Supplementary Information: Assessment of van der Waals inclusive density functional theory methods for layered electroactive materials

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Average redox potentials

The average redox potential for the Li intercalation process can be approximated by the difference in the total energy between the delithiated and lithiated systems (formation energy), since vibrational and configurational entropy contributions to redox potentials at room temperature are expected to be small.[1] For example, in the case of the $Li_{0\to1}TiTe_2$ system, we computed the average redox potential (Φ) as

$$\Phi = -\frac{E[\mathrm{LiTiTe_2}] - E[\mathrm{TiTe_2}] - E[\mathrm{Li}]}{1e} \tag{S1}$$

where $E[\mathrm{LiTiTe_2}]$ is the total energy per formula unit of $LiTiTe_2$, $E[\mathrm{TiTe_2}]$ is the total energy per formula unit of the fully delithiated system ($TiTe_2$), $E[\mathrm{Li}]$ is the total energy per Li atom of bulk *bcc* Li, and e is the electron charge. Table S3 summarizes all of the computed Φ values for the studied layered materials. In general, this expression can be applied to obtain the average redox potential for any two compositions between x_i and x_j:

$$\Phi = -\frac{E[\mathrm{Li}_{x_j}\mathrm{TiTe_2}] - E[\mathrm{Li}_{x_i}\mathrm{TiTe_2}] - (x_j - x_i)E[\mathrm{Li}]}{(x_j - x_i)e} \tag{S2}$$

Data records

The DFT runs of the entire set of layered materials (all input and output files) are hosted by NoMaD (Novel Materials Discovery) Repository in the following link http://dx.doi.org/10.17172/NOMAD/2016.12.01-1.

System	Method	Structure	E_{tot}	Structure Exp.	Ref.	ICSD
C	PBE	(2.47, 2.47, 8.34) (90.0, 90.0, 120.0)	-55.36	(2.46, 2.46, 6.71)	2	193439
$P6_3/mmmc$	D3	(2.47, 2.47, 6.92) (90.0, 90.0, 120.0)	-55.85	(90.0, 90.0, 120.0)		
	D3BJ	(2.47, 2.47, 6.70) (90.0, 90.0, 120.0)	-56.21			
	dDsC	(2.46, 2.46, 6.70) (90.0, 90.0, 120.0)	-56.10			
	optB86b-vdW	(2.47, 2.47, 6.60) (90.0, 90.0, 120.0)	-48.82			
	optB88-vdW	(2.47, 2.47, 6.70) (90.0, 90.0, 120.0)	-48.17			
	optPBE-vdW	(2.47, 2.47, 6.85) (90.0, 90.0, 120.0)	-47.23			
	BEEF	(2.47, 2.47, 7.26) (90.0, 90.0, 120.0)	-47.65			
	vdW-DF2	(2.48, 2.48, 7.00) (90.0, 90.0, 120.0)	-45.71			
$TiTe_2$	PBE	(3.78, 3.78, 6.81) (90.0, 90.0, 120.0)	-16.18	(3.777, 3.777, 6.498)	3	15543
$P\bar{3}m1$	D3	(3.76, 3.76, 6.46) (90.0, 90.0, 120.0)	-17.00	(90.0, 90.0, 120.0)		
	D3BJ	(3.71, 3.71, 6.35) (90.0, 90.0, 120.0)	-17.68			
	dDsC	(3.74, 3.74, 6.47) (90.0, 90.0, 120.0)	-16.88			
	optB86b-vdW	(3.76, 3.76, 6.47) (90.0, 90.0, 120.0)	-10.15			
	optB88-vdW	(3.81, 3.81, 6.57) (90.0, 90.0, 120.0)	-9.71			
	optPBE-vdW	(3.82, 3.82, 6.75) (90.0, 90.0, 120.0)	-9.29			
	BEEF	(3.81, 3.81, 6.83) (90.0, 90.0, 120.0)	-9.54			
	vdW-DF2	(3.96, 3.96, 6.98) (90.0, 90.0, 120.0)	-8.57			
SnS_2	PBE	(3.70, 3.70, 6.98) (90.0, 90.0, 120.0)	-13.23			
$P\bar{3}m1$	D3	(3.68, 3.68, 5.97) (90.0, 90.0, 120.0)	-13.75			
	D3BJ	(3.67, 3.67, 5.82) (90.0, 90.0, 120.0)	-14.14			
	dDsC	(3.67, 3.67, 6.00) (90.0, 90.0, 120.0)	-13.85			
	optB86b-vdW	(3.68, 3.68, 5.89) (90.0, 90.0, 120.0)	-7.26			
	optB88-vdW	(3.71, 3.71, 5.90) (90.0, 90.0, 120.0)	-6.91			
	optPBE-vdW	(3.72, 3.72, 6.04) (90.0, 90.0, 120.0)	-6.60			
	BEEF	(3.72, 3.72, 6.37) (90.0, 90.0, 120.0)	-7.05			
	vdW-DF2	(3.83, 3.83, 6.04) (90.0, 90.0, 120.0)	-6.06			
VS_2	PBE	(3.20, 3.20, 6.65) (90.0, 90.0, 120.0)	-19.78	(3.217, 3.217, 5.755)	4	651361
$P\bar{3}m1$	D3	(3.18, 3.18, 5.86) (90.0, 90.0, 120.0)	-20.41	(90.0, 90.0, 120.0)		
	D3BJ	(3.15, 3.15, 5.63) (90.0, 90.0, 120.0)	-20.99			
	dDsC	(3.16, 3.16, 5.87) (90.0, 90.0, 120.0)	-20.44			
	optB86b-vdW	(3.18, 3.18, 5.79) (90.0, 90.0, 120.0)	-14.19			
	optB88-vdW	(3.21, 3.21, 5.85) (90.0, 90.0, 120.0)	-13.72			
	optPBE-vdW	(3.23, 3.23, 5.97) (90.0, 90.0, 120.0)	-13.29			
	BEEF	(3.24, 3.24, 6.30) (90.0, 90.0, 120.0)	-13.60			
	vdW-DF2	(3.38, 3.38, 5.97) (90.0, 90.0, 120.0)	-12.52			
TiO_2	PBE	(3.00, 3.00, 15.23) (90.0, 90.0, 120.0)	-26.39			
$R\bar{3}m$	D3	(2.99, 2.99, 13.33) (90.0, 90.0, 120.0)	-26.82			
	D3BJ	(2.99, 2.99, 13.23) (90.0, 90.0, 120.0)	-27.00			
	dDsC	(2.98, 2.98, 13.61) (90.0, 90.0, 120.0)	-26.89			
	optB86b-vdW	(2.98, 2.98, 13.40) (90.0, 90.0, 120.0)	-20.93			
	optB88-vdW	(3.00, 3.00, 13.42) (90.0, 90.0, 120.0)	-20.78			
	optPBE-vdW	(3.01, 3.01, 13.66) (90.0, 90.0, 120.0)	-20.30			
	BEEF	(3.01, 3.01, 14.38) (90.0, 90.0, 120.0)	-20.58			
	vdW-DF2	(3.05, 3.05, 13.72) (90.0, 90.0, 120.0)	-20.26			
TiS_2	PBE	(3.42, 3.42, 6.42) (90.0, 90.0, 120.0)	-19.90	(3.412, 3.412, 5.695)	5	651217
$P\bar{3}m1$	D3	(3.40, 3.40, 5.71) (90.0, 90.0, 120.0)	-20.52	(90.0, 90.0, 120.0)		
	D3BJ	(3.36, 3.36, 5.53) (90.0, 90.0, 120.0)	-21.05			
	dDsC	(3.38, 3.38, 5.71) (90.0, 90.0, 120.0)	-20.53			
	optB86b-vdW	(3.39, 3.39, 5.67) (90.0, 90.0, 120.0)	-14.74			
	optB88-vdW	(3.42, 3.42, 5.73) (90.0, 90.0, 120.0)	-14.38			
	optPBE-vdW	(3.44, 3.44, 5.87) (90.0, 90.0, 120.0)	-13.99			
	BEEF	(3.43, 3.43, 6.19) (90.0, 90.0, 120.0)	-14.29			
	vdW-DF2	(3.52, 3.52, 5.95) (90.0, 90.0, 120.0)	-13.44			
$Ba_8Nb_7O_{24}$	PBE	(5.93, 5.93, 19.30) (90.0, 90.0, 120.0)	-313.25			
$P\bar{3}m1$	D3	(5.91, 5.91, 19.19) (90.0, 90.0, 120.0)	-320.15			
	D3BJ	(5.89, 5.89, 19.14) (90.0, 90.0, 120.0)	-322.52			
	dDsC	(5.87, 5.87, 19.08) (90.0, 90.0, 120.0)	-325.04			
	optB86b-vdW	(5.89, 5.89, 19.12) (90.0, 90.0, 120.0)	-245.85			
	optB88-vdW	(5.91, 5.91, 19.19) (90.0, 90.0, 120.0)	-244.44			
	optPBE-vdW	(5.94, 5.94, 19.30) (90.0, 90.0, 120.0)	-237.83			
	BEEF	(5.96, 5.96, 19.36) (90.0, 90.0, 120.0)	-240.99			
	vdW-DF2	(6.03, 6.03, 19.57) (90.0, 90.0, 120.0)	-238.05			

