Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.
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Electronic Supplementary Information

Finite-temperature property-maps of Li-Mn-Ni-O cathode materials from ab-initio calculations

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Choice of U parameter

For choosing the value of U_{eff} for Mn and Ni we determined the band-gap for Li_2MnO_3, $LiMnO_2$ and $LiNiO_2$ for different choices of U_{eff} in previous works.

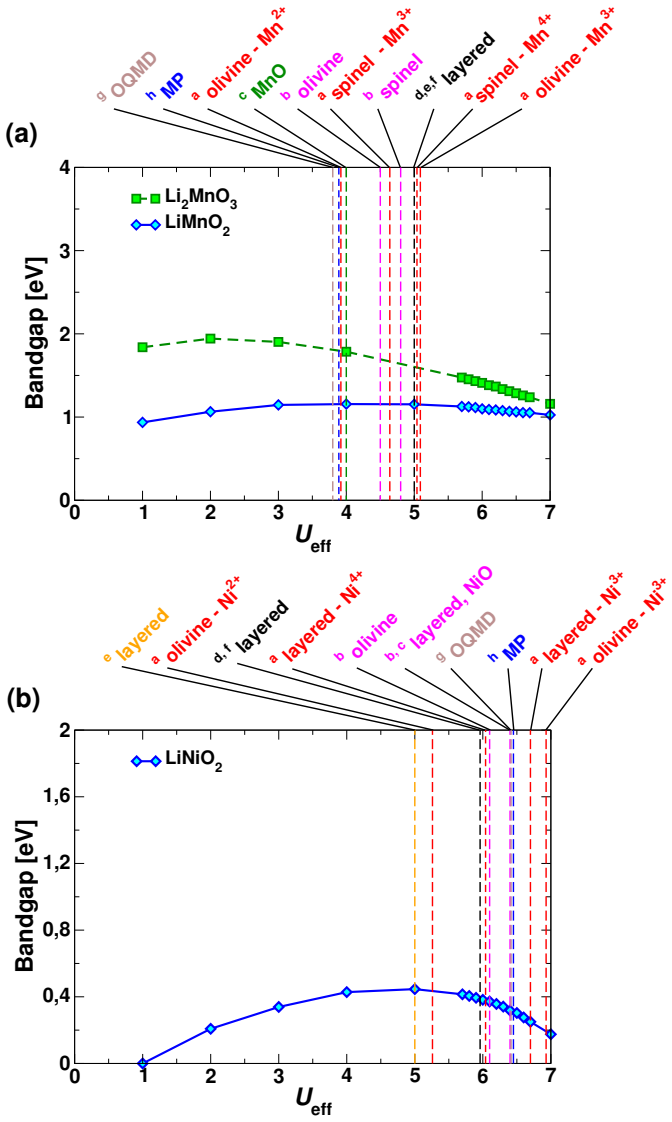

Figure 1: Band gap as a function of U_{eff} for (a) Li_2MnO_3, $LiMnO_2$ and (b) $LiNiO_2$. [a] Ref. 1; [b] Ref. 2; [c] Ref. 3; [d] Ref. 4; [e] Ref. 5; [f] Ref. 6; [g] Ref. 7; [h] Ref. 8.

Ternary phase diagram for the Li-Mn-O system at T=0 K

The ternary Phase diagram presented in Fig. 2 is evaluated from first-principles calculations at T=0 K. The reported result does not include entropic contributions.

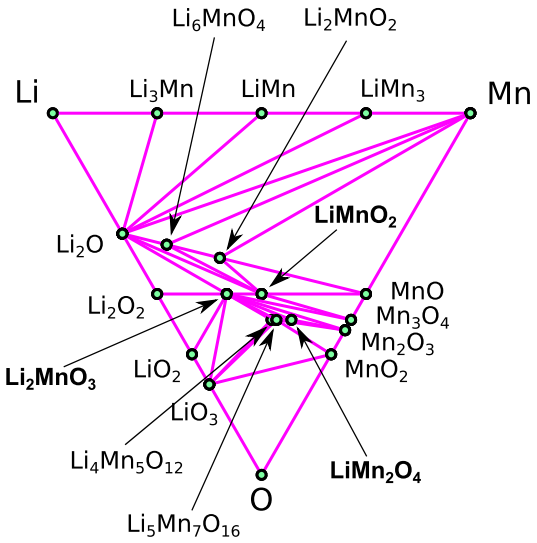

Figure 2: Ternary phase diagram at T=0 K (without zero-point energy corrections) for the Li-Mn-O system.

