

SUPPLEMENTARY INFORMATION

Unraveling the Role of Structural Water in Bilayer V_2O_5 during Zn^{2+} -Intercalation: Insights from DFT Calculations

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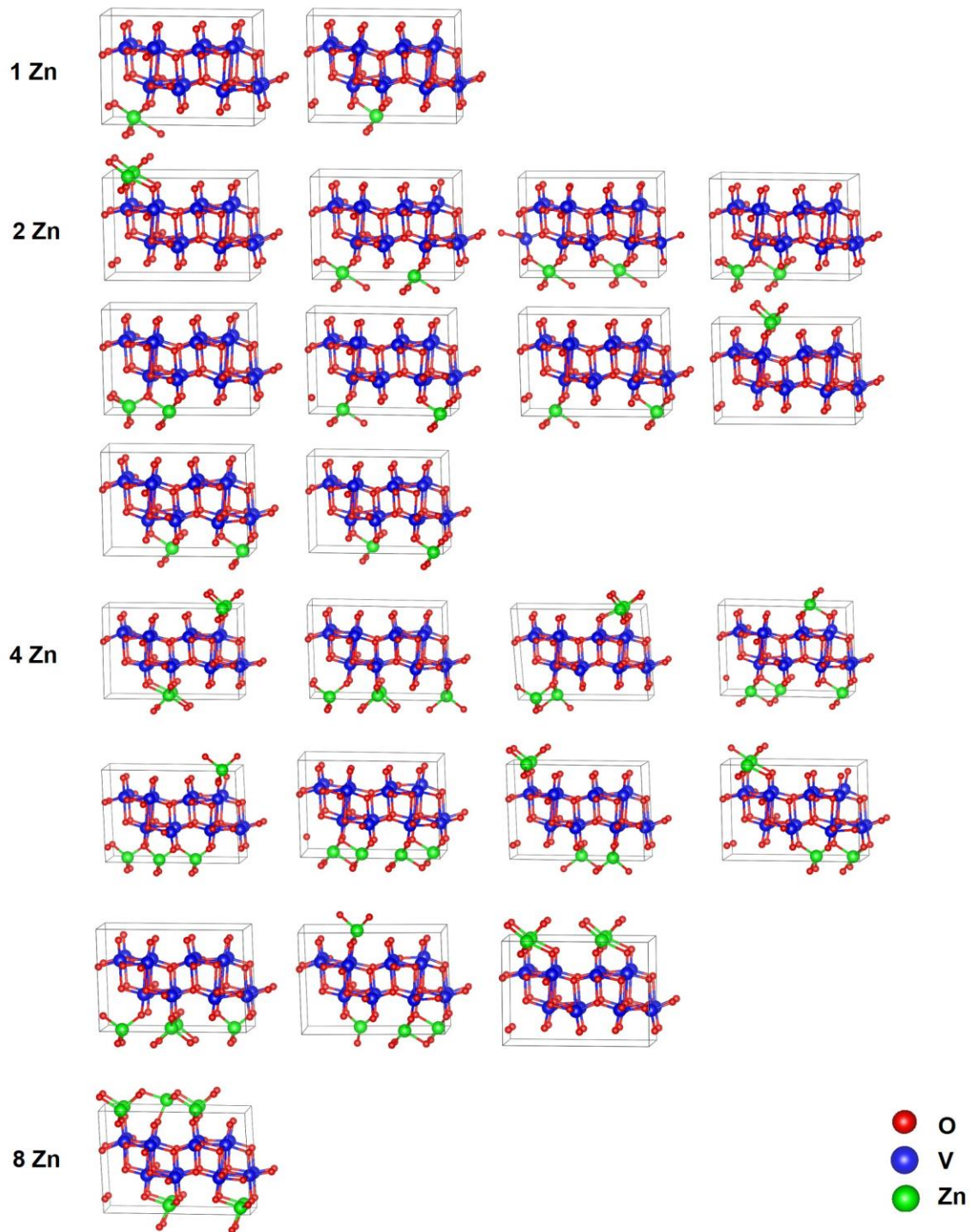


Fig. S1 The optimized different configurations for bilayer V_2O_5 with different numbers of Zn-ion intercalation.