System	Method	Structure	E_{tot}	Structure Exp.	Ref.	ICSD
MnO_2	PBE	(2.92, 2.92, 5.18) (90.0, 90.0, 120.0)	-21.26			
$P\bar{3}m1$	D3	(2.91, 2.91, 4.60) (90.0, 90.0, 120.0)	-21.52			
	D3BJ	(2.91, 2.91, 4.57) (90.0, 90.0, 120.0)	-21.62			
	dDsC	(2.90, 2.90, 4.51) (90.0, 90.0, 120.0)	-21.80			
	optB86b-vdW	(2.90, 2.90, 4.46) (90.0, 90.0, 120.0)	-14.97			
	optB88-vdW	(2.91, 2.91, 4.44) (90.0, 90.0, 120.0)	-14.75			
	optPBE-vdW	(2.93, 2.93, 4.55) (90.0, 90.0, 120.0)	-14.31			
	BEEF	(2.94, 2.94, 4.77) (90.0, 90.0, 120.0)	-14.78			
	vdW-DF2	(2.97, 2.97, 4.55) (90.0, 90.0, 120.0)	-14.10			
CrS_2	PBE	(3.33, 3.33, 5.65) (90.0, 90.0, 120.0)	-19.41			
$P\bar{3}m1$	D3	(3.31, 3.31, 5.29) (90.0, 90.0, 120.0)	-20.06			
	D3BJ	(3.29, 3.29, 5.23) (90.0, 90.0, 120.0)	-20.45			
	dDsC	(3.30, 3.30, 5.34) (90.0, 90.0, 120.0)	-20.09			
	optB86b-vdW	(3.31, 3.31, 5.32) (90.0, 90.0, 120.0)	-13.79			
	optB88-vdW	(3.33, 3.33, 5.39) (90.0, 90.0, 120.0)	-13.37			
	optPBE-vdW	(3.35, 3.35, 5.52) (90.0, 90.0, 120.0)	-12.95			
	BEEF	(3.35, 3.35, 5.56) (90.0, 90.0, 120.0)	-13.30			
	vdW-DF2	(3.45, 3.45, 5.61) (90.0, 90.0, 120.0)	-12.22			
$Sr_3Nb_4O_{13}$	PBE	(3.98, 3.98, 36.90) (90.0, 90.0, 90.0)	-164.21			
I4/mmm	D3	(3.97, 3.97, 34.94) (90.0, 90.0, 90.0)	-168.07			
	D3BJ	(3.96, 3.96, 34.43) (90.0, 90.0, 90.0)	-168.63			
	dDsC	(3.96, 3.96, 34.52) (90.0, 90.0, 90.0)	-167.37			
	optB86b-vdW	(3.96, 3.96, 34.17) (90.0, 90.0, 90.0)	-128.71			
	optB88-vdW	(3.97, 3.97, 34.37) (90.0, 90.0, 90.0)	-127.96			
	optPBE-vdW	(3.99, 3.99, 34.86) (90.0, 90.0, 90.0)	-124.83			
	BEEF	(4.00, 4.00, 36.50) (90.0, 90.0, 90.0)	-126.65			
	vdW-DF2	(4.03, 4.03, 35.75) (90.0, 90.0, 90.0)	-124.98			
V_2O_5	PBE	(3.62, 4.75, 11.56) (90.0, 90.0, 90.0)	-51.83	(3.56, 4.37, 11.56)	6	41030
Pmnm	D3	(3.61, 4.38, 11.66) (90.0, 90.0, 90.0)	-52.61	(90.0, 90.0, 90.0)		
	D3BJ	(3.61, 4.34, 11.65) (90.0, 90.0, 90.0)	-52.89			
	dDsC	(3.61, 4.23, 11.71) (90.0, 90.0, 90.0)	-52.74			
	optB86b-vdW	(3.61, 4.20, 11.72) (90.0, 90.0, 90.0)	-38.15			
	optB88-vdW	(3.61, 4.23, 11.74) (90.0, 90.0, 90.0)	-37.81			
	optPBE-vdW	(3.62, 4.44, 11.69) (90.0, 90.0, 90.0)	-36.86			
	BEEF	(3.62, 4.82, 11.61) (90.0, 90.0, 90.0)	-37.77			
	vdW-DF2	(3.65, 4.51, 11.83) (90.0, 90.0, 90.0)	-36.98			
VO_2	PBE	(2.94, 2.94, 15.37) (90.0, 90.0, 120.0)	-22.43			
$R\bar{3}m$	D3	(2.93, 2.93, 13.60) (90.0, 90.0, 120.0)	-22.83			
	D3BJ	(2.93, 2.93, 13.50) (90.0, 90.0, 120.0)	-23.00			
	dDsC	(2.92, 2.92, 13.76) (90.0, 90.0, 120.0)	-22.94			
	optB86b-vdW	(2.92, 2.92, 13.55) (90.0, 90.0, 120.0)	-16.47			
	optB88-vdW	(2.95, 2.95, 13.46) (90.0, 90.0, 120.0)	-16.29			
	optPBE-vdW	(2.96, 2.96, 13.87) (90.0, 90.0, 120.0)	-15.83			
	BEEF	(2.97, 2.97, 14.38) (90.0, 90.0, 120.0)	-16.17			
	vdW-DF2	(3.02, 3.02, 13.71) (90.0, 90.0, 120.0)	-15.75			
NiO_2	PBE	(2.80, 2.80, 4.72) (90.0, 90.0, 120.0)	-13.57	(2.82, 2.82, 4.37)	7	
$P\bar{3}m1$	D3	(2.79, 2.79, 4.34) (90.0, 90.0, 120.0)	-13.91	(90.0, 90.0, 120.0)		
	D3BJ	(2.79, 2.79, 4.36) (90.0, 90.0, 120.0)	-14.03			
	dDsC	(2.78, 2.78, 4.33) (90.0, 90.0, 120.0)	-14.15			
	optB86b-vdW	(2.78, 2.78, 4.31) (90.0, 90.0, 120.0)	-6.65			
	optB88-vdW	(2.79, 2.79, 4.31) (90.0, 90.0, 120.0)	-6.47			
	optPBE-vdW	(2.80, 2.80, 4.41) (90.0, 90.0, 120.0)	-5.95			
	BEEF	(2.84, 2.84, 4.59) (90.0, 90.0, 120.0)	-6.22			
	vdW-DF2	(2.96, 2.96, 4.20) (90.0, 90.0, 120.0)	-6.06			
V_2O_5	PBE	(3.64, 10.24, 10.95) (90.0, 90.0, 90.0)	-51.77	(3.585, 9.946, 10.042)	8	80594
Pnma	D3	(3.63, 10.05, 10.15) (90.0, 90.0, 90.0)	-52.54	(90.0, 90.0, 90.0)		
	D3BJ	(3.62, 10.03, 10.08) (90.0, 90.0, 90.0)	-52.82			
	dDsC	(3.62, 10.05, 10.04) (90.0, 90.0, 90.0)	-52.65			
	optB86b-vdW	(3.62, 9.99, 9.93) (90.0, 90.0, 90.0)	-38.08			
	optB88-vdW	(3.63, 10.03, 9.95) (90.0, 90.0, 90.0)	-37.73			
	optPBE-vdW	(3.64, 10.11, 10.22) (90.0, 90.0, 90.0)	-36.80			
	BEEF	(3.64, 10.20, 10.83) (90.0, 90.0, 90.0)	-37.72			
	vdW-DF2	(3.67, 10.27, 10.32) (90.0, 90.0, 90.0)	-36.89			

