Supplemental Information: Electronic and structural properties of V_2O_5 layered polymorphs

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TABLE S1. Lattice parameters and percentage deviations for the α and β polymorphs using different van der Waals; interactions.

polymorph		a (Å)	b (Å)	c (Å)	β (deg.)	Δ a (%)	Δ b (%)	Δ c (%)	Δ β (%)
	experimental (Ref. 66)	11.512	3.564	4.368*					
	HSE06	11.362	3.545	4.689*		-1.30	-0.53	7.35*	
	HSE-D2	11.438	3.512	4.415*		-0.64	-1.46	1.08*	
	HSE-D3+damping	11.428	3.527	4.331*		-0.73	-1.04	-0.86*	
α	HSE-D3	11.434	3.532	4.363*		-0.67	-0.90	-0.11*	
	HSE-D4	11.431	3.527	4.359*		-0.70	-1.04	-0.21*	
	HSE-TS	11.448	3.521	4.347*		-0.56	-1.19	-0.49*	
	HSE-TSH	11.458	3.518	4.337*		-0.47	-1.30	-0.71*	
	HSE-rVV10	11.479	3.528	4.215*		-0.29	-1.01	-3.51*	
	HSE-rVV10L	11.450	3.533	4.339*		-0.53	-0.86	-0.66*	
	experimental (Ref. 39)	7.112*	3.579	6.290	90.15				
	HSE06	7.863*	3.539	6.278	91.14	10.56*	-1.13	-0.19	1.10
	HSE-D2	7.092*	3.526	6.237	90.48	-0.28*	-1.49	-0.85	0.37
	HSE-D3+damping	7.079*	3.535	6.231	90.40	-0.46*	-1.24	-0.95	0.27
β	HSE-D3	7.119*	3.529	6.261	90.39	0.10*	-1.41	-0.47	0.27
	HSE-D4	7.149*	3.523	6.245	90.28	0.52*	-1.57	-0.73	0.15
	HSE-TS	7.066*	3.530	6.249	90.07	-0.64*	-1.38	-0.65	-0.08
	HSE-TSH	7.145*	3.529	6.236	90.11	0.47*	-1.41	-0.86	-0.05
	HSE-rVV10	6.990*	3.533	6.213	90.428	-1.71*	-1.30	-1.22	0.31
	HSE-rVV10L	7.153*	3.532	6.250	90.385	0.57*	-1.31	-0.65	0.26

I. LATTICE CONSTANTS

This section has tables, S1 and S2, detailing the lattice constants of the α, β and non-layered B polymorphs as obtained with HSE06 in combination with various approaches to include van der Waals interactions.

II. UNINTERCALATED BANDSTRUCTURES

Bandstructures of the unintercalated layered polymorphs of V_2O_5 are shown in Figs. S1-S8. The color scale indicates the bands' orbital character, where red indicates vanadium and blue oxygen character. All band structures were calculated with HSE06 with Grimme D3 to describe the van der Waals interactions, as described in the main manuscript.

III. LI BANDSTRUCTURES

Bandstructures of the Li intercalated α and ϵ-$Cu_{0.85}$ polymorphs (Fig S9-12) at two concentrations described in their captions. Dark grey bands are V-character, light grey bands are O-character, and red bands are Li-character.

IV. MG BANDSTRUCTURES

Bandstructures of the Mg intercalated α and ϵ-$Cu_{0.85}$ polymorphs (Fig. S13-14). Dark grey bands are V-character, light grey bands are O-character, and green bands are Mg-character. The dashed and solid lines represent the two spins.

V. K BANDSTRUCTURES

Bandstructures of the K intercalated α and ϵ-$Cu_{0.85}$ polymorphs (Fig. S15-16). Dark grey bands are V-character, light grey bands are O-character, and blue bands are K-character. The dashed and solid lines represent the two spins.

VI. ZN BANDSTRUCTURES

Bandstructures of the Zn intercalated α and ϵ-$Cu_{0.85}$ polymorphs (Fig. S17-18). Dark grey bands are V-character, light grey bands are O-character, and bright purple bands are Zn-character. The dashed and solid lines represent the two spins.

TABLE S2. Lattice parameters and percentage deviations for the B polymorph using different van der Waals interactions.

polymorph		a (Å)	b (Å)	c (Å)	β (deg.)	Δ a (%)	Δ b (%)	Δ c (%)	Δ β (%)
	experimental (Ref. 39)	11.972	4.702	5.325	104.41				
	HSE06	11.801	4.644	5.361	103.60	-1.43	-1.24	0.68	-0.78
	HSE-D2	11.761	4.619	5.296	104.20	-1.77	-1.78	-0.54	-0.20
B	HSE-D3+damping	11.766	4.613	5.284	104.06	-1.72	-1.90	-0.78	-0.33
(nonlayered)	HSE-D3	11.807	4.626	5.333	103.97	-1.38	-1.61	0.14	-0.42
	HSE-D4	11.544	4.673	5.305	105.28	-3.57	-0.61	-0.38	0.83
	HSE-TS	11.798	4.603	5.293	103.92	-1.46	-2.10	-0.60	-0.47
	HSE-TSH	11.770	4.611	5.284	103.95	-1.68	-1.94	-0.78	-0.45
	HSE-rVV10	11.768	4.605	5.256	104.23	-1.70	-2.06	-1.30	-0.17
	HSE-rVV10L	11.784	4.623	5.302	103.94	-1.57	-1.68	-0.43	-0.45