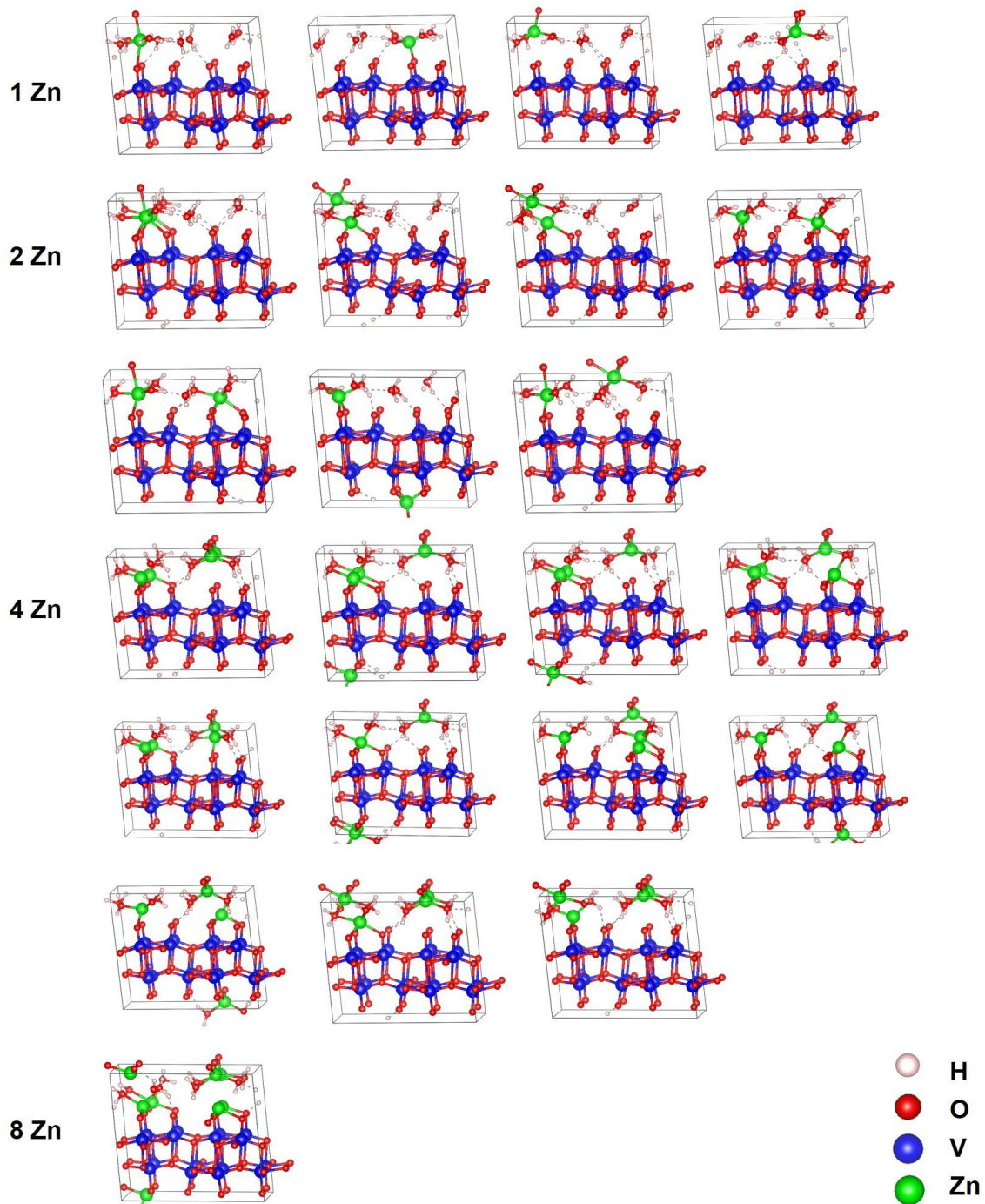


Fig. S2 The optimized different configurations for $V_2O_5 \cdot H_2O$ with different numbers of Zn-ion intercalation.

