Supplemental Materials for "A Rapid Lithium-ion Cathode Discovery Pipeline and Its Exemplary Application"

1 Energy Evolution of Migration Hops calculated with ApproxNEB in Some Representative Structure Types

1.1 VBO_4 (mp-754594, space group $I\bar{4}$), tunnel

FIG. S1 shows the energy landscape plots and visualizations of sample migration hops in VBO_4(mp-754594), calculated with ApproxNEB.

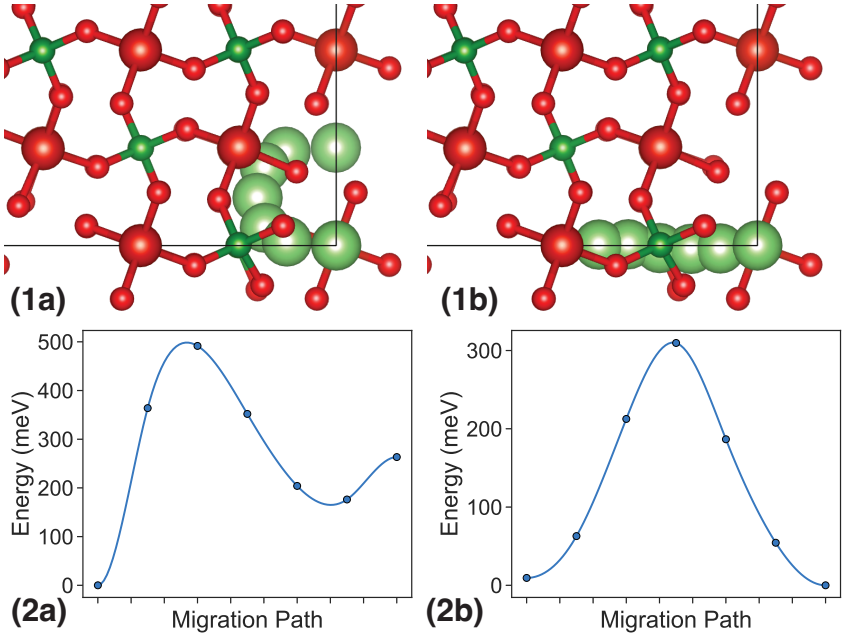

Figure S1: Path visualization and energy evolution as a function of migration distance for two sample migration hops in VBO_4(mp-754594).

1.2 $MnPO_4$ (mp-777460, space group Pnma), tunnel

FIG. S2 shows the energy landscape plots and visualizations of sample migration hops in $MnPO_4$(mp-777460), calculated with ApproxNEB.

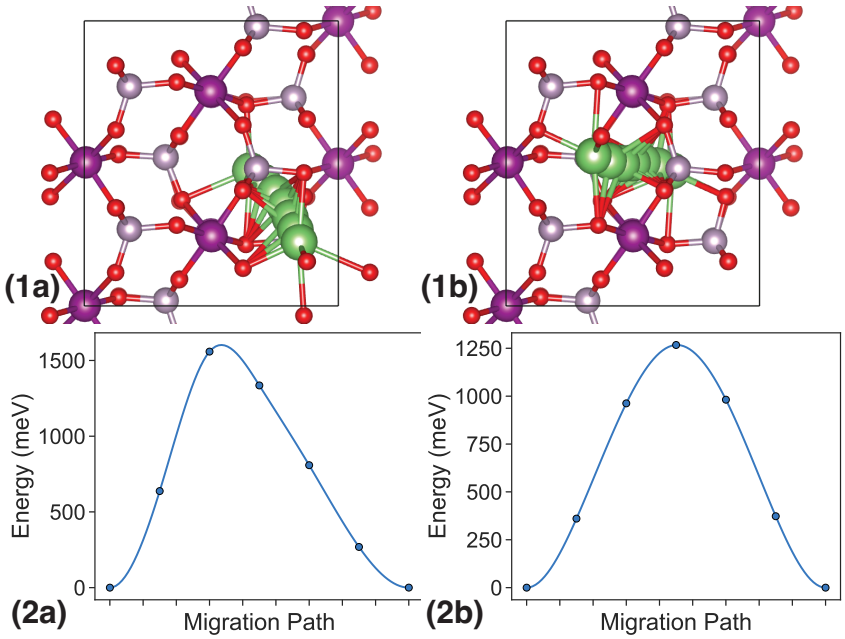

Figure S2: Path visualization and energy evolution as a function of migration distance for two sample migration hops in $MnPO_4$(mp-777460).