System	Method	Structure	E_{tot}	Structure Exp.	Ref.	ICSD
CoO_2	PBE	(2.83, 2.83, 15.18) (90.0, 90.0, 120.0)	-17.21	(2.84, 2.84, 13.44)	9	
R$\bar{3}$m	D3	(2.82, 2.82, 13.51) (90.0, 90.0, 120.0)	-17.51	(90.0, 90.0, 120.0)		
	D3BJ	(2.82, 2.82, 13.48) (90.0, 90.0, 120.0)	-17.62			
	dDsC	(2.81, 2.81, 13.31) (90.0, 90.0, 120.0)	-17.80			
	optB86b-vdW	(2.81, 2.81, 13.21) (90.0, 90.0, 120.0)	-11.71			
	optB88-vdW	(2.83, 2.83, 13.14) (90.0, 90.0, 120.0)	-11.51			
	optPBE-vdW	(2.84, 2.84, 13.47) (90.0, 90.0, 120.0)	-11.02			
	BEEF	(2.86, 2.86, 14.11) (90.0, 90.0, 120.0)	-11.18			
	vdW-DF2	(2.91, 2.91, 13.50) (90.0, 90.0, 120.0)	-10.88			
NiO_2	PBE	(2.80, 2.80, 14.30) (90.0, 90.0, 120.0)	-13.58	(2.835, 2.835, 14.332)	10	78698
R$\bar{3}$m	D3	(2.79, 2.79, 13.18) (90.0, 90.0, 120.0)	-13.91	(90.0, 90.0, 120.0)		
	D3BJ	(2.79, 2.79, 13.18) (90.0, 90.0, 120.0)	-14.03			
	dDsC	(2.78, 2.78, 13.14) (90.0, 90.0, 120.0)	-14.15			
	optB86b-vdW	(2.78, 2.78, 13.06) (90.0, 90.0, 120.0)	-6.65			
	optB88-vdW	(2.79, 2.79, 13.06) (90.0, 90.0, 120.0)	-6.47			
	optPBE-vdW	(2.80, 2.80, 13.33) (90.0, 90.0, 120.0)	-5.95			
	BEEF	(2.84, 2.84, 13.79) (90.0, 90.0, 120.0)	-6.22			
	vdW-DF2	(2.86, 2.86, 13.42) (90.0, 90.0, 120.0)	-5.99			
$V(CO_3)_2$	PBE	(4.85, 4.85, 16.76) (90.0, 90.0, 120.0)	-68.66			
R$\bar{3}$	D3	(4.82, 4.82, 15.79) (90.0, 90.0, 120.0)	-69.34			
	D3BJ	(4.82, 4.82, 15.72) (90.0, 90.0, 120.0)	-69.58			
	dDsC	(4.79, 4.79, 15.50) (90.0, 90.0, 120.0)	-69.64			
	optB86b-vdW	(4.77, 4.77, 15.25) (90.0, 90.0, 120.0)	-53.84			
	optB88-vdW	(4.78, 4.78, 15.23) (90.0, 90.0, 120.0)	-53.26			
	optPBE-vdW	(4.81, 4.81, 15.55) (90.0, 90.0, 120.0)	-52.09			
	BEEF	(4.83, 4.83, 16.01) (90.0, 90.0, 120.0)	-53.31			
	vdW-DF2	(4.86, 4.86, 15.67) (90.0, 90.0, 120.0)	-51.38			
$Co_2C_2O_7$	PBE	(4.84, 8.48, 16.99) (90.0, 95.7, 90.0)	-75.02			
C2/c	D3	(4.80, 8.49, 16.09) (90.0, 107.1, 90.0)	-75.75			
	D3BJ	(4.80, 8.48, 16.08) (90.0, 107.0, 90.0)	-75.97			
	dDsC	(4.77, 8.46, 15.91) (90.0, 107.5, 90.0)	-76.03			
	optB86b-vdW	(4.77, 8.46, 15.68) (90.0, 108.1, 90.0)	-55.94			
	optB88-vdW	(4.77, 8.48, 15.71) (90.0, 108.2, 90.0)	-55.21			
	optPBE-vdW	(4.80, 8.51, 16.02) (90.0, 107.8, 90.0)	-53.97			
	BEEF	(4.85, 8.55, 16.53) (90.0, 107.4, 90.0)	-55.86			
	vdW-DF2	(4.85, 8.62, 16.21) (90.0, 107.6, 90.0)	-53.21			
$Ba_4Nb_3O_{12}$	PBE	(5.92, 5.92, 19.49) (90.0, 90.0, 120.0)	-148.55			
P63mc	D3	(5.89, 5.89, 19.36) (90.0, 90.0, 120.0)	-151.66			
	D3BJ	(5.87, 5.87, 19.29) (90.0, 90.0, 120.0)	-152.74			
	dDsC	(5.84, 5.84, 19.19) (90.0, 90.0, 120.0)	-154.15			
	optB86b-vdW	(5.86, 5.86, 19.23) (90.0, 90.0, 120.0)	-115.84			
	optB88-vdW	(5.89, 5.89, 19.31) (90.0, 90.0, 120.0)	-115.31			
	optPBE-vdW	(5.92, 5.92, 19.45) (90.0, 90.0, 120.0)	-112.28			
	BEEF	(5.94, 5.94, 19.58) (90.0, 90.0, 120.0)	-114.02			
	vdW-DF2	(6.01, 6.01, 19.75) (90.0, 90.0, 120.0)	-112.88			
$Fe(CO_3)_2$	PBE	(4.78, 4.78, 17.00) (90.0, 90.0, 120.0)	-64.33			
R$\bar{3}$	D3	(4.75, 4.75, 16.10) (90.0, 90.0, 120.0)	-65.02			
	D3BJ	(4.75, 4.75, 16.03) (90.0, 90.0, 120.0)	-65.23			
	dDsC	(4.71, 4.71, 15.80) (90.0, 90.0, 120.0)	-65.35			
	optB86b-vdW	(4.69, 4.69, 15.45) (90.0, 90.0, 120.0)	-48.83			
	optB88-vdW	(4.70, 4.70, 15.45) (90.0, 90.0, 120.0)	-48.17			
	optPBE-vdW	(4.74, 4.74, 15.76) (90.0, 90.0, 120.0)	-47.13			
	BEEF	(4.89, 4.89, 16.36) (90.0, 90.0, 120.0)	-48.48			
	vdW-DF2	(4.80, 4.80, 15.92) (90.0, 90.0, 120.0)	-46.26			

Table S1: Lattice parameters (a, b, c) and (α, β, γ) in Å and degrees of different empty hosts using different vdW-inclusive methods and PBE. In addition, we show the computed total energies in eV per formula unit (E_{tot}) and the experimental structural parameters taken from the specified references. When available, the corresponding collection code assigned to each entry in the inorganic crystal structure database (ICSD) is also provided.

System	Method	Structure	E_{tot}	Structure Exp.	Ref.	ICSD
LiC_6	PBE	(4.33, 4.33, 3.74) (90.0, 90.0, 120.0)	-57.34	(4.301, 4.301, 3.687)	2	193441
P6/mmm	D3	(4.32, 4.32, 3.64) (90.0, 90.0, 120.0)	-57.95	(90.0, 90.0, 120.0)		
	D3BJ	(4.31, 4.31, 3.59) (90.0, 90.0, 120.0)	-58.37			
	dDsC	(4.31, 4.31, 3.60) (90.0, 90.0, 120.0)	-58.25			
	optB86b-vdW	(4.33, 4.33, 3.61) (90.0, 90.0, 120.0)	-50.06			
	optB88-vdW	(4.33, 4.33, 3.63) (90.0, 90.0, 120.0)	-49.38			
	optPBE-vdW	(4.34, 4.34, 3.67) (90.0, 90.0, 120.0)	-48.37			
	BEEF	(4.32, 4.32, 3.67) (90.0, 90.0, 120.0)	-48.93			
	vdW-DF2	(4.35, 4.35, 3.73) (90.0, 90.0, 120.0)	-46.83			
$LiTiTe_2$	PBE	(3.99, 3.99, 6.89) (90.0, 90.0, 120.0)	-19.31	(3.82, 3.82, 6.925)	11	44908
$P\bar{3}m1$	D3	(3.95, 3.95, 6.80) (90.0, 90.0, 120.0)	-20.43	(90.0, 90.0, 120.0)		
	D3BJ	(3.90, 3.90, 6.68) (90.0, 90.0, 120.0)	-21.07			
	dDsC	(3.94, 3.94, 6.79) (90.0, 90.0, 120.0)	-20.08			
	optB86b-vdW	(3.96, 3.96, 6.84) (90.0, 90.0, 120.0)	-12.40			
	optB88-vdW	(4.00, 4.00, 6.85) (90.0, 90.0, 120.0)	-12.00			
	optPBE-vdW	(4.02, 4.02, 6.90) (90.0, 90.0, 120.0)	-11.53			
	BEEF	(4.02, 4.02, 6.89) (90.0, 90.0, 120.0)	-11.94			
	vdW-DF2	(4.14, 4.14, 7.05) (90.0, 90.0, 120.0)	-10.91			
$LiSnS_2$	PBE	(3.77, 3.77, 6.51) (90.0, 90.0, 120.0)	-16.72			
$P\bar{3}m1$	D3	(3.73, 3.73, 6.40) (90.0, 90.0, 120.0)	-17.47			
	D3BJ	(3.70, 3.70, 6.35) (90.0, 90.0, 120.0)	-17.98			
	dDsC	(3.72, 3.72, 6.41) (90.0, 90.0, 120.0)	-17.47			
	optB86b-vdW	(3.74, 3.74, 6.45) (90.0, 90.0, 120.0)	-10.02			
	optB88-vdW	(3.77, 3.77, 6.49) (90.0, 90.0, 120.0)	-9.75			
	optPBE-vdW	(3.79, 3.79, 6.51) (90.0, 90.0, 120.0)	-9.36			
	BEEF	(3.79, 3.79, 6.50) (90.0, 90.0, 120.0)	-9.89			
	vdW-DF2	(3.90, 3.90, 6.62) (90.0, 90.0, 120.0)	-9.15			
$LiVS_2$	PBE	(3.48, 3.48, 6.04) (90.0, 90.0, 120.0)	-23.49	(3.390, 3.390, 6.100)	4	642325
$P\bar{3}m1$	D3	(3.44, 3.44, 5.92) (90.0, 90.0, 120.0)	-24.51	(90.0, 90.0, 120.0)		
	D3BJ	(3.42, 3.42, 5.88) (90.0, 90.0, 120.0)	-25.03			
	dDsC	(3.44, 3.44, 5.96) (90.0, 90.0, 120.0)	-24.25			
	optB86b-vdW	(3.45, 3.45, 6.00) (90.0, 90.0, 120.0)	-17.01			
	optB88-vdW	(3.48, 3.48, 6.02) (90.0, 90.0, 120.0)	-16.67			
	optPBE-vdW	(3.50, 3.50, 6.04) (90.0, 90.0, 120.0)	-16.21			
	BEEF	(3.49, 3.49, 6.02) (90.0, 90.0, 120.0)	-16.78			
	vdW-DF2	(3.57, 3.57, 6.13) (90.0, 90.0, 120.0)	-15.73			
$LiTiO_2$	PBE	(2.91, 2.91, 14.99) (90.0, 90.0, 120.0)	-30.10			
$R\bar{3}m$	D3	(2.88, 2.88, 14.79) (90.0, 90.0, 120.0)	-31.09			
	D3BJ	(2.88, 2.88, 14.73) (90.0, 90.0, 120.0)	-31.29			
	dDsC	(2.89, 2.89, 14.82) (90.0, 90.0, 120.0)	-30.78			
	optB86b-vdW	(2.90, 2.90, 14.87) (90.0, 90.0, 120.0)	-23.98			
	optB88-vdW	(2.91, 2.91, 14.88) (90.0, 90.0, 120.0)	-23.88			
	optPBE-vdW	(2.92, 2.92, 14.97) (90.0, 90.0, 120.0)	-23.27			
	BEEF	(2.95, 2.95, 14.86) (90.0, 90.0, 120.0)	-23.66			
	vdW-DF2	(2.99, 2.99, 15.01) (90.0, 90.0, 120.0)	-23.38			
$LiTiS_2$	PBE	(3.45, 3.45, 6.20) (90.0, 90.0, 120.0)	-23.69	(3.459, 3.459, 6.188)	12	200709
$P\bar{3}m1$	D3	(3.41, 3.41, 6.10) (90.0, 90.0, 120.0)	-24.75	(90.0, 90.0, 120.0)		
	D3BJ	(3.38, 3.38, 6.06) (90.0, 90.0, 120.0)	-25.30			
	dDsC	(3.41, 3.41, 6.14) (90.0, 90.0, 120.0)	-24.44			
	optB86b-vdW	(3.42, 3.42, 6.17) (90.0, 90.0, 120.0)	-17.74			
	optB88-vdW	(3.45, 3.45, 6.17) (90.0, 90.0, 120.0)	-17.39			
	optPBE-vdW	(3.48, 3.48, 6.19) (90.0, 90.0, 120.0)	-16.92			
	BEEF	(3.48, 3.48, 6.16) (90.0, 90.0, 120.0)	-17.40			
	vdW-DF2	(3.57, 3.57, 6.25) (90.0, 90.0, 120.0)	-16.45			
$LiBa_8Nb_7O_{24}$	PBE	(5.92, 5.92, 19.24) (90.0, 90.0, 120.0)	-317.11			
$P\bar{3}m1$	D3	(5.89, 5.89, 19.14) (90.0, 90.0, 120.0)	-324.33			
	D3BJ	(5.88, 5.88, 19.11) (90.0, 90.0, 120.0)	-326.88			
	dDsC	(5.86, 5.86, 19.06) (90.0, 90.0, 120.0)	-329.22			
	optB86b-vdW	(5.88, 5.88, 19.10) (90.0, 90.0, 120.0)	-249.16			
	optB88-vdW	(5.90, 5.90, 19.17) (90.0, 90.0, 120.0)	-247.77			
	optPBE-vdW	(5.93, 5.93, 19.26) (90.0, 90.0, 120.0)	-240.95			
	BEEF	(5.94, 5.94, 19.28) (90.0, 90.0, 120.0)	-244.09			
	vdW-DF2	(6.02, 6.02, 19.54) (90.0, 90.0, 120.0)	-241.27			