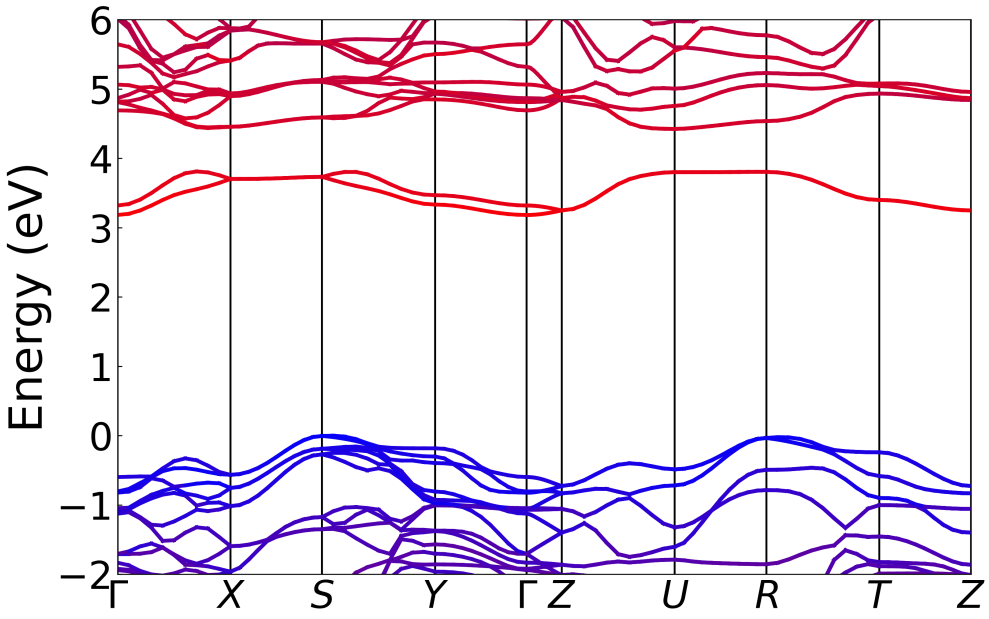

Fig. S1. Calculated bandstructure for the α polymorph (delithiated $Li_xV_2O_5$ for $0 < x < 0.1$).

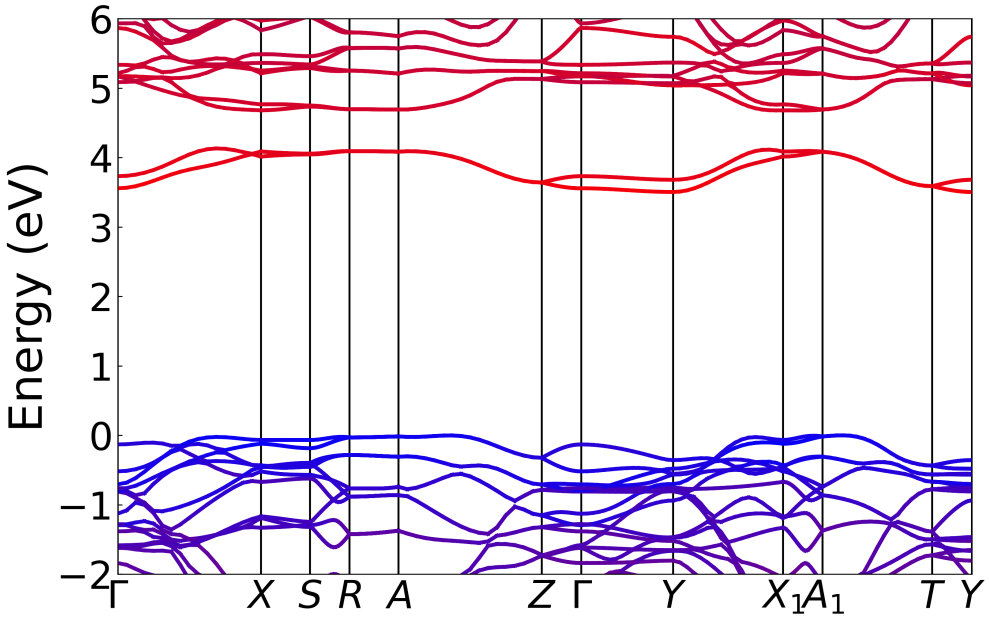

Fig. S2. Calculated bandstructure for the δ polymorph (delithiated $Li_xV_2O_5$ for $0.7 < x < 1$).

