Supporting Information

Investigating the Role of Structural Water on the Electrochemical Properties of $\alpha - V_2O_5$ through Density Functional Theory

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Diffusion Calculations

The physical diffusion pathway for Mg in the 2×1×1 supercell of α-V_2O_5 without H_2O molecules present is shown in Fig. S1. The same diffusion pathway was used for all ions and structures with H_2O present. The energy barriers for all ions investigated as a function of the path distance for a) V_2O_5 and b) V_2O_5-$(H_2O)_1$ are shown in Fig. S2. The energy barriers for Zn and Al in V_2O_5-$(H_2O)_1$ are not shown since such calculations failed to converge.

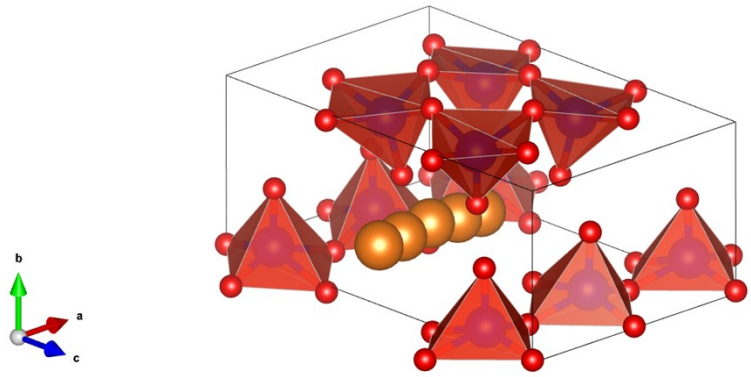

Fig. S1: The ion migration pathway along the *a* lattice vector for α-V_2O_5 with H_2O molecules not shown.

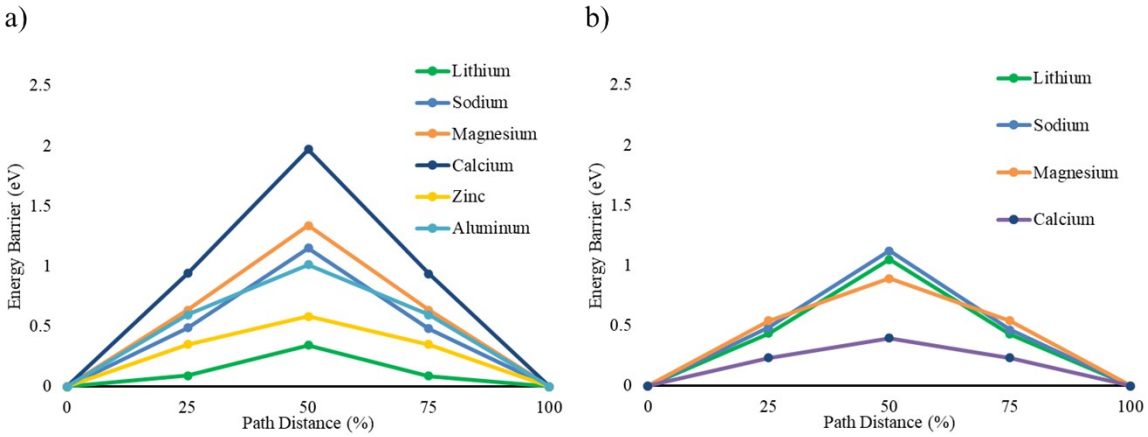

Fig S2: Corresponding ion migration energy barriers in α-V_2O_5 utilizing PBE-D3 for a) V_2O_5 and b) V_2O_5-$(H_2O)_1$.