1.3 $VCuO_4$ (mp-25196, space group Imma), layered

FIG. S3 shows the energy landscape plots and visualizations of sample migration hops in $VCuO_4$(mp-25196), calculated with ApproxNEB.

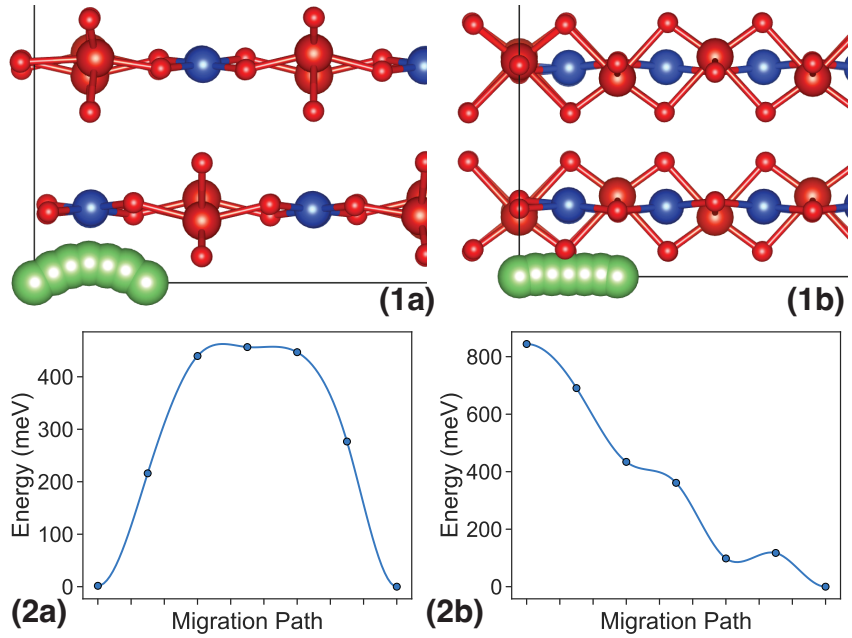

Figure S3: Path visualization and energy evolution as a function of migration distance for two sample migration hops in $VCuO_4$(mp-25196).

1.4 MnO_2 (mp-510732, space group Pmmn), layered

FIG. S4 shows the energy landscape plots and visualizations of sample migration hops in MnO_2(mp-510732), calculated with ApproxNEB.