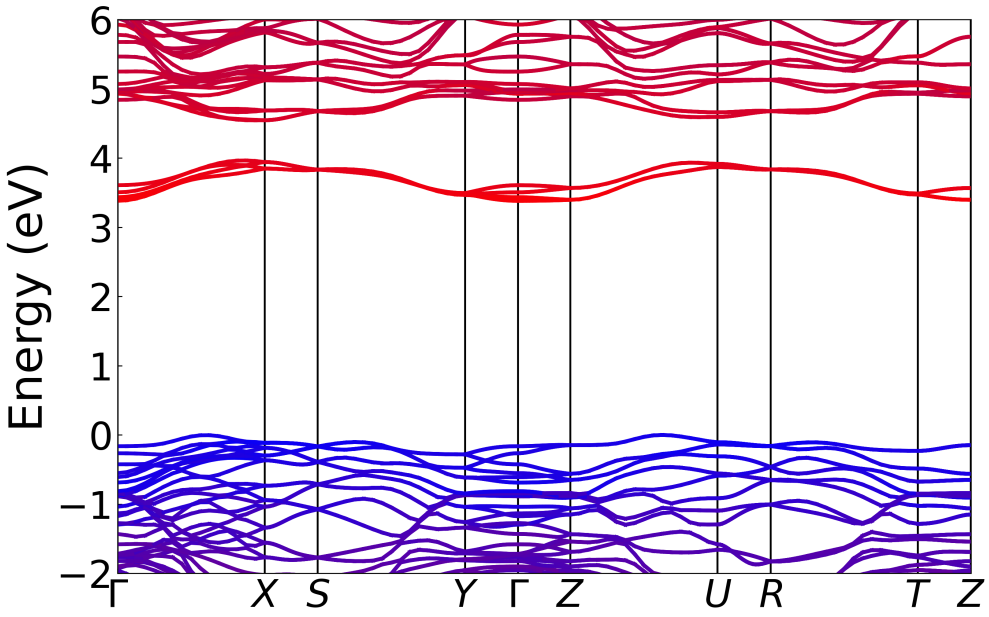

Fig. S3. Calculated bandstructure for the γ polymorph (delithiated $Li_xV_2O_5$ for $1 < x < 2$).

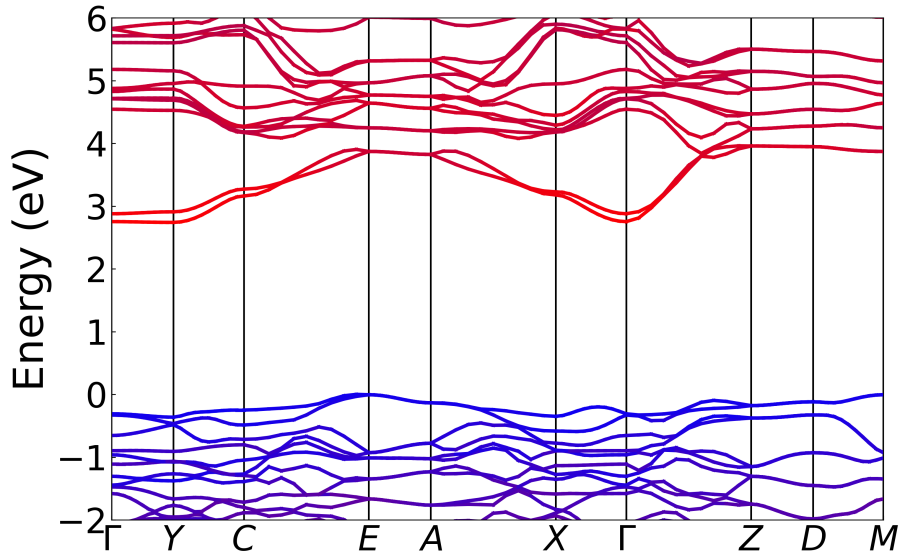

Fig. S4. Calculated bandstructure for the β polymorph (a high temperature and high pressure polymorph of V_2O_5).