System	Method	Structure	E_{tot}	Structure Exp.	Ref.	ICSD
Li_2MnO_2	PBE	(3.22, 3.22, 5.31) (90.0, 90.0, 120.0)	-29.88			
P$\bar{3}$m1	D3	(3.19, 3.19, 5.22) (90.0, 90.0, 120.0)	-30.84			
	D3BJ	(3.18, 3.18, 5.24) (90.0, 90.0, 120.0)	-30.96			
	dDsC	(3.19, 3.19, 5.26) (90.0, 90.0, 120.0)	-30.70			
	optB86b-vdW	(3.20, 3.20, 5.28) (90.0, 90.0, 120.0)	-21.92			
	optB88-vdW	(3.20, 3.20, 5.28) (90.0, 90.0, 120.0)	-21.89			
	optPBE-vdW	(3.22, 3.22, 5.31) (90.0, 90.0, 120.0)	-21.38			
	BEEF	(3.23, 3.23, 5.33) (90.0, 90.0, 120.0)	-22.52			
	vdW-DF2	(3.25, 3.25, 5.35) (90.0, 90.0, 120.0)	-21.76			
$LiCrS_2$	PBE	(3.50, 3.50, 5.97) (90.0, 90.0, 120.0)	-23.72	(3.451, 3.451, 6.021)	13	626233
P$\bar{3}$m1	D3	(3.48, 3.48, 5.84) (90.0, 90.0, 120.0)	-24.62	(90.0, 90.0, 120.0)		
	D3BJ	(3.45, 3.45, 5.81) (90.0, 90.0, 120.0)	-25.06			
	dDsC	(3.47, 3.47, 5.88) (90.0, 90.0, 120.0)	-24.49			
	optB86b-vdW	(3.48, 3.48, 5.92) (90.0, 90.0, 120.0)	-17.20			
	optB88-vdW	(3.50, 3.50, 5.94) (90.0, 90.0, 120.0)	-16.86			
	optPBE-vdW	(3.51, 3.51, 5.98) (90.0, 90.0, 120.0)	-16.41			
	BEEF	(3.51, 3.51, 5.97) (90.0, 90.0, 120.0)	-17.03			
	vdW-DF2	(3.58, 3.58, 6.08) (90.0, 90.0, 120.0)	-15.88			
$Li_2Sr_3Nb_4O_{13}$	PBE	(4.05, 4.05, 34.70) (90.0, 90.0, 90.0)	-172.86			
I4/mmm	D3	(4.05, 4.05, 34.09) (90.0, 90.0, 90.0)	-177.15			
	D3BJ	(4.03, 4.03, 34.02) (90.0, 90.0, 90.0)	-178.05			
	dDsC	(4.04, 4.04, 34.25) (90.0, 90.0, 90.0)	-176.30			
	optB86b-vdW	(4.04, 4.04, 34.23) (90.0, 90.0, 90.0)	-136.03			
	optB88-vdW	(4.04, 4.04, 34.34) (90.0, 90.0, 90.0)	-135.35			
	optPBE-vdW	(4.06, 4.06, 34.52) (90.0, 90.0, 90.0)	-131.90			
	BEEF	(4.06, 4.06, 34.73) (90.0, 90.0, 90.0)	-133.75			
	vdW-DF2	(4.11, 4.11, 35.15) (90.0, 90.0, 90.0)	-132.27			
LiV_2O_5	PBE	(3.63, 4.75, 11.46) (90.0, 90.0, 90.0)	-56.69	(3.557, 4.371, 11.555)	6	41030
Pmnm	D3	(3.64, 4.61, 11.37) (90.0, 90.0, 90.0)	-57.94	(90.0, 90.0, 90.0)		
	D3BJ	(3.63, 4.58, 11.36) (90.0, 90.0, 90.0)	-58.12			
	dDsC	(3.60, 4.56, 11.43) (90.0, 90.0, 90.0)	-57.76			
	optB86b-vdW	(3.60, 4.57, 11.42) (90.0, 90.0, 90.0)	-42.31			
	optB88-vdW	(3.61, 4.58, 11.44) (90.0, 90.0, 90.0)	-42.07			
	optPBE-vdW	(3.62, 4.68, 11.48) (90.0, 90.0, 90.0)	-41.02			
	BEEF	(3.63, 4.84, 11.49) (90.0, 90.0, 90.0)	-42.04			
	vdW-DF2	(3.65, 4.75, 11.60) (90.0, 90.0, 90.0)	-41.42			
$LiVO_2$	PBE	(2.99, 2.99, 14.67) (90.0, 90.0, 120.0)	-27.64	(2.837, 2.837, 14.773)	14	202540
R$\bar{3}$m	D3	(2.96, 2.96, 14.50) (90.0, 90.0, 120.0)	-28.55	(90.0, 90.0, 120.0)		
	D3BJ	(2.96, 2.96, 14.39) (90.0, 90.0, 120.0)	-28.72			
	dDsC	(2.97, 2.97, 14.48) (90.0, 90.0, 120.0)	-28.34			
	optB86b-vdW	(2.97, 2.97, 14.55) (90.0, 90.0, 120.0)	-20.95			
	optB88-vdW	(2.98, 2.98, 14.57) (90.0, 90.0, 120.0)	-20.90			
	optPBE-vdW	(3.00, 3.00, 14.65) (90.0, 90.0, 120.0)	-20.34			
	BEEF	(3.00, 3.00, 14.63) (90.0, 90.0, 120.0)	-20.90			
	vdW-DF2	(3.04, 3.04, 14.78) (90.0, 90.0, 120.0)	-20.59			
Li_2NiO_2	PBE	(3.12, 3.12, 5.08) (90.0, 90.0, 120.0)	-24.05	(3.080, 3.080, 5.06)	15	73874
P$\bar{3}$m1	D3	(3.08, 3.08, 4.97) (90.0, 90.0, 120.0)	-25.22	(90.0, 90.0, 120.0)		
	D3BJ	(3.08, 3.08, 4.99) (90.0, 90.0, 120.0)	-25.34			
	dDsC	(3.09, 3.09, 5.02) (90.0, 90.0, 120.0)	-24.89			
	optB86b-vdW	(3.10, 3.10, 5.04) (90.0, 90.0, 120.0)	-15.38			
	optB88-vdW	(3.10, 3.10, 5.05) (90.0, 90.0, 120.0)	-15.49			
	optPBE-vdW	(3.12, 3.12, 5.08) (90.0, 90.0, 120.0)	-14.87			
	BEEF	(3.13, 3.13, 5.10) (90.0, 90.0, 120.0)	-15.74			
	vdW-DF2	(3.16, 3.16, 5.15) (90.0, 90.0, 120.0)	-15.76			
LiV_2O_5	PBE	(3.64, 9.83, 10.98) (90.0, 90.0, 90.0)	-57.17	(3.607, 9.702, 10.664)	16	25384
Pnma	D3	(3.63, 9.78, 10.77) (90.0, 90.0, 90.0)	-58.42	(90.0, 90.0, 90.0)		
	D3BJ	(3.61, 9.75, 10.72) (90.0, 90.0, 90.0)	-58.58			
	dDsC	(3.61, 9.75, 10.77) (90.0, 90.0, 90.0)	-58.21			
	optB86b-vdW	(3.61, 9.75, 10.78) (90.0, 90.0, 90.0)	-42.77			
	optB88-vdW	(3.62, 9.78, 10.78) (90.0, 90.0, 90.0)	-42.55			
	optPBE-vdW	(3.63, 9.83, 10.90) (90.0, 90.0, 90.0)	-41.53			
	BEEF	(3.64, 9.88, 11.02) (90.0, 90.0, 90.0)	-42.60			
	vdW-DF2	(3.67, 9.95, 10.99) (90.0, 90.0, 90.0)	-41.99			