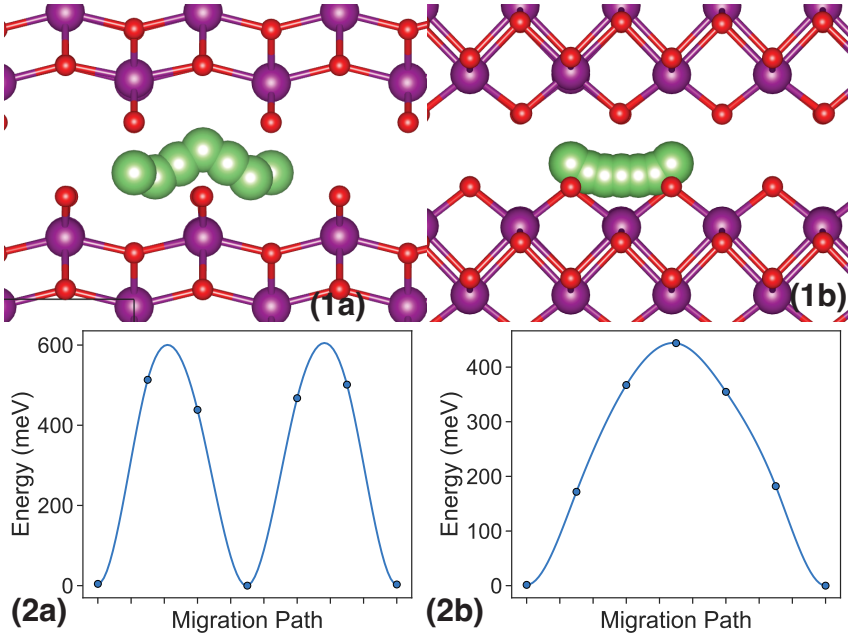

Figure S4: Path visualization and energy evolution as a function of migration distance for two sample migration hops in MnO_2(mp-510732).

1.5 VOF_3 (mp-764274, space group $P\bar{4}2_1m$), tunnel

FIG. S5 shows the energy landscape plots and visualizations of sample migration hops in VOF_3(mp-764274), calculated with ApproxNEB.

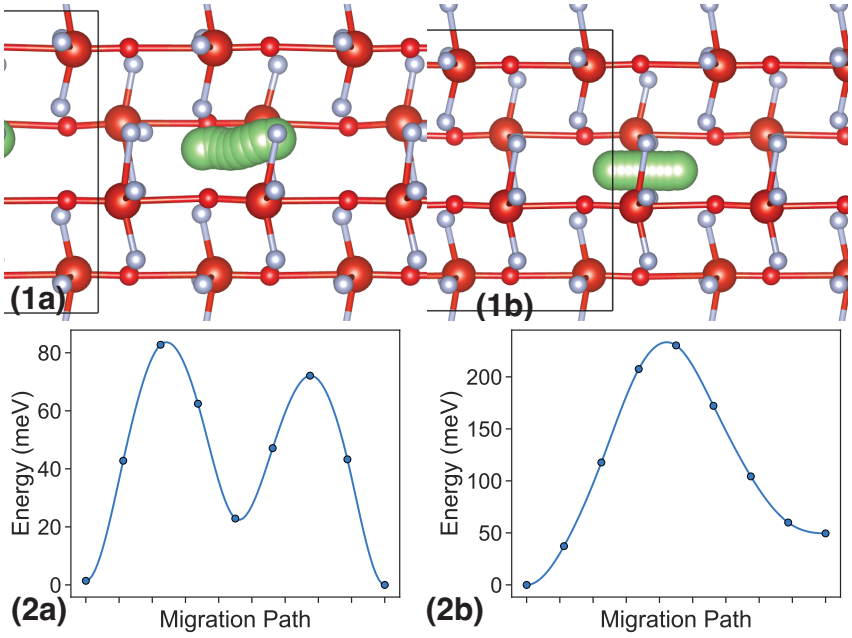

Figure S5: Path visualization and energy evolution as a function of migration distance for two sample migration hops in VOF_3(mp-764274).

2 Structure Information of MnP_2O_7, $LiMnP_2O_7$ and $Li_2MnP_2O_7$

2.1 Lattice Parameters and Site Positions of charged MnP_2O_7

Table 1: Calculated lattice parameters of MnP_2O_7 from VASP

a(Å)	b(Å)	c(Å)	alpha(^{o})	beta(^{o})	gamma(^{o})
6.90764	7.87549	4.77603	90.0000	106.1555	89.9999

