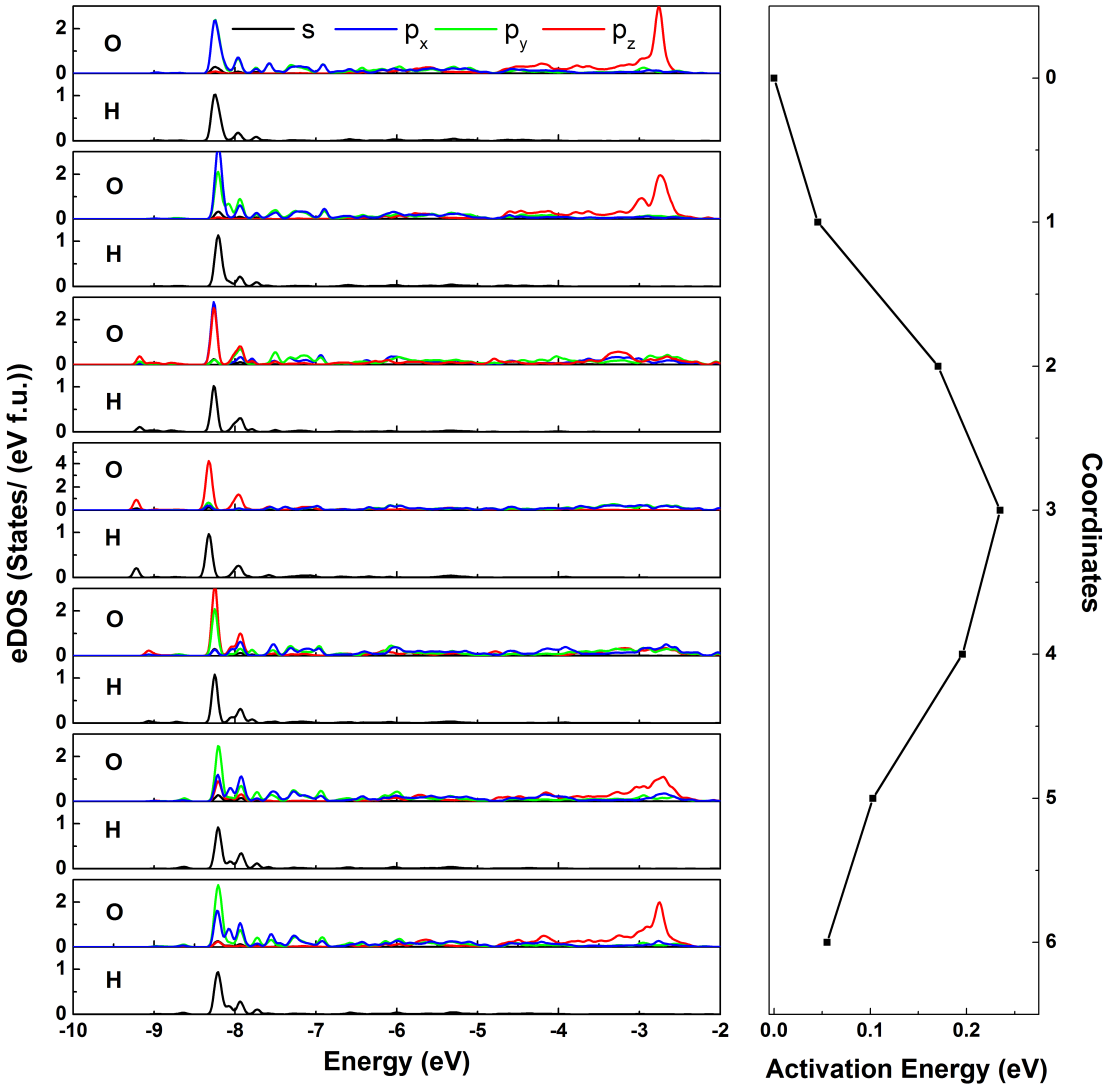

Fig. 5S Atom- and momentum-decomposed eDOS of the O_b-H dimer during proton rotation. This rotation is facilitated by the fact that the proton remains bonded to one of the bridging oxygen's nonbonding 2*p* orbitals.

Movie S1 NEB images movie corresponding to proton rotation.

Movie S2 NEB images movie corresponding to the supercell calculation.

Movie S3 NEB images movie corresponding to large octahedral distortion.