Phonon density-of-states

The phonon density of states (DOS) for selected compounds forming/disappearing along the Li_2MnO_3 delithiation path are plotted in Fig. 3. The DOS for Li_2MnO_3 and $LiMn_{0.5}Ni_{0.5}O_2$ (Fig. 3 (a)) exhibit similar shapes while $LiMnO_2$ shows a greater degree of splitting. The dissimilarity comes most likely from the additional Li in the TM layer of Li_2MnO_3 and $LiMn_{0.5}Ni_{0.5}O_2$ which is absent in the $LiMnO_2$ material. As for the spinel-like structures (Fig. 3 (b)), the DOS are remarkably similar, reflecting the three-dimensional character of spinel-like compounds. Regarding the DOS for Mn-O compounds, two subgroups are identified with the Mn_2O_3 and Mn_3O_4 phases (Fig. 3 (c))on one hand, and the MnO_2 and $MnNiO_3$ phases (Fig. 3 (d)) on the other hand.

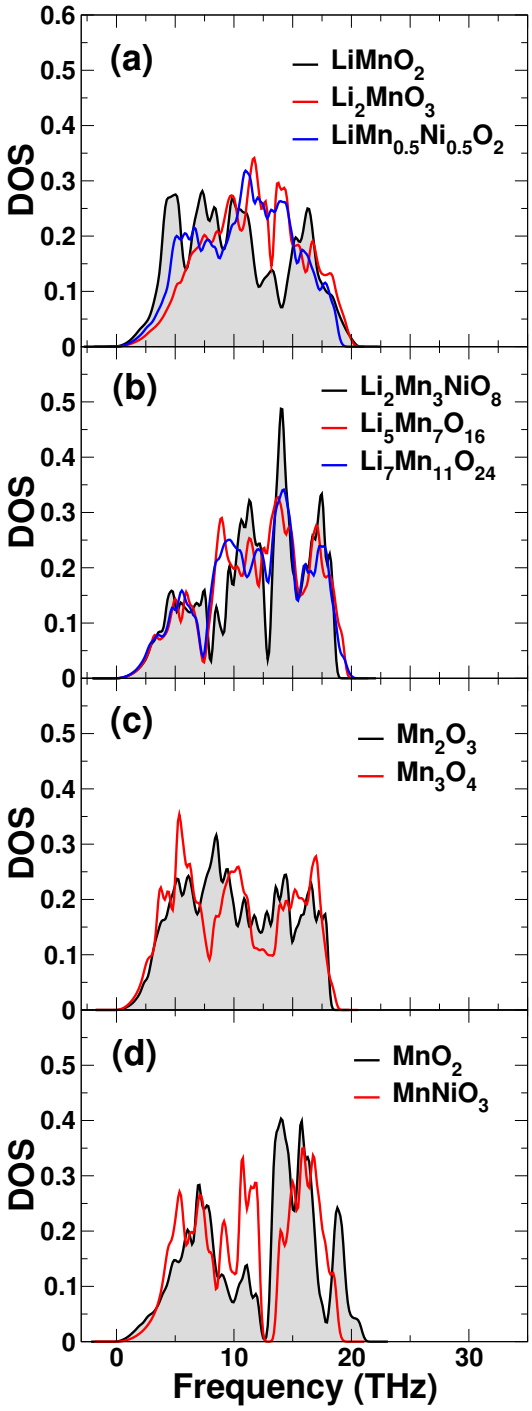

Figure 3: Phonon density of states for selected compounds forming/disappearing along the Li_2MnO_3 delithiation path.

Properties computed from the convex hull

Chemical potentials

The total formation energy of a point located on a facet is related to the formation energies of each individual phase through the weight coefficients. The concentration of an element k is expressed as the sum of the relative concentration of the element in each phase weighted by the factor w_i of the phase i.

$$C_k = \sum_i w_i c_{ik} \tag{1}$$

Therefore, the total formation energy, which is also the product of the number of particles times the formation energy per atom of each individual phase, can be rewritten as:

$$\begin{aligned} E_f = N\varepsilon_f &= \sum_i w_i \varepsilon_{f,i} N \\ &= \sum_{ik} \varepsilon_{f,i} (c^{-1})_{ik} C_k N \\ &= \sum_{ik} \varepsilon_{f,i} (c^{-1})_{ik} N_k \end{aligned} \tag{2}$$

with $w_i = \underline{C}\ \underline{C_i}^{-1} = \sum_k C_k (c^{-1})_{ik}$

where the -1 superscript denotes the inverse matrix. N_k is the number of particles of the species k.