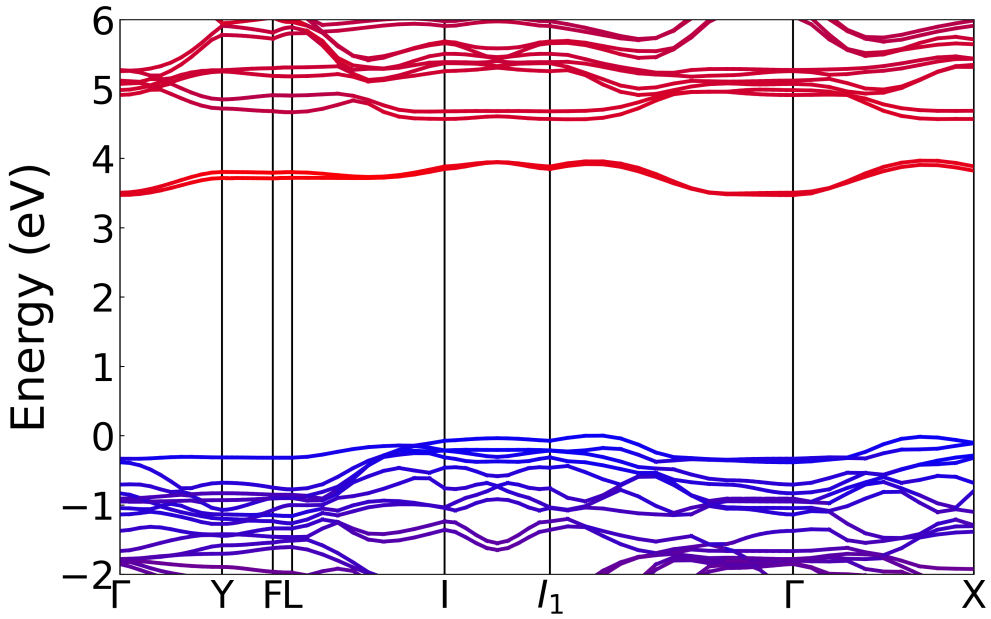

Fig. S5. Calculated bandstructure for the double-layer δ-$Ag_{0.84}$ polymorph (unintercalated $Ag_{0.84}V_2O_5$).

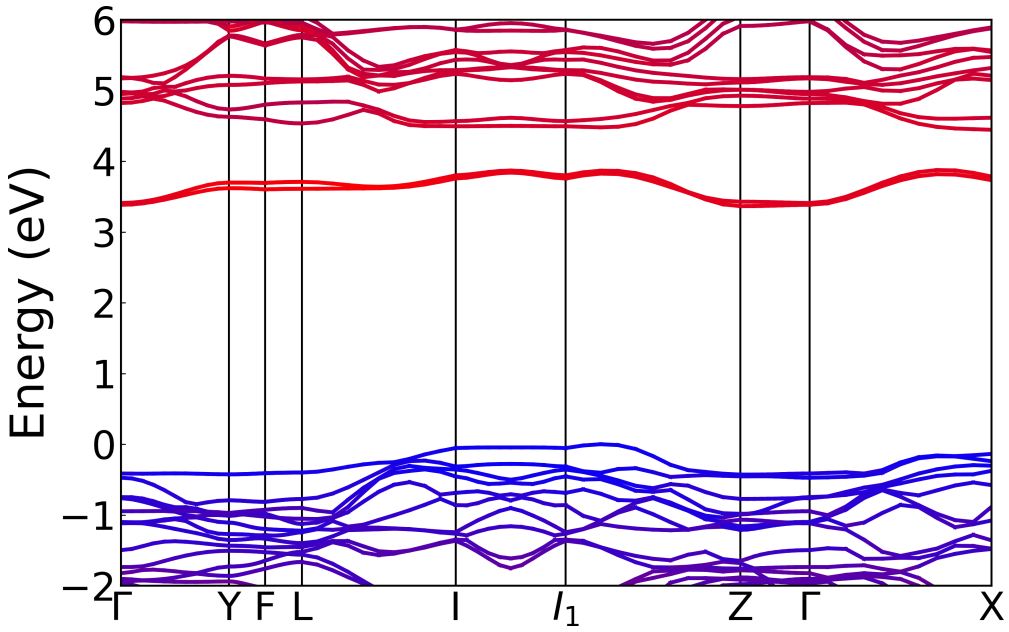

Fig. S6. Calculated bandstructure for the double-layer ϵ-$Cu_{0.85}$ polymorph (unintercalated $Cu_{0.85}V_2O_5$.

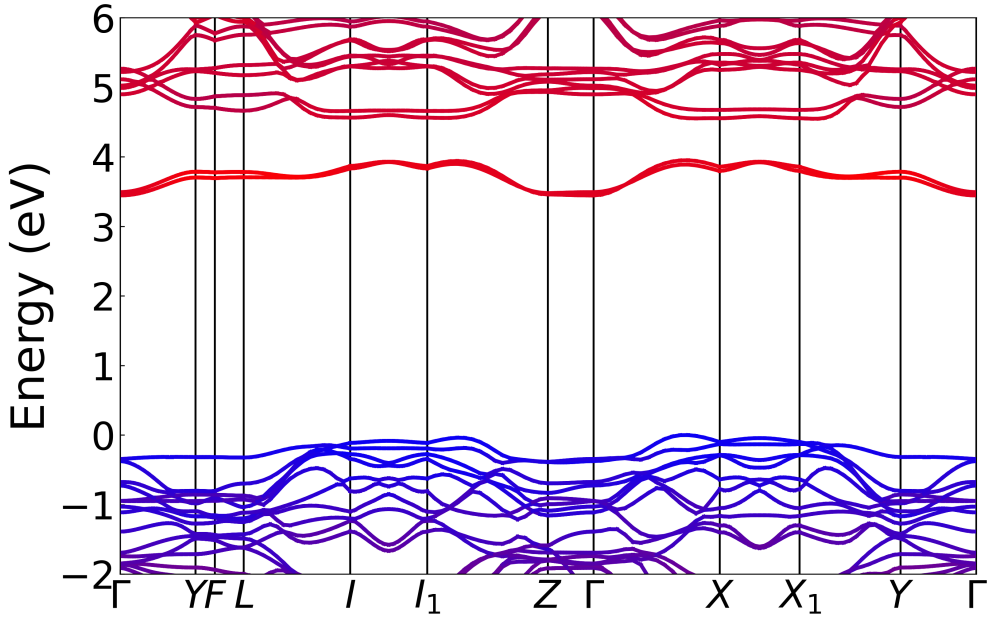

Fig. S7. Calculated bandstructure for the double-layer ν-$Ca_{0.6}$ polymorph (unintercalated $Ca_{0.6}V_2O_5$).