System	Method	Structure	E_{tot}	Structure Exp.	Ref.	ICSD
$LiCoO_2$	PBE	(2.83, 2.83, 14.13) (90.0, 90.0, 120.0)	-22.92	(2.815, 2.815, 14.047)	17	51767
R$\overline{3}$m	D3	(2.81, 2.81, 13.96) (90.0, 90.0, 120.0)	-23.74	(90.0, 90.0, 120.0)		
	D3BJ	(2.81, 2.81, 13.91) (90.0, 90.0, 120.0)	-23.85			
	dDsC	(2.81, 2.81, 13.95) (90.0, 90.0, 120.0)	-23.70			
	optB86b-vdW	(2.81, 2.81, 14.01) (90.0, 90.0, 120.0)	-16.87			
	optB88-vdW	(2.82, 2.82, 14.05) (90.0, 90.0, 120.0)	-16.79			
	optPBE-vdW	(2.84, 2.84, 14.13) (90.0, 90.0, 120.0)	-16.15			
	BEEF	(2.84, 2.84, 14.14) (90.0, 90.0, 120.0)	-16.41			
	vdW-DF2	(2.89, 2.89, 14.31) (90.0, 90.0, 120.0)	-16.31			
$LiNiO_2$	PBE	(2.90, 2.90, 14.33) (90.0, 90.0, 120.0)	-19.39	(2.883, 2.883, 14.199)	10	78687
R$\overline{3}$m	D3	(2.87, 2.87, 14.19) (90.0, 90.0, 120.0)	-20.18	(90.0, 90.0, 120.0)		
	D3BJ	(2.87, 2.87, 14.10) (90.0, 90.0, 120.0)	-20.28			
	dDsC	(2.87, 2.87, 14.14) (90.0, 90.0, 120.0)	-20.11			
	optB86b-vdW	(2.87, 2.87, 14.19) (90.0, 90.0, 120.0)	-11.66			
	optB88-vdW	(2.89, 2.89, 14.24) (90.0, 90.0, 120.0)	-11.62			
	optPBE-vdW	(2.90, 2.90, 14.33) (90.0, 90.0, 120.0)	-11.05			
	BEEF	(2.92, 2.92, 14.35) (90.0, 90.0, 120.0)	-11.57			
	vdW-DF2	(2.97, 2.97, 14.52) (90.0, 90.0, 120.0)	-11.53			
$LiV(CO_3)_2$	PBE	(4.69, 4.69, 15.28) (90.0, 90.0, 120.0)	-74.62			
R$\overline{3}$	D3	(4.67, 4.67, 15.01) (90.0, 90.0, 120.0)	-75.86			
	D3BJ	(4.66, 4.66, 14.99) (90.0, 90.0, 120.0)	-76.04			
	dDsC	(4.64, 4.64, 14.92) (90.0, 90.0, 120.0)	-75.92			
	optB86b-vdW	(4.65, 4.65, 14.91) (90.0, 90.0, 120.0)	-59.36			
	optB88-vdW	(4.66, 4.66, 14.93) (90.0, 90.0, 120.0)	-58.91			
	optPBE-vdW	(4.68, 4.68, 15.11) (90.0, 90.0, 120.0)	-57.62			
	BEEF	(4.69, 4.69, 15.35) (90.0, 90.0, 120.0)	-58.95			
	vdW-DF2	(4.75, 4.75, 15.22) (90.0, 90.0, 120.0)	-56.46			
$LiCo_2C_2O_7$	PBE	(4.80, 8.34, 15.62) (90.0, 92.7, 90.0)	-81.38			
Cc	D3	(4.78, 8.30, 15.45) (90.0, 93.1, 90.0)	-82.53			
	D3BJ	(4.78, 8.30, 15.38) (90.0, 93.1, 90.0)	-82.72			
	dDsC	(4.75, 8.27, 15.32) (90.0, 93.4, 90.0)	-82.59			
	optB86b-vdW	(4.76, 8.26, 15.27) (90.0, 93.4, 90.0)	-61.74			
	optB88-vdW	(4.76, 8.27, 15.34) (90.0, 93.4, 90.0)	-61.18			
	optPBE-vdW	(4.79, 8.32, 15.49) (90.0, 93.2, 90.0)	-59.80			
	BEEF	(4.81, 8.37, 15.75) (90.0, 93.1, 90.0)	-61.78			
	vdW-DF2	(4.83, 8.40, 15.75) (90.0, 93.1, 90.0)	-59.46			
$LiBa_4Nb_3O_{12}$	PBE	(5.88, 5.88, 19.40) (90.0, 90.0, 120.0)	-155.11	(5.803, 5.803, 19.076)	18	19009
P63mc	D3	(5.85, 5.85, 19.29) (90.0, 90.0, 120.0)	-158.54	(90.0, 90.0, 120.0)		
	D3BJ	(5.84, 5.84, 19.23) (90.0, 90.0, 120.0)	-159.79			
	dDsC	(5.82, 5.82, 19.18) (90.0, 90.0, 120.0)	-160.94			
	optB86b-vdW	(5.84, 5.84, 19.22) (90.0, 90.0, 120.0)	-121.82			
	optB88-vdW	(5.86, 5.86, 19.28) (90.0, 90.0, 120.0)	-121.32			
	optPBE-vdW	(5.89, 5.89, 19.40) (90.0, 90.0, 120.0)	-118.10			
	BEEF	(5.90, 5.90, 19.44) (90.0, 90.0, 120.0)	-119.88			
	vdW-DF2	(5.97, 5.97, 19.68) (90.0, 90.0, 120.0)	-118.75			
$LiFe(CO_3)_2$	PBE	(4.69, 4.69, 15.25) (90.0, 90.0, 120.0)	-71.13			
R$\overline{3}$	D3	(4.69, 4.69, 15.07) (90.0, 90.0, 120.0)	-72.36			
	D3BJ	(4.68, 4.68, 15.09) (90.0, 90.0, 120.0)	-72.51			
	dDsC	(4.64, 4.64, 14.88) (90.0, 90.0, 120.0)	-72.44			
	optB86b-vdW	(4.64, 4.64, 14.86) (90.0, 90.0, 120.0)	-55.20			
	optB88-vdW	(4.65, 4.65, 14.89) (90.0, 90.0, 120.0)	-54.62			
	optPBE-vdW	(4.68, 4.68, 15.07) (90.0, 90.0, 120.0)	-53.41			
	BEEF	(4.69, 4.69, 15.31) (90.0, 90.0, 120.0)	-54.88			
	vdW-DF2	(4.72, 4.72, 15.24) (90.0, 90.0, 120.0)	-52.73			

Table S2: Lattice parameters (a, b, c) and (α, β, γ) in Å and degrees of different Li-intercalated compounds using different vdW-inclusive methods and PBE. In addition, we show the computed total energies in eV per formula unit (E_{tot}) and the experimental structural parameters taken from the specified references. When available, the corresponding collection code assigned to each entry in the inorganic crystal structure database (ICSD) is also provided.

System	Space Group	PBE	vdW-DF2	optB86b vdW	optB88 vdW	optPBE vdW	BEEF	D3	D3BJ	dDsC	Exp.
$Li_{0\to1}C_6$	P6/mmm	0.08	0.08	0.23	0.23	0.17	0.08	0.10	0.08	0.20	0.14 [19]
$Li_{0\to1}TiTe_2$	P$\bar{3}$m1	1.22	1.30	1.24	1.31	1.27	1.21	1.42	1.31	1.25	
$Li_{0\to1}SnS_2$	P$\bar{3}$m1	1.59	2.06	1.75	1.86	1.79	1.64	1.71	1.76	1.67	1.95 [20]
$Li_{0\to1}VS_2$	P$\bar{3}$m1	1.80	2.17	1.81	1.97	1.96	1.98	2.10	1.96	1.87	
$Li_{0\to1}TiO_2$	R$\bar{3}$m	1.80	2.09	2.04	2.12	2.01	1.87	2.26	2.21	1.95	
$Li_{0\to1}TiS_2$	P$\bar{3}$m1	1.89	1.97	1.99	2.03	1.96	1.91	2.22	2.18	1.97	2.10 [21]
$Li_{0\to1}Ba_8Nb_7O_{24}$	P$\bar{3}$m1	1.95	2.19	2.30	2.36	2.16	1.90	2.18	2.28	2.23	
$Li_{0\to2}MnO_2$	P$\bar{3}$m1	2.40	2.79	2.46	2.59	2.57	2.67	2.66	2.59	2.50	
$Li_{0\to1}CrS_2$	P$\bar{3}$m1	2.41	2.63	2.39	2.51	2.50	2.53	2.56	2.53	2.45	
$Li_{0\to2}Sr_3Nb_4O_{13}$	I4/mmm	2.42	2.61	2.65	2.71	2.57	2.36	2.53	2.63	2.52	
$Li_{0\to1}V_2O_5$	Pmnm	2.96	3.41	3.15	3.29	3.19	3.07	3.32	3.15	3.07	
$Li_{0\to1}VO_2$	R$\bar{3}$m	3.30	3.81	3.46	3.63	3.55	3.54	3.71	3.64	3.45	
$Li_{0\to2}NiO_2$	P$\bar{3}$m1	3.34	3.82	3.35	3.53	3.50	3.56	3.65	3.57	3.43	
$Li_{0\to1}V_2O_5$	Pmna	3.50	4.06	3.68	3.85	3.77	3.68	3.87	3.68	3.61	3.60 [22]
$Li_{0\to1}CoO_2$	R$\bar{3}$m	3.81	4.39	4.15	4.30	4.17	4.04	4.22	4.14	3.95	4.10 [23]
$Li_{0\to1}NiO_2$	R$\bar{3}$m	3.90	4.51	3.99	4.18	4.13	4.15	4.26	4.17	4.01	3.85 [24]
$Li_{0\to1}V(CO_3)_2$	R$\bar{3}$	4.06	4.04	4.50	4.67	4.57	4.44	4.51	4.38	4.34	
$Li_{0\to1}Co_2C_2O_7$	Cc	4.45	5.22	4.79	4.99	4.87	4.72	4.77	4.67	4.62	
$Li_{0\to1}Ba_4Nb_3O_{12}$	P6_3mc	4.66	4.84	4.97	5.03	4.85	4.66	4.88	4.97	4.84	
$Li_{0\to1}Fe(CO_3)_2$	R$\bar{3}$	4.89	5.43	5.36	5.47	5.32	5.20	5.33	5.20	5.14	

Table S3: Computed average redox potentials in V for Li intercalation using different vdW-inclusive DFT methods and PBE. The values are compared to available experimental data.