Relation between open circuit voltage and formation energies

The average voltage is the energy difference between two composition limits divided by the charge transfer between these limits.

$$V = -\frac{\Delta E}{\Delta Q} = -\frac{E_2 - E_1}{Q_2 - Q_1} \tag{3}$$

where E_1 and E_2 are the energies of structure 1 and 2 plus a pure lithium contribution given by:

$$\begin{aligned} E_1 &= E_1(N_k^{(1)}) + N_{Li}^{(2)}\varepsilon_{Li} \\ E_2 &= E_2(N_k^{(2)}) + N_{Li}^{(1)}\varepsilon_{Li} \end{aligned} \tag{4}$$

N_k is the number of atoms for the component k and ε_{Li} is the energy per lithium atom of the reference phase (lithium bcc obtained by DFT).

Q_1 and Q_2 are expressed as:

$$Q_i = eN_{Li}^{(i)} \quad \text{and} \quad i = 1, 2 \tag{5}$$

with the electron charge e.

The energy difference can be expressed in terms of the formation energies ε_f

$$\Delta E = E_2 - E_1 = N_2\varepsilon_{f,2} - N_1\varepsilon_{f,1} \tag{6}$$

with N_1 and N_2 the total number of atoms in the structure 1 and 2, respectively.

$$N_1 = N_{Li}^{(i)} + N_{Mn} + N_{Ni} + N_O \quad \text{and} \quad i = 1, 2 \tag{7}$$

Note that the number of atoms for the components other than lithium remains unchanged in the structure 1 and 2.

Using the definition of concentration for the Li component $C_{Li}^{(i)} = (N_{Li}^{(i)}/N_i)$, the difference in energy can be further rewritten as:

$$\begin{aligned} \Delta E = E_2 - E_1 &= N_{Li}^{(2)} \frac{N_2}{N_{Li}^{(2)}} \varepsilon_{f,2} - N_{Li}^{(1)} \frac{N_1}{N_{Li}^{(1)}} \varepsilon_{f,1} \\ &= N_{Li}^{(2)} \frac{\varepsilon_{f,2}}{C_{Li}^{(2)}} - N_{Li}^{(1)} \frac{\varepsilon_{f,1}}{C_{Li}^{(1)}} \end{aligned} \tag{8}$$

We define $\tilde{N} = N_{Mn} + N_{\mathrm{Ni}} + N_O$ thus:

$$N_i = N_{Li}^{(i)} + \tilde{N} \quad \text{and} \quad i = 1, 2 \tag{9}$$

and therefore:

$$N_{Li}^{(i)} = (N_{Li}^{(i)} + \tilde{N}) C_{Li}^{(i)} \quad \text{and} \quad i = 1, 2 \tag{10}$$

which is rewritten as:

$$N_{Li}^{(i)} = \frac{\tilde{N} C_{Li}^{(i)}}{(1 - C_{Li}^{(i)})} \quad \text{and} \quad i = 1, 2 \tag{11}$$

Inserting Eq. 11 into Eq. 8 and dividing by ΔQ, the average voltage is eventually expressed by:

$$V = -\frac{\Delta E}{\Delta Q} = -\frac{[(1 - C_{Li}^{(1)})\varepsilon_{f,2} - (1 - C_{Li}^{(2)})\varepsilon_{f,1}]}{e(C_{Li}^{(2)} - C_{Li}^{(1)})} \tag{12}$$

The contribution from each phase i to the voltage can be estimated independently using the formation energy $\varepsilon_{f,i}$ with the total voltage being the sum of the individual phase voltages:

$$V = \sum_i V_i \tag{13}$$

with

$$V_i = -\frac{[(1 - C_{Li}^{(1)}) w_{i,2} \varepsilon_{fi,2} - (1 - C_{Li}^{(2)}) w_{i,1} \varepsilon_{fi,1}]}{e(C_{Li}^{(2)} - C_{Li}^{(1)})} \tag{14}$$

List of phases and formation energies

Table 1: Phase formula, space group, and calculated formation energies with GGA+U in Li-Mn-Ni oxides at T=0 K without zero-point energy corrections. Phases with multiple space group entries have similar formation energies (within less than 1 meV/atom). Partly delithiated phases (*e.g.*, $Li_{1.5}MnO_3$ - $C2/m$) are not included in this table.

