

Investigation of Hydrogen Diffusion in Zirconia under Extreme Conditions

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S1. The test on different effects to barriers

The van der Waals interactions and zero-point vibrational energy effects show only minor impacts on the energy barrier, as presented in Fig. S1. We also tested the finite-size effect under extreme pressure conditions, and the results for a H^+ diffusion path calculation under 220 GPa in different supercells are presented in Tab. S1.

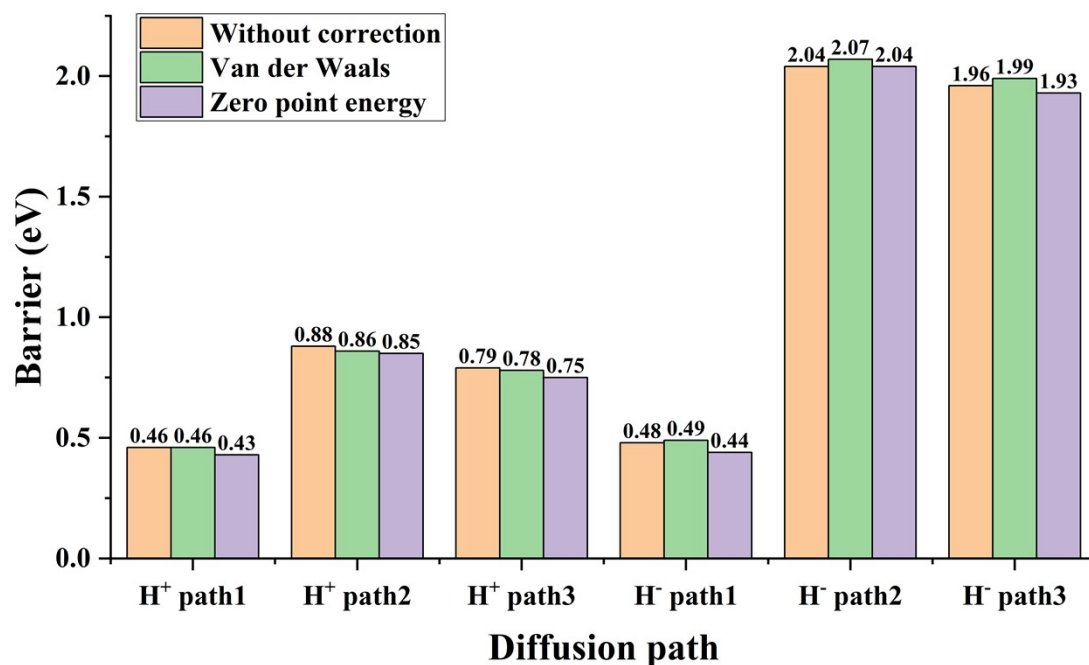


FIG. S1. The van der Waals interactions and zero-point vibrational energy effects for different charged defects and pressures. H^+ path1 is at 0 GPa, H^+ path2 is at 10 GPa, and H^+ path3 is

at 60 GPa. All H^- paths are at 0 GPa.

Expansion factor	Atom number	Barrier (eV)
10	90	2.787
12	108	2.802
14	126	2.809

Tab. S1. Diffusion barrier of H^+ towards the second-nearest neighbour position in different supercells at 220 GPa.