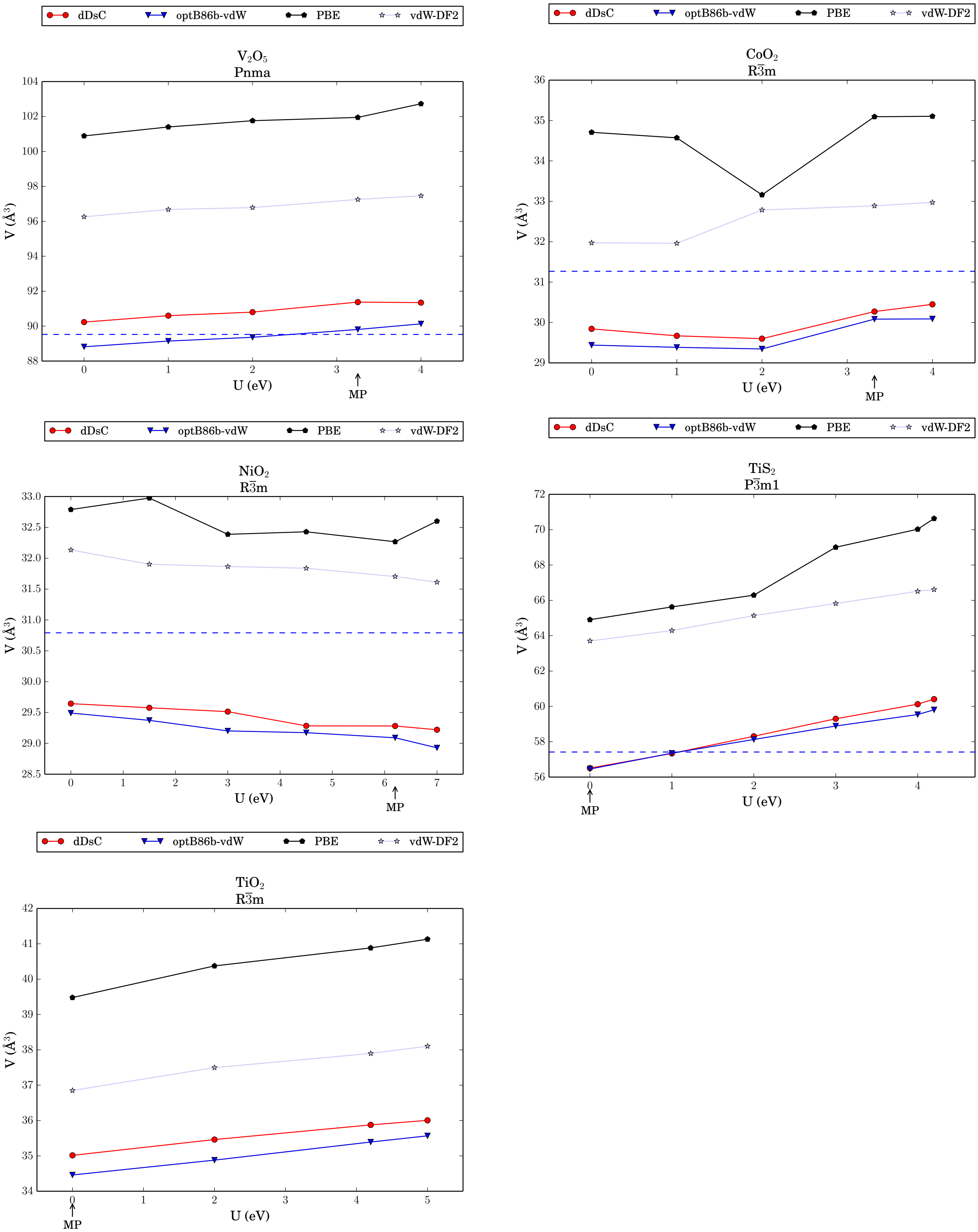

Figure S1: Unit cell volume as a function of the U parameter for the empty hosts where the GGA+U correction was analyzed. The U value recommended by Materials Project is pointed with an arrow on the x axis. When present, the horizontal dashed lines correspond to the experimental result.

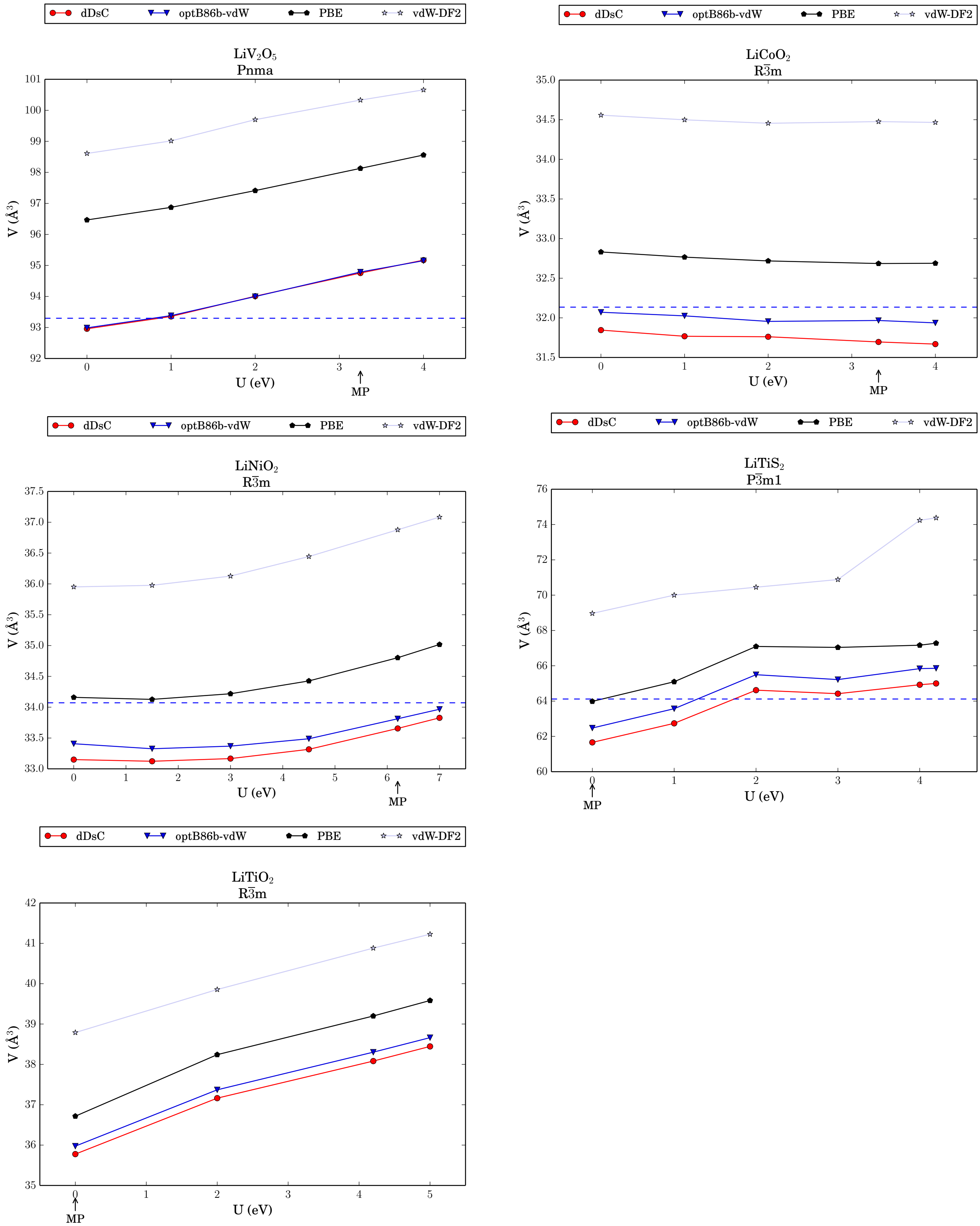

Figure S2: Unit cell volume as a function of the U parameter for the Li-intercalated systems where the GGA+U correction was analyzed. The U value recommended by Materials Project is pointed with an arrow on the x axis. When present, the horizontal dashed lines correspond to the experimental result.