Table 2: Calculated site positions (fractional) of MnP_2O_7 from VASP

Site Index	Species	x	y	z
0	Mn	0.77151	0.73544	0.78042
1	Mn	0.22849	0.23544	0.21958
2	P	0.60232	0.96855	0.22916
3	P	0.39768	0.46855	0.77084
4	P	0.99106	0.05481	0.61095
5	P	0.00894	0.55480	0.38905
6	O	0.59099	0.81198	0.41867
7	O	0.40902	0.31198	0.58133
8	O	0.40779	0.07040	0.13018
9	O	0.59221	0.57040	0.86982
10	O	0.66502	0.92218	0.95498
11	O	0.33497	0.42218	0.04502
12	O	0.98573	0.87195	0.72148
13	O	0.01427	0.37196	0.27852
14	O	0.03695	0.18954	0.84835
15	O	0.96305	0.68954	0.15165
16	O	0.13224	0.05346	0.41242
17	O	0.86776	0.55346	0.58758
18	O	0.76577	0.10010	0.41904
19	O	0.23423	0.60010	0.58096

2.2 Lattice Parameters and Site Positions of intermediately discharged $LiMnP_2O_7$

Table 3: Calculated lattice parameters of $LiMnP_2O_7$ from VASP

a(Å)	b(Å)	c(Å)	alpha(^{o})	beta(^{o})	gamma(^{o})
7.11689	8.35112	4.80612	90.0001	109.0151	90.0000

Table 4: Calculated site positions of $LiMnP_2O_7$ from VASP

Site Index	Species	x	y	z
0	Li	0.17741	0.88269	0.17735
1	Li	0.82259	0.38269	0.82265
2	Mn	0.77438	0.74310	0.79108
3	Mn	0.22562	0.24310	0.20892
4	P	0.59424	0.95328	0.21479
5	P	0.40576	0.45328	0.78521
6	P	0.98560	0.06367	0.59893
7	P	0.01440	0.56368	0.40107
8	O	0.60250	0.80187	0.40180
9	O	0.39750	0.30188	0.59819
10	O	0.39394	0.03503	0.13940
11	O	0.60606	0.53503	0.86060
12	O	0.64968	0.91444	0.93925
13	O	0.35031	0.41445	0.06075
14	O	0.01108	0.90342	0.75578
15	O	0.98892	0.40342	0.24421
16	O	0.02176	0.20882	0.80879
17	O	0.97824	0.70882	0.19121
18	O	0.10627	0.06983	0.38472
19	O	0.89373	0.56983	0.61528
20	O	0.75374	0.08493	0.40432
21	O	0.24626	0.58494	0.59568

2.3 Lattice Parameters and Site Positions of Discharged γ-$Li_2MnP_2O_7$

Table 5: Calculated lattice parameters of γ-$Li_2MnP_2O_7$ from VASP

a(Å)	b(Å)	c(Å)	alpha(^{o})	beta(^{o})	gamma(^{o})
7.26778	8.55198	5.12016	90.0004	110.1515	89.9994

Table 6: Calculated site positions of γ-$Li_2MnP_2O_7$ from VASP

Site Index	Species	x	y	z
0	Li	0.14719	0.89158	0.18599
1	Li	0.85281	0.39159	0.81401
2	Li	0.59310	0.56297	0.35483
3	Li	0.40690	0.06297	0.64517
4	Mn	0.77464	0.75171	0.81436
5	Mn	0.22536	0.25171	0.18564
6	P	0.58026	0.94736	0.22121
7	P	0.41975	0.44737	0.77879
8	P	0.97681	0.05643	0.61209
9	P	0.02319	0.55645	0.38791
10	O	0.60256	0.79231	0.37759
11	O	0.39744	0.29231	0.62241
12	O	0.39251	0.03217	0.21900
13	O	0.60749	0.53218	0.78100
14	O	0.58991	0.92880	0.92823
15	O	0.41009	0.42880	0.07178
16	O	0.99249	0.91009	0.79035
17	O	0.00751	0.41010	0.20965
18	O	0.00272	0.20617	0.78545
19	O	0.99727	0.70618	0.21455
20	O	0.11395	0.04966	0.44243
21	O	0.88605	0.54967	0.55758
22	O	0.75279	0.06683	0.39392
23	O	0.24721	0.56684	0.60608