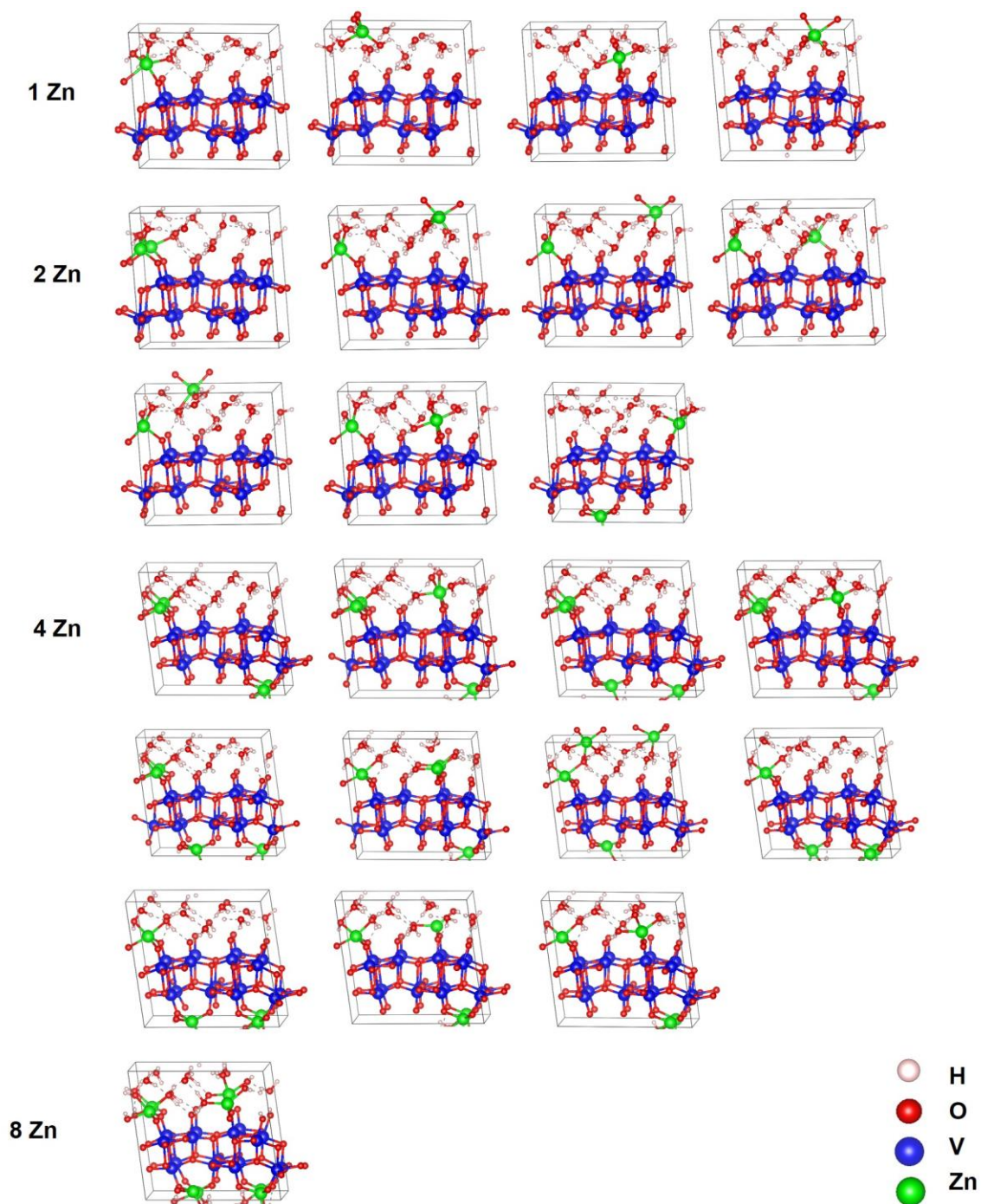


Fig. S3 The optimized different configurations for $V_2O_5 \cdot 1.75H_2O$ with different numbers of Zn-ion intercalation.