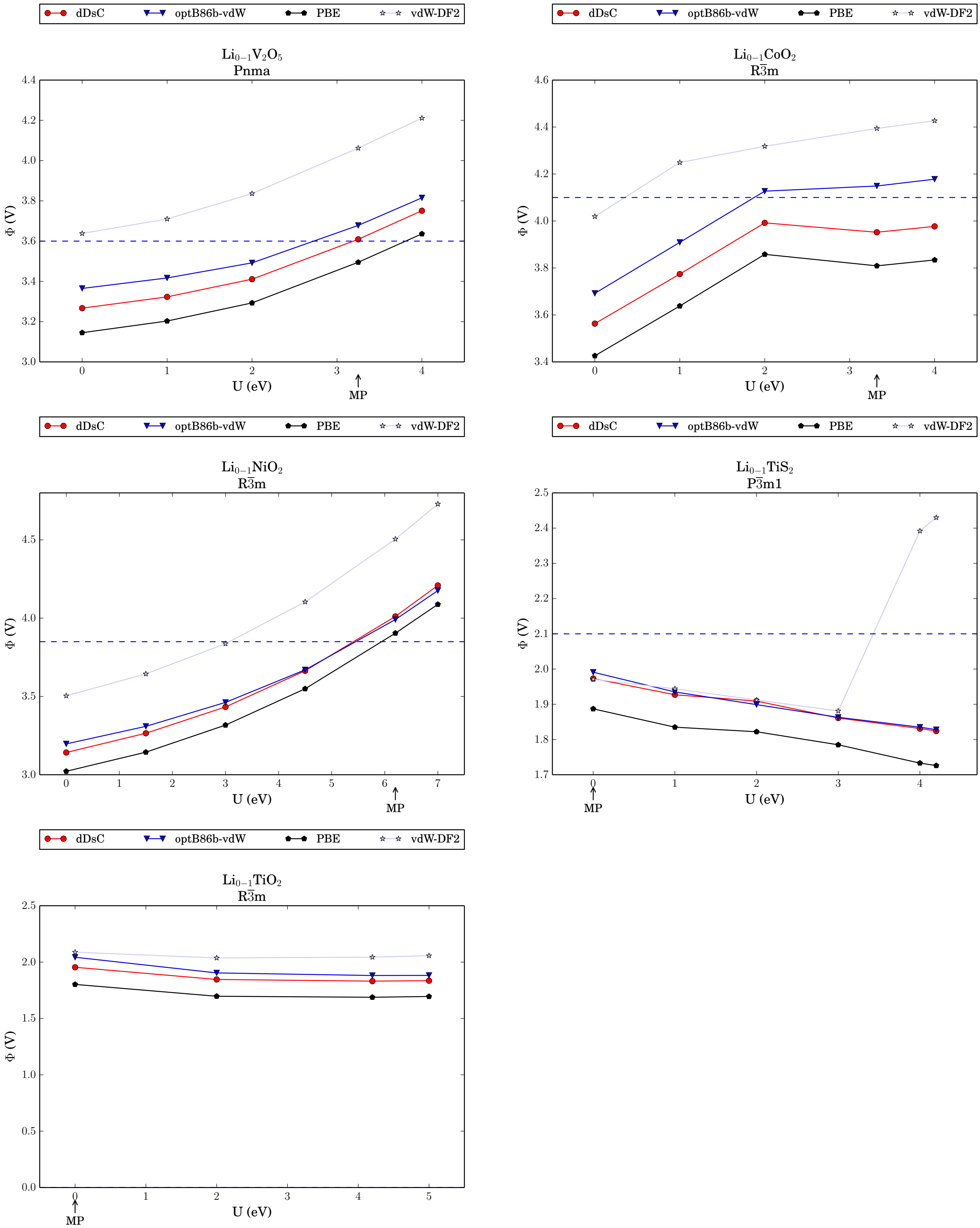

Figure S3: Redox potentials as a function of the U parameter for the systems where the GGA+U correction was analyzed. The U value recommended by Materials Project is pointed with an arrow on the x axis. When present, the horizontal dashed lines correspond to the experimental result.

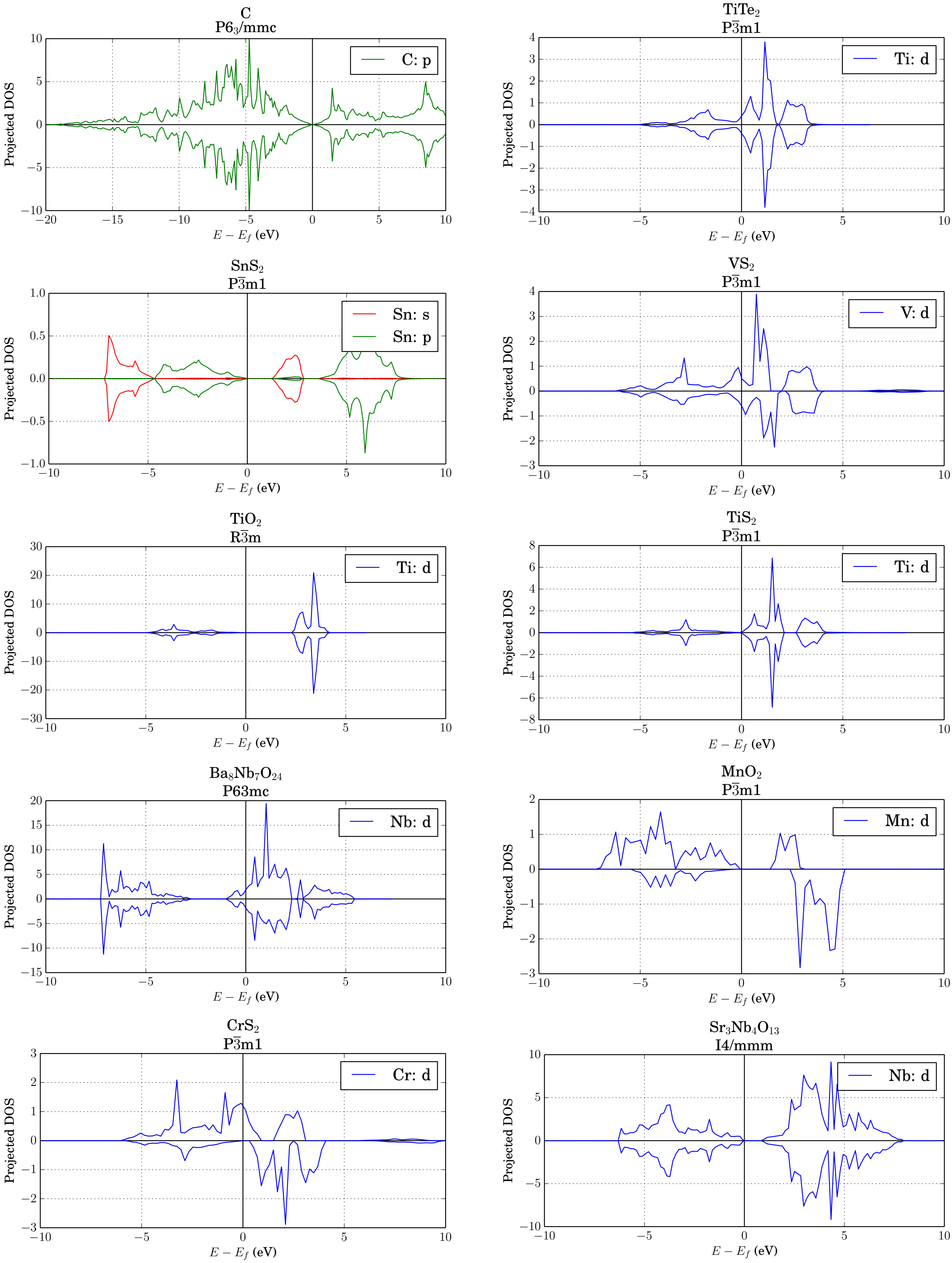

Figure S4: Density of states projected onto the s, p, or d orbitals of the indicated atoms for the empty hosts with $\Phi \lesssim 2.5$ V, obtained with the optB86b-vdW method. Positive (negative) values correspond to spin up (down) states. The energy zero is the Fermi level.