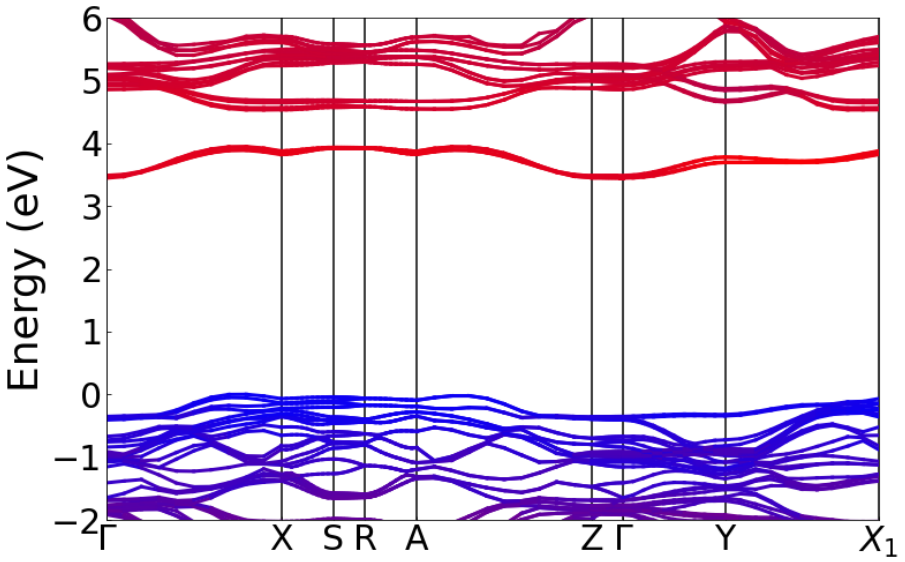

Fig. S8. Calculated bandstructure for the double-layer ρ-$K_{0.5}$ polymorph (unintercalated $K_{0.5}V_2O_5$).

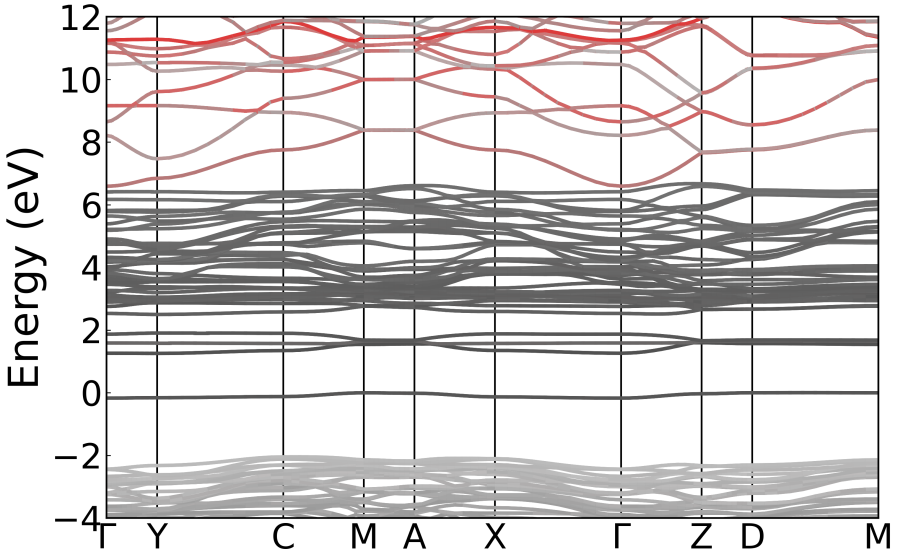

Fig. S9. Calculated bandstructure of α-$Li_{0.5}V_2O_5$ with AFM ordering.