Phase	Crystal structure	E_f (eV)
Li	$Im\bar{3}m$	0.0000
$Li_{10}Mn_{23}O_{48}$	Cm	-2.1273
$Li_{10}Ni_4O_9$	$P4_2/nmc$	-2.0337
$Li_{11}Mn_{13}O_{32}$	$C2/m$	-2.1689
$Li_{11}Mn_2O_8$	$C2$	-2.1383
$Li_{11}Mn_6O_{16}$	$P1$	-2.2528
$Li_{11}Ni_{13}O_{24}$	$C2/m$	-1.9592
$Li_{11}(NiO_2)_{12}$	$C2/m$	-1.9097
$Li_{11}(NiO_4)_2$	$C2$	-2.0278
$Li_{12}Mn_2O_9$	$P1$	-2.1082
$Li_{13}Mn_{17}O_40$	$C2/m$	-2.1956
$Li_{13}Mn_{21}O_{48}$	Cm	-2.1691
$Li_{13}Mn_2O_9$	$P1$	-2.1100
$Li_{13}Mn_8O_{24}$	$C2$	-2.1234
$Li_{13}Mn_8O_{24}$	$P\bar{1}$ - $P2/m$	-2.1211
$Li_{13}Ni_{15}O_{28}$	$P\bar{1}$	-1.9621
$Li_{13}Ni_9O_{22}$	$P\bar{1}$	-1.9100
$Li_{14}Mn_2O_9$	$P\bar{3}$	-2.1006
$Li_{17}Ni_{11}O_{28}$	$P\bar{1}$	-1.8930
$Li_{19}Ni_{23}O_{42}$	$P\bar{1}$	-1.9652
Li_1MnO_3	$C2/m$	-1.8324

Table 1 *(Continued)*

Phase	Crystal structure	E_f (eV)
$Li_{23}Ni_{17}O_{40}$	$P\bar{1}$	-1.9168
$Li_2Mn_2Ni_3O_{12}$	$Pbcn$	-1.3313
$Li_2Mn_2Ni_3O_{12}$	$Pnma$	-1.3631
$Li_2Mn_2NiO_6$	$Cmce$	-2.1465
$Li_2Mn_2NiO_8$	$P\bar{1}$	-1.6989
$Li_2Mn_2O_5$	$P4/mmm$	-1.8705
$Li_2Mn_3Ni_2O_{12}$	$Pnma$	-1.6032
$Li_2Mn_3NiO_8$	$Fd\bar{3}m$	-2.2076
$Li_2Mn_3NiO_8$	$P2_13$	-2.1517
$Li_2Mn_3O_6$	$C2/m$	-2.2626
$Li_2Mn_3O_6$	$Cmce$	-2.2077
$Li_2Mn_3O_6$	$P1$	-2.2170
$Li_2Mn_3O_7$	$P\bar{1}$	-2.1605
$Li_2Mn_3O_7$	$P2_1/m$	-1.9975
Li_2Mn_3	$R\bar{3}c$	-0.0063
$Li_2Mn_4O_9$	$P\bar{3}c1$	-2.0590
$Li_2Mn_5O_{10}$	$P\bar{1}$	-2.1752
$Li_2Mn_5O_{12}$	Cc	-1.9174
$Li_2Mn_7O_{12}$	$P2_1$	-2.2532
$Li_2MnNi_2O_8$	$P\bar{1}$	-1.6746
$Li_2MnNi_3O_8$	$C2/m$	-1.8454
$Li_2MnNi_3O_8$	$P1$	-1.8872
$Li_2MnNi_3O_8$	$R\bar{3}m$	-1.8952
$Li_2Mn(NiO_3)_2$	$C2$	-1.9813
$Li_2Mn(NiO_3)_2$	$Cmce$	-1.9698