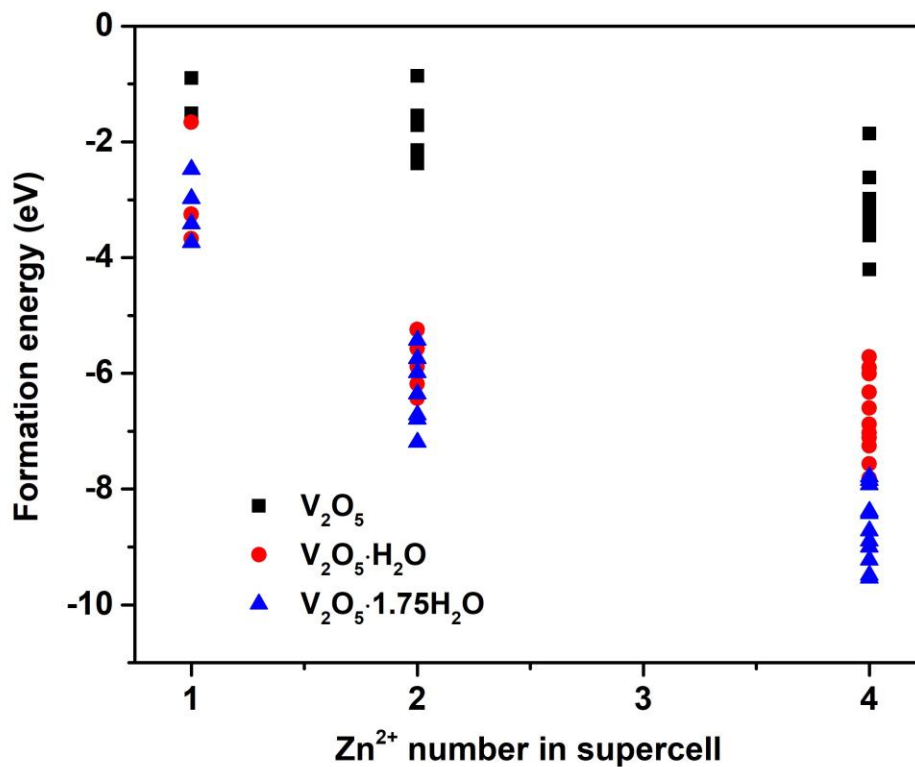


Fig. S4 The formation energies of Zn for V_2O_5 , $V_2O_5 \cdot H_2O$ and $V_2O_5 \cdot 1.75 H_2O$ with different numbers of Zn intercalation. The formation energies of Zn can be calculated using equation $\Delta E_f(Zn) = E(Zn_y V_{16} O_{40} \cdot x H_2 O) - E(V_{16} O_{40} \cdot x H_2 O) - y E(Zn)$.

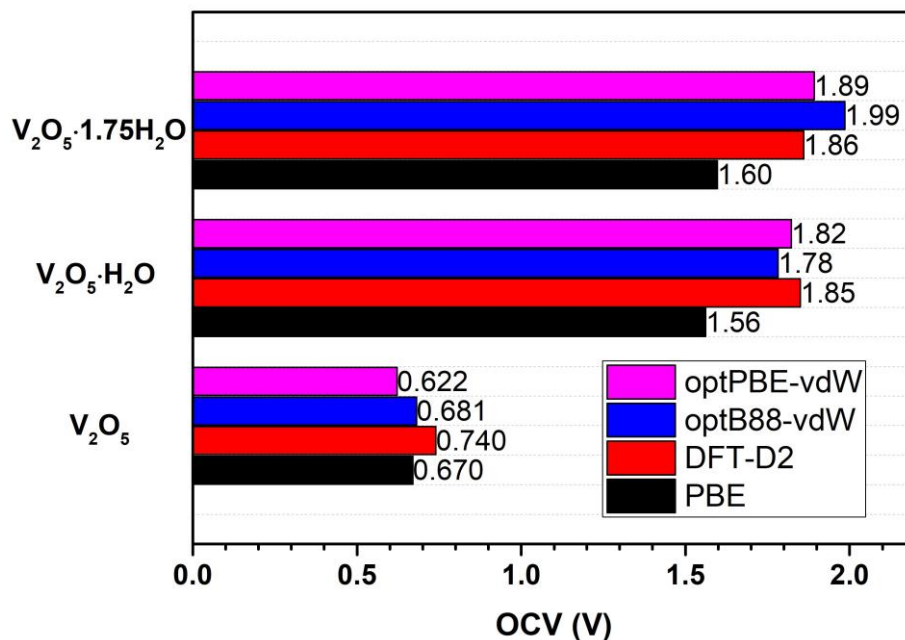


Fig. S5 The calculated OCV by different functional for V_2O_5 , $V_2O_5 \cdot H_2O$ and $V_2O_5 \cdot 1.75 H_2O$.

Table S1 Comparison of calculated lattice parameters of $V_2O_5 \cdot 1.75H_2O$ by different functionals.

Method	a (Å)	b (Å)	c (Å)
PBE	11.82	3.66	11.84
optB88-vdW	11.68	3.64	11.13
optPBE-vdW	11.62	3.63	11.26
DFT-D2	11.63	3.61	11.35
$V_2O_5 \cdot nH_2O$ (exp.)	11.72	3.57	11.52