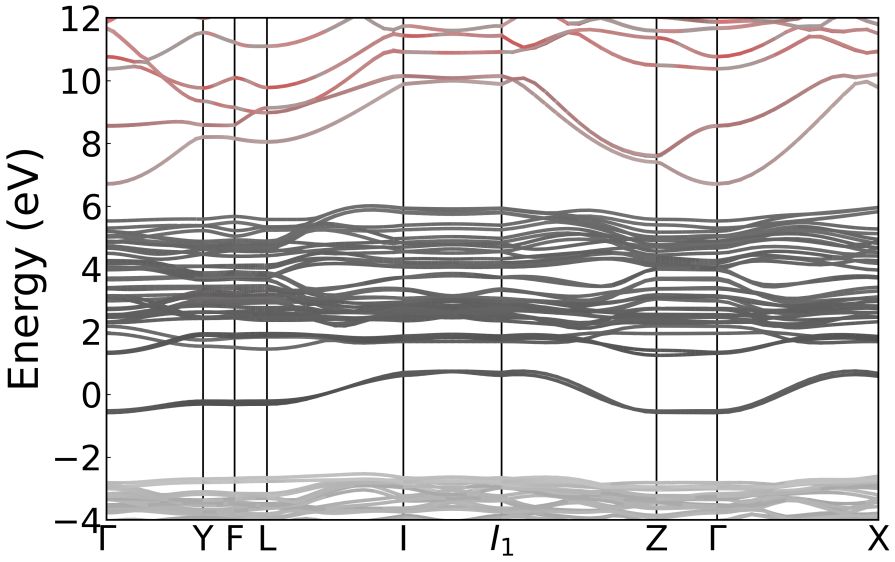

Fig. S10. Calculated bandstructure of $Li_{0.5}V_2O_5$ in the ϵ-$Cu_{0.85}$ polymorph.

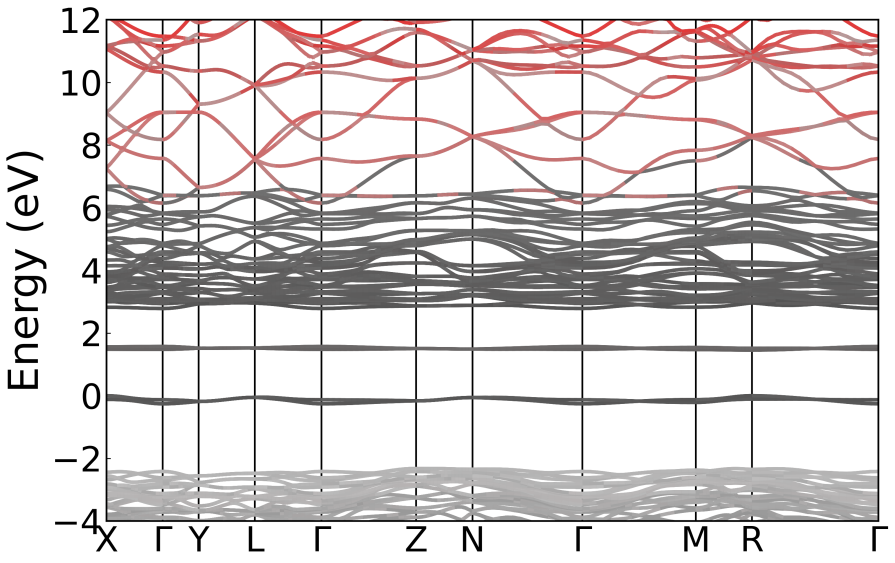

Fig. S11. Calculated bandstructure of α-$Li_1V_2O_5$ with AFM ordering.

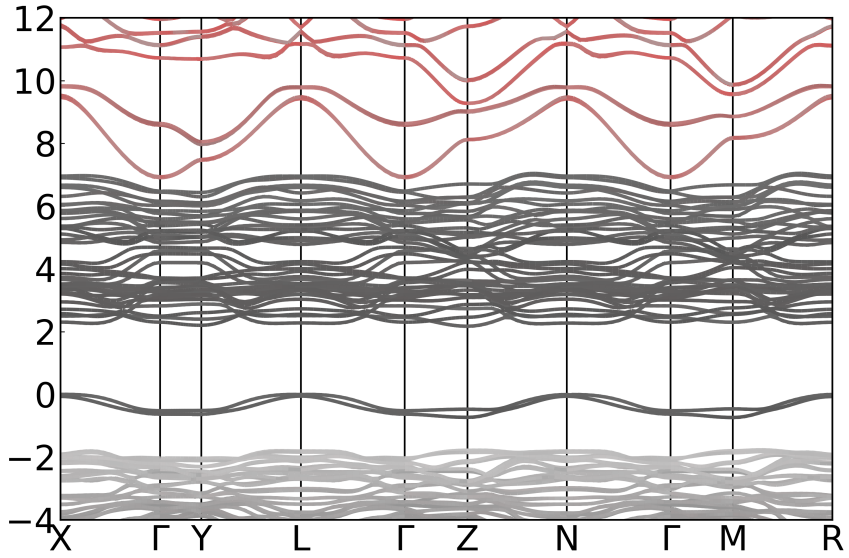

Fig. S12. Calculated bandstructure of $Li_1V_2O_5$ in the ϵ-$Cu_{0.85}$ polymorph.