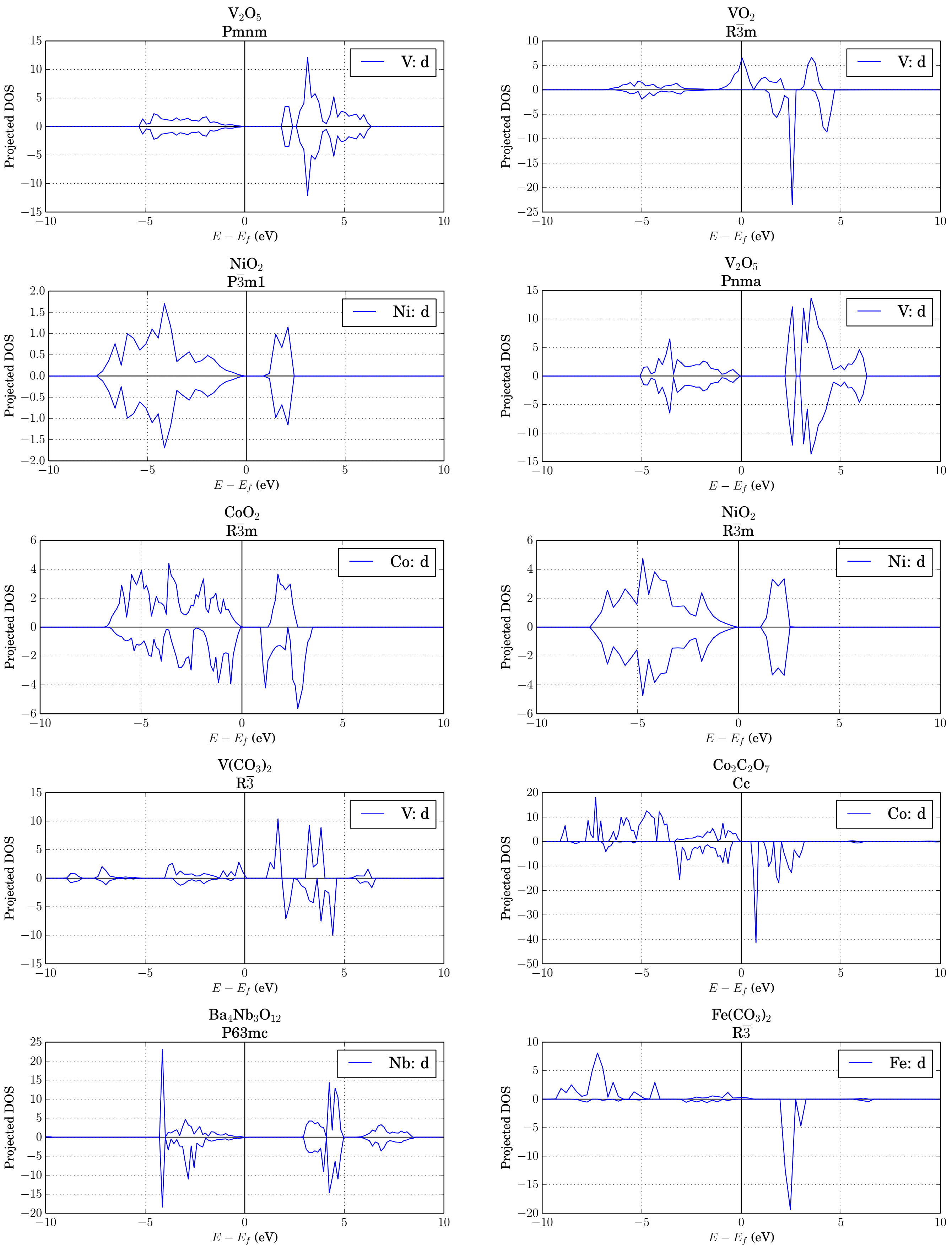

Figure S5: Density of states projected onto the d orbitals of the indicated atoms for the empty hosts with $\Phi \gtrsim 3$ V, obtained with the optB86b-vdW method. Positive (negative) values correspond to spin up (down) states. The energy zero is the Fermi level.

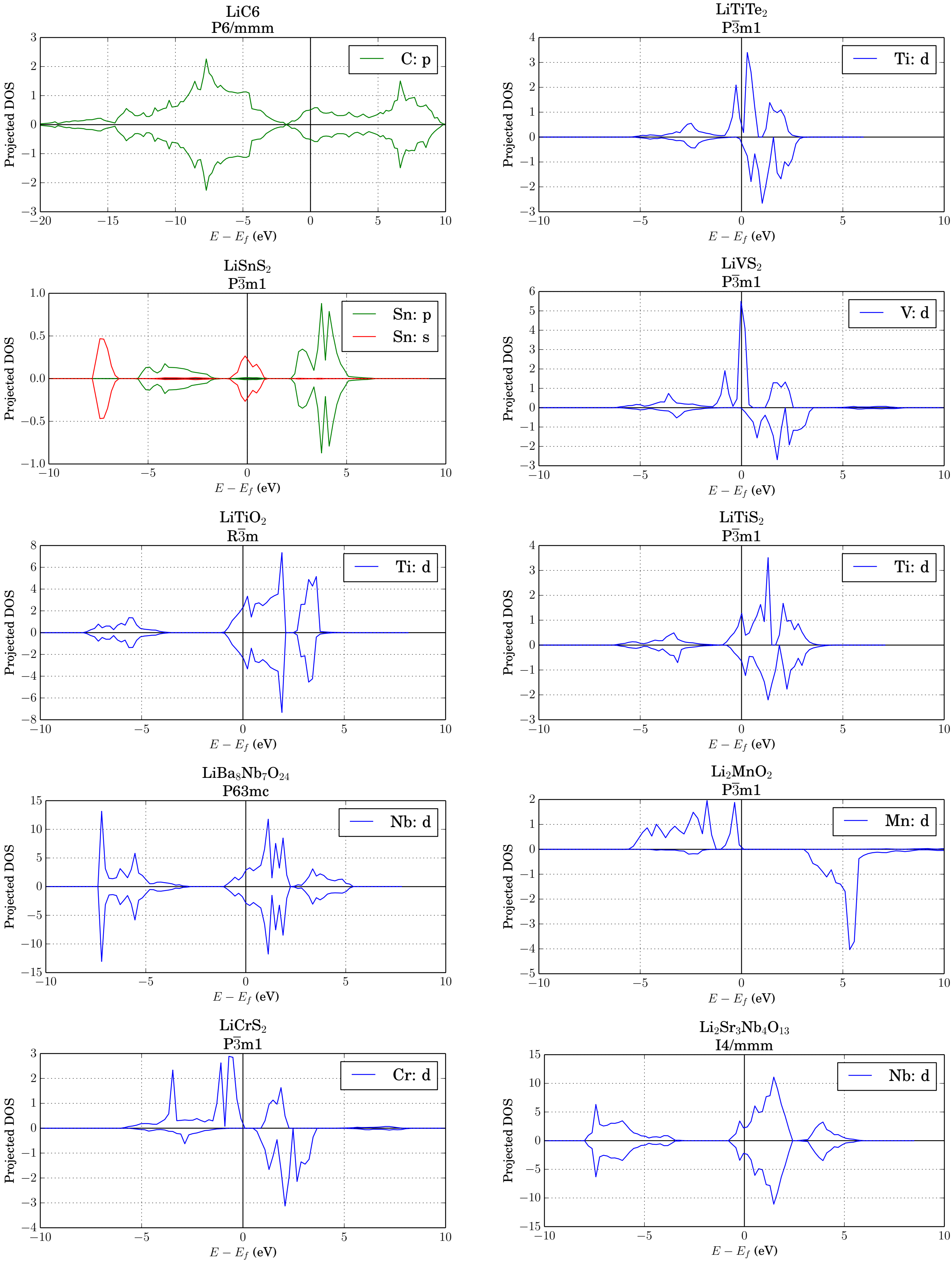

Figure S6: Density of states projected onto the s, p, or d orbitals of the indicated atoms for the Li-intercalated systems with $\Phi \lesssim 2.5$ V, obtained with the optB86b-vdW method. Positive (negative) values correspond to spin up (down) states. The energy zero is the Fermi level.

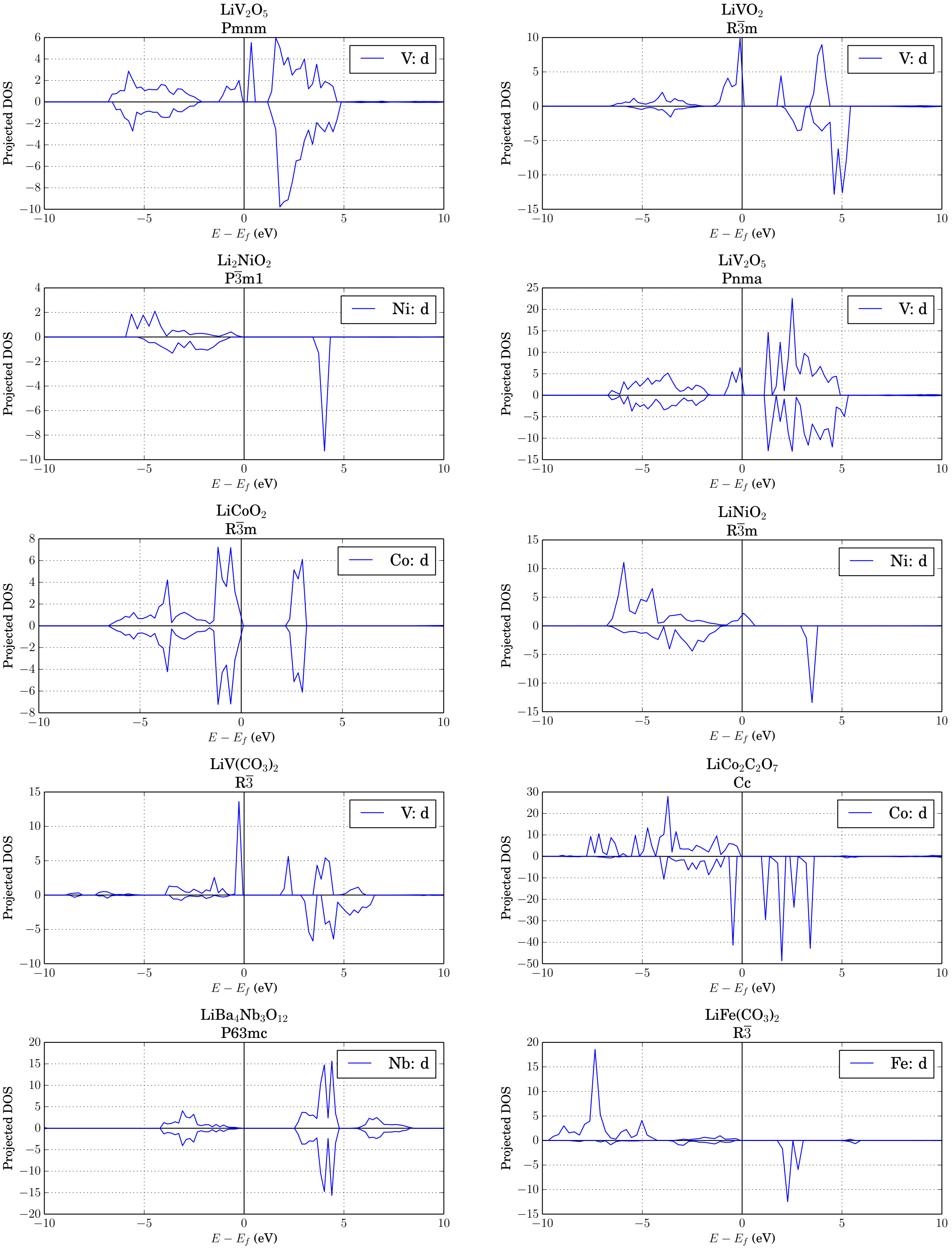

Figure S7: Density of states projected onto the d orbitals of the indicated atoms for the Li-intercalated systems with $\Phi \gtrsim 3$ V, obtained with the optB86b-vdW method. Positive (negative) values correspond to spin up (down) states. The energy zero is the Fermi level.

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