Table 1 *(Continued)*

Phase	Crystal structure	E_f (eV)
Li_2MnNiO_4	$Fm\bar{3}m$	-2.0684
Li_2MnNiO_4	$Imcm$ - $P2/m$	-2.2018
Li_2MnNiO_6	$Fm\bar{3}m$	-1.3501
Li_2MnO_2	$Immm$	-2.1700
Li_2MnO_2	$P\bar{3}m1$	-2.2241
Li_2MnO_3	$C2/m$	-2.2829
$Li_2Ni_5O_7$	$C2/m$	-2.0015
$Li_2(NiO_2)_{21}$	$P\bar{1}$	-1.3730
$Li_2(NiO_2)_3$	$Aea2$	-1.7233
$Li_2(NiO_2)_3$	$C2/m$	-1.7847
$Li_2(NiO_2)_3$	Cc	-1.7405
$Li_2(NiO_2)_3$	$P\bar{1}$	-1.7976
$Li_2(NiO_2)_5$	$P\bar{1}$	-1.6476
Li_2NiO_2	$Immm$	-2.0295
Li_2NiO_2	$P\bar{3}m1$	-2.0970
Li_2NiO_2	$R\bar{3}m$	-2.0235
Li_2NiO_3	$C/2m$ - $C/2c$	-1.9034
Li_2O_2	Cm	-1.6719
Li_2O_2	$Cmcm$	-1.6364
Li_2O_2	$F\bar{4}3m$	-1.1042
Li_2O_2	$Fm\bar{3}m$	-1.2937
Li_2O_2	$P4/mmm$	-1.3633
Li_2O_2	$P6_3mc$	-1.2797
Li_2O_2	$P6_3/mmc$	-1.7746
Li_2O_2	$P\bar{6}m2$	-1.4766

Table 1 *(Continued)*

Phase	Crystal structure	E_f (eV)
Li_2O_2	$Pm\bar{3}m$	-1.3306
Li_2O_2	$Pmma$	-1.3956
Li_2O_3	$Pm\bar{3}m$	-0.5037
Li_2O_3	$R\bar{3}c$	-1.4723
Li_2O	$Fm\bar{3}m$ - $R\bar{3}m$	-2.0867
Li_2O	$P4_2/mnm$	-2.0389
Li_2O	$Pnma$	-2.0008
$Li_3Mn_2Ni_5O_{12}$	$C2$	-1.9882
$Li_3Mn_2(NiO_4)_2$	$P\bar{1}$	-1.8875
$Li_3Mn_2NiO_6$	$C2/m$	-2.2341
$Li_3Mn_2O_4$	$C2/c$	-2.1039
$Li_3Mn_2O_4$	$Imma$	-2.0892
$Li_3Mn_3NiO_8$	$C2/m$	-2.1661
$Li_3Mn_3NiO_8$	Cc	-2.1585
$Li_3Mn_3NiO_8$	$P\bar{1}$	-2.2224
$Li_3Mn_3O_8$	$C2$	-2.0672
$Li_3Mn_3O_8$	$P4_332$	-2.1049
$Li_3Mn_3O_8$	$P6_3mc$	-2.0644
$Li_3Mn_3O_8$	$R\bar{3}m$	-2.0934
$Li_3Mn_4NiO_8$	$C2/m$	-2.3205
$Li_3Mn_4O_8$	$C2/m$	-2.2860
$Li_3Mn_4O_8$	$P\bar{1}$	-2.2607
$Li_3Mn_4O_8$	$R\bar{3}m$	-2.2666
$Li_3Mn_5O_{10}$	$P\bar{1}$	-2.2275
$Li_3Mn_5O_8$	$R\bar{3}m$	-2.3258

Table 1 *(Continued)*

Phase	Crystal structure	E_f (eV)
$Li_3Mn_7O_{16}$	$R3m$	-2.0453
$Li_3Mn_8O_{16}$	$Pmmn$	-2.1842
Li_3Mn	$Fm\bar{3}m$	-0.0066
Li_3Mn	$I4/mmm$	-0.0185
$Li_3MnNi_3O_8$	$C2/m$	-1.9883
$Li_3MnNi_3O_8$	$R\bar{3}m$	-1.9648
$Li_3Mn(NiO_2)_4$	$C2/m$	-2.1167
$Li_3Mn(NiO_3)_2$	$C2/c$	-2.1087
$Li_3Mn(NiO_3)_2$	$C2/m$	-2.1192
Li_3MnO_3	$P2_1/c$	-2.1722
Li_3MnO_3	$P321$	-2.1746
Li_3MnO_3	$P4_2/mnm$	-2.2243
Li_3MnO_4	$Cmmm$	-2.0611
Li_3MnO_4	$I\bar{4}3m$	-2.0592
Li_3MnO_4	$Pmn2_1$	-2.0758
Li_3MnO_4	$Pnma$	-2.0703
Li_3Mn	$P6_3/mmc$	-0.0128
Li_3Mn	$Pm\bar{3}m$	-0.0143
$Li_3Ni_5O_8$	$C2/m$	-1.9825
$Li_3Ni_5O_8$	$R\bar{3}m$	-1.9806
$Li_3(NiO_2)_4$	$C2/m$	-1.8476
$Li_3(NiO_2)_4$	$P\bar{1}$	-1.8042
$Li_3(NiO_2)_5$	$P\bar{1}$	-1.7614
$Li_3(NiO_2)_8$	$P\bar{1}$	-1.6166
Li_3NiO_3	$P4_2/mnm$	-1.9042