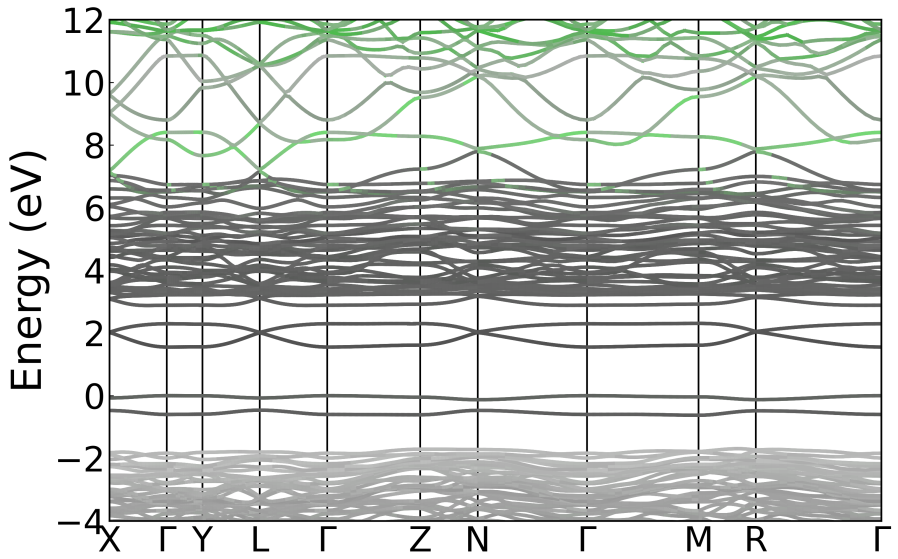

Fig. S13. Calculated bandstructure of α-$Mg_{0.5}V_2O_5$ with AFM ordering.

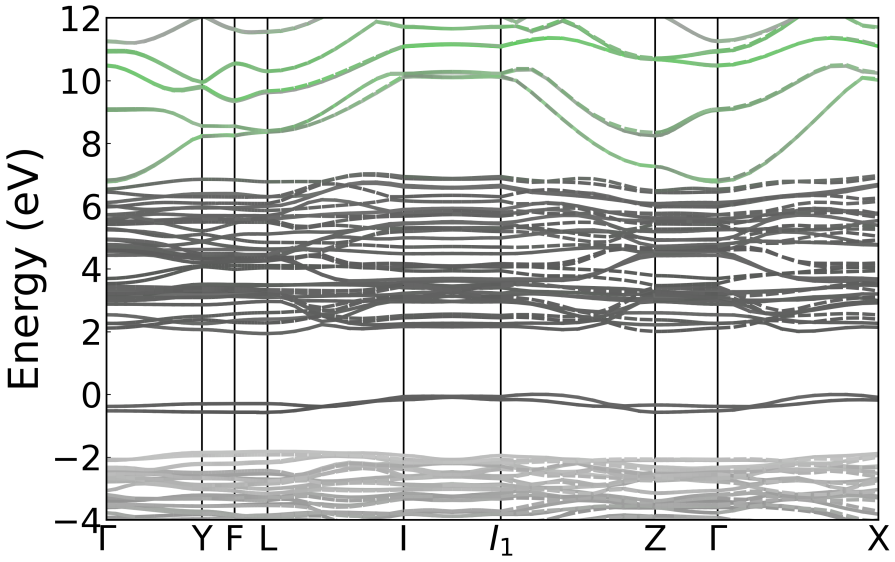

Fig. S14. Calculated bandstructure of $Mg_{0.5}V_2O_5$ in the ϵ-$Cu_{0.85}$ polymorph.

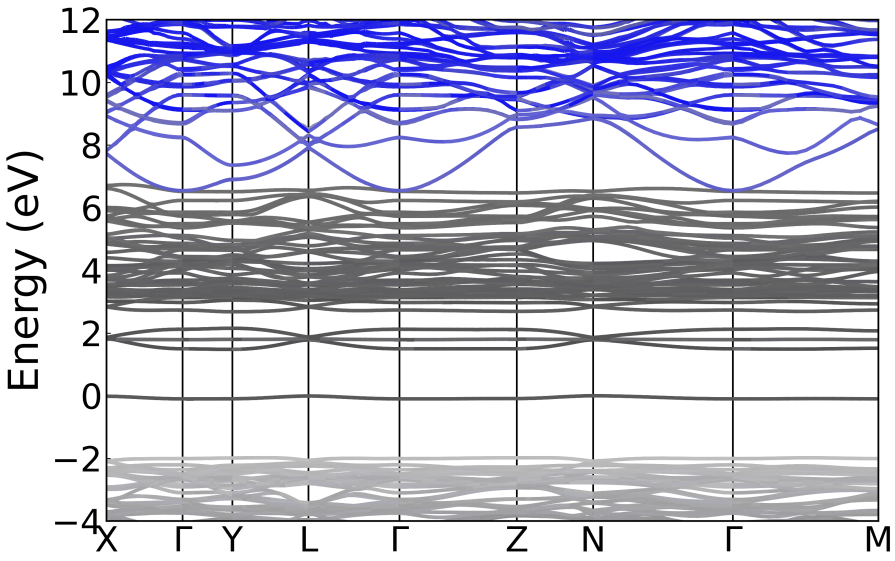

Fig. S15. Calculated bandstructure for the α-$K_{0.5}V_2O_5$ polymorph with AFM ordering.

