Investigating the Role of Structural Water on the Electrochemical Properties of $\alpha-\text{V}_2\text{O}_5$ through Density Functional Theory

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Diffusion Calculations

The physical diffusion pathway for Mg in the 2×1×1 supercell of $\alpha$-V$_2$O$_5$ without H$_2$O molecules present is shown in Fig. S1. The same diffusion pathway was used for all ions and structures with H$_2$O present. The energy barriers for all ions investigated as a function of the path distance for a) V$_2$O$_5$ and b) V$_2$O$_5^-$ (H$_2$O)$_1$ are shown in Fig. S2. The energy barriers for Zn and Al in V$_2$O$_5^-$ (H$_2$O)$_1$ are not shown since such calculations failed to converge.

Fig. S1: The ion migration pathway along the $a$ lattice vector for $\alpha$-V$_2$O$_5$ with H$_2$O molecules not shown.

![Diffusion Diagram](image)

![Energy Barriers](image)
**Fig S2:** Corresponding ion migration energy barriers in α-V₂O₅ utilizing PBE-D3 for a) V₂O₅ and b) V₂O₅-(H₂O)₁.