Table 1 *(Continued)*

Phase	Crystal structure	E_f (eV)
Li_3O	$Fm\bar{3}m$	-0.7343
Li_3O	$I4/mmm$	-0.7444
Li_3O	$P6_3/mmc$	-1.4064
Li_3O	$Pm\bar{3}m$	-0.8992
$Li_{47}(NiO_4)_8$	$P1$	-2.0491
$Li_4Mn_{13}O_{24}$	$P1$	-2.2394
$Li_4Mn_2Ni_3O_{10}$	$P\bar{1}$	-2.0535
$Li_4Mn_2Ni_5O_{12}$	$P2_1$	-2.0714
$Li_4Mn_3(NiO_4)_3$	$P\bar{1}$	-2.0850
$Li_4Mn_3NiO_8$	$C2/m$	-2.2713
$Li_4Mn_3O_7$	$P2_1/m$	-2.2723
$Li_4Mn_3O_8$	$R32$	-2.2183
$Li_4Mn_3O_8$	$R\bar{3}m$	-2.2055
$Li_4Mn_5Ni_3O_{16}$	Cm	-2.0757
$Li_4Mn_5NiO_{12}$	$C2/m$	-2.1838
$Li_4Mn_5(NiO_6)_2$	$P2_1$	-2.2485
$Li_4Mn_5O_{10}$	$P\bar{1}$	-2.2953
$Li_4Mn_5O_{12}$	$C2/c$	-2.1997
$Li_4Mn_7O_{12}$	$P1$	-2.3169
$Li_4Mn_7O_{16}$	$C2/m$	-2.0884
$Li_4Mn(Ni_2O_5)_2$	$P\bar{1}$	-1.9658
$Li_4MnNi_5O_{12}$	$C2$	-1.8827
Li_4MnO_3	Cc	-2.1272
$Li_4Ni_5O_9$	$P\bar{1}$	-1.9668
$Li_4Ni_7O_{11}$	$P\bar{1}$	-1.9921

Table 1 *(Continued)*

Phase	Crystal structure	E_f (eV)
$Li_4(NiO_2)_{11}$	$P\bar{1}$	-1.6150
$Li_4(NiO_2)_5$	$P\bar{1}$	-1.8673
$Li_4(NiO_2)_7$	$P\bar{1}$	-1.7479
Li_4O_5	$P4/mmm$	-1.5153
$Li_5Mn_2Ni_3O_{10}$	$P\bar{1}$	-2.1680
$Li_5Mn_2Ni_5O_{12}$	$C2$	-2.1521
$Li_5Mn_3(NiO_5)_2$	$P\bar{1}$	-2.1123
$Li_5Mn_4O_8$	$C2/m$	-2.2471
$Li_5Mn_4O_8$	$Cmc2_1$	-2.2676
$Li_5Mn_5(NiO_6)_2$	$C2$	-2.2872
$Li_5Mn_5O_{12}$	$P1$	-2.1942
$Li_5Mn_6O_{12}$	$P\bar{1}$	-2.2890
$Li_5Mn_6O_{16}$	$R\bar{3}m$	-1.9957
$Li_5Mn_7O_{12}$	$C2$	-2.3306
$Li_5Mn_7O_{15}$	Cm	-2.1963
$Li_5Mn_7O_{16}$	$Pnnm$	-2.2236
$Li_5Mn(Ni_2O_5)_2$	$P\bar{1}$	-2.0537
Li_5MnO_4	$Aea2$	-2.1509
Li_5MnO_4	$P2_1/mn$	-2.1292
Li_5MnO_4	$P4_2/nmc$	-2.1014
Li_5MnO_4	$Pbca$	-2.1493
Li_5MnO_4	$Pmmn$	-2.1241
Li_5MnO_5	$C2/m$	-2.0572
$Li_5Ni_7O_{12}$	$C2$	-1.9693
$Li_5Ni_9O_{16}$	$P\bar{1}$	-1.8089

Table 1 *(Continued)*

Phase	Crystal structure	E_f (eV)
$Li_5(NiO_2)_4$	Cc	-1.9390
$Li_5(NiO_2)_4$	$P4_332$	-1.9284
$Li_5(NiO_2)_6$	$P1$	-1.8772
$Li_5(NiO_2)_8$	$P1$	-1.7727
Li_5NiO_4	$Aea2$	-2.0096
Li_5NiO_4	$Pbca$	-2.0328
$Li_6Mn_5Ni_3O_{16}$	Cm	-2.1479
$Li_6Mn_5O_{10}$	Cm	-2.2824
$Li_6Mn_5O_{12}$	$C2$	-2.2487
$Li_6Mn_5O_{12}$	$P1$	-2.2516
$Li_6Mn_9O_{20}$	$C2/m$	-2.2123
$Li_6MnNi_7O_{16}$	$P\bar{1}$	-1.9044
Li_6MnO_4	$P4_2/nmc$	-2.1520
$Li_6(NiO_2)_{13}$	$P\bar{1}$	-1.6764
$Li_6(NiO_2)_5$	$P\bar{1}$	-1.9427
Li_6NiO_4	$Pmmn$	-2.0711
$Li_7Mn_{10}O_{20}$	$P1$	-2.1192
$Li_7Mn_{10}O_{24}$	$C2$	-2.1341
$Li_7Mn_{11}O_{24}$	$C2$	-2.2370
$Li_7Mn_{11}O_{24}$	$C2/m$	-2.1799
$Li_7Mn_{11}O_{24}$	$P\bar{1}$	-2.1967
$Li_7(NiO_2)_{10}$	$C2/m$	-1.8104
$Li_7(NiO_2)_{11}$	$P\bar{1}$	-1.7799
$Li_7(NiO_2)_{12}$	$C2$	-1.7475
$Li_7(NiO_2)_9$	$P\bar{1}$	-1.8566

Table 1 *(Continued)*

Phase	Crystal structure	E_f (eV)
$Li_8Mn_{15}NiO_{32}$	$R32$	-2.2463
$Li_8Mn_2O_7$	$P2_1/c$	-2.1027
$Li_8Mn_5O_{10}$	$P1$	-2.2420
$Li_8Mn_9O_{18}$	$P1$	-2.3100
$Li_8MnNi_7O_{16}$	$P\bar{1}$	-2.0184
Li_8MnO_6	$P6\bar{3}cm$	-2.0889
Li_8MnO_6	$R\bar{3}$	-2.1397
$Li_8(NiO_2)_5$	$P\bar{1}$	-2.0181
$Li_{95}Mn_{16}O_{64}$	$Pmm2$	-2.1482
$Li_9Mn_{10}O_{20}$	$P1$	-2.2959
$Li_9Mn_{12}Ni_3O_{32}$	$C2$	-2.1867
$Li_9Mn_{14}O_{32}$	Cm	-2.1771
$Li_9Mn_{15}O_{32}$	$P1$	-2.2385
$Li_9(NiO_2)_{10}$	$P\bar{1}$	-1.9120
$Li_9(NiO_4)_2$	$Pca2_1$	-1.9236
$LiMn_{0.5}Ni_{0.5}O_2$	$R\bar{3}m$ (SQS)	-2.2266
$LiMn_{12}O_{24}$	$P2/c$	-2.0255
$LiMn_2Ni_3O_6$	$C2/m$	-1.8234
$LiMn_2Ni$	$Fm\bar{3}m$	-0.2014
$LiMn_2NiO_6$	$C2/c$	-2.0014
$LiMn_2NiO_6$	$Fm\bar{3}m$	-1.3724
$LiMn_2NiO_6$	$I4mm$	-1.5204
$LiMn_2NiO_6$	$P\bar{1}$	-1.9901
$LiMn_2NiO_8$	$C2/c$	-1.4799
$LiMn_2NiO_8$	$P\bar{1}$	-1.4535

Table 1 *(Continued)*

Phase	Crystal structure	E_f (eV)
$LiMn_2O_3$	$C2/c$	-2.3493
$LiMn_2O_4$	$C2/c$	-2.2134
$LiMn_2O_4$	$Fd\bar{3}m$	-2.2223
$LiMn_2O_4$	$I4_1/amd$	-2.2643
$LiMn_2O_4$	$Fddd$	-2.2389
$LiMn_2O_4$	$P1$	-2.2045
$LiMn_2O_4$	$P6_3mc$	-2.2414
$LiMn_2O_4$	$R3m$	-2.2163
$LiMn_3Ni_2O_6$	$C2/m$	-2.1406
$LiMn_3Ni_4O_{12}$	$I\bar{4}2d$	-1.7805
$LiMn_3(NiO_4)_2$	$Imm2$	-2.1463
$LiMn_3NiO_8$	$C2/m$	-1.9730
$LiMn_3O_4$	$C2/m$	-2.3595
$LiMn_3O_5$	$Pbam$	-2.2942
$LiMn_3O_6$	$C2/m$	-2.1571
$LiMn_3O_6$	Cc	-2.1479
$LiMn_3O_6$	$P1$	-2.1745
$LiMn_3$	$P6_3/mmc$	-0.0320
$LiMn_3$	$Pm\bar{3}m$ - $I4/mmm$	-0.0369
$LiMn_4Ni_3O_{12}$	$I\bar{4}2d$	-1.8449
$LiMn_4O_8$	$C2$	-2.0803
$LiMn_4O_8$	$C2/m$	-2.1146
$LiMn_4O_8$	$F\bar{4}3m$	-2.1089
$LiMn_4O_8$	$R\bar{3}m$	-2.1115
$LiMn_5O_{10}$	$P\bar{1}$	-2.0358

Table 1 *(Continued)*

Phase	Crystal structure	E_f (eV)
$LiMn_5O_8$	$P4_332$	-2.2942
$LiMn_7O_{12}$	$C2$	-2.1877
$LiMn_7O_{12}$	$I4_1/acd$	-2.2083
$LiMn_7O_{12}$	$Im\bar{3}$	-2.1907
$LiMn_8O_{16}$	$Pmmn$	-2.0445
$LiMnNi_2$	$Fm\bar{3}m$	-0.1693
$LiMnNi_2O_6$	$Fm\bar{3}m$	-0.8418
$LiMnNi_2O_6$	$I4mm$	-1.4063
$LiMnNi_2O_8$	$C2/c$	-1.2417
$LiMnNi_2O_8$	$P\bar{1}$	-1.1354
$LiMnNiO_4$	$C2/m$	-1.9721
$LiMnNiO_4$	$Cmcm$	-1.8609
$LiMnNiO_4$	$Imma$	-2.0529
$LiMnO_2$	$C2/c$	-2.2829
$LiMnO_2$	Cc	-2.3117
$LiMnO_2$	Cm	-2.3269
$LiMnO_2$	$I4_1/amd$	-2.3384
$LiMnO_2$	$P\bar{1}$	-2.3302
$LiMnO_2$	$Pmm2$ - $Pmmn$	-2.3372
$LiMnO_2$	$Pmmn$	-2.2950
$LiMnO_2$	$R\bar{3}m$	-2.2604
$LiMnO_2$	$C2/m$	-2.3399
$LiMnO_3$	$Pm\bar{3}m$	-1.5904
$LiMnO_4$	$Cmcm$	-1.4558
LiMn	$Pm\bar{3}m$ - $P\bar{6}m2$	-0.0248

Table 1 *(Continued)*

Phase	Crystal structure	E_f (eV)
LiMn	$Pmma$ - $P4/mmm$	-0.0321
LiMn	$R\bar{3}m$	-0.0224
$LiNi_2O_3$	$C2/c$	-2.0033
$LiNi_2O_4$	$Fd\bar{3}m$	-1.7193
$LiNi_2O_4$	$Fd\bar{3}m$	-1.7458
$LiNi_2O_4$	$I4_1/amd$	-1.7247
$LiNi_3$	$Fm\bar{3}m$	-0.0034
$LiNi_3$	$I4/mmm$	-0.1988
$LiNi_3O_4$	$Cmmm$	-2.0147
$LiNi_3$	$P6_3/mmc$	-0.3499
$LiNi_3$	$Pm\bar{3}m$	-0.0288
$LiNi_4O_5$	$I4/m$	-2.0295
$LiNi_6O_7$	$P\bar{1}$	-2.0460
$LiNi_9O_{10}$	$P\bar{1}$	-2.0528
$Li(NiO_2)_2$	$P\bar{1}$	-1.7091
$Li(NiO_2)_2$	$P6_3mc$	-1.6909
$Li(NiO_2)_2$	$R\bar{3}$	-1.7365
$LiNiO_2$	$C2/m$	-1.9514
$LiNiO_2$	Cm	-1.9239
$LiNiO_2$	$I4