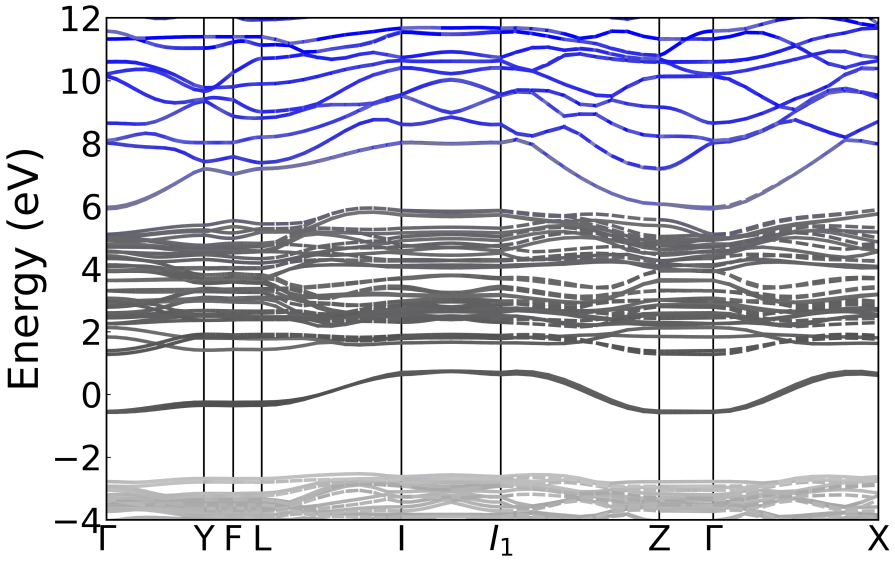

Fig. S16. Calculated bandstructure for $K_{0.5}V_2O_5$ in the ϵ-$Cu_{0.85}$ polymorph.

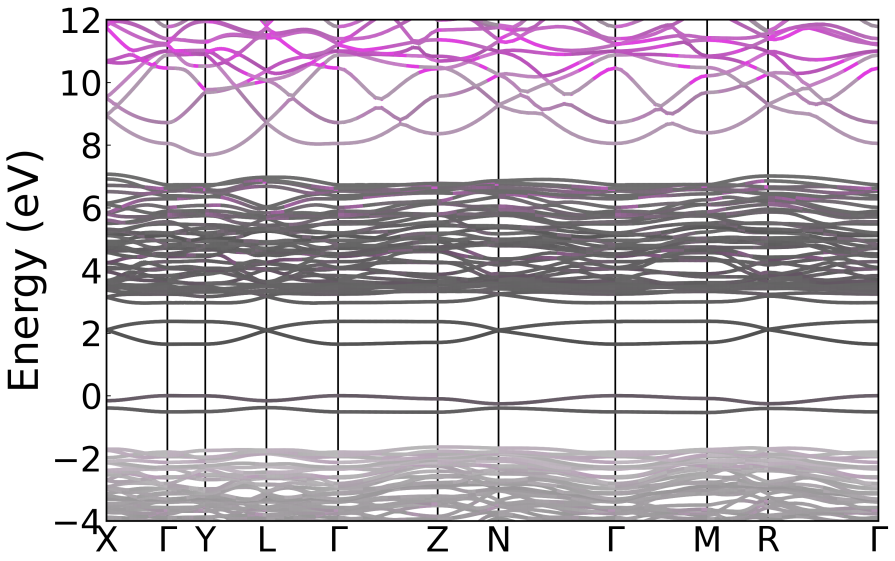

Fig. S17. Calculated bandstructure for the α-$Zn_{0.5}V_2O_5$ polymorph with AFM ordering.

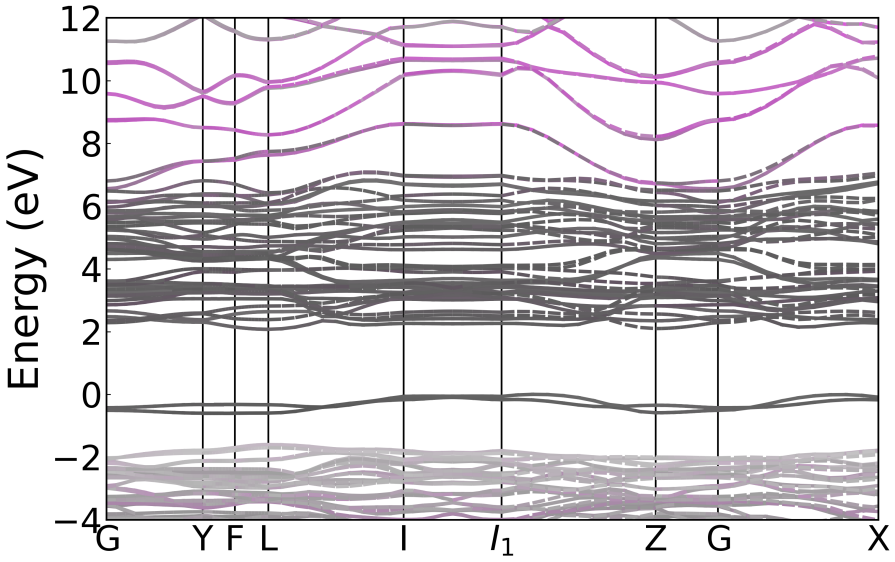

Fig. S18. Calculated bandstructure for $Zn_{0.5}V_2O_5$ in the ϵ-$Cu_{0.85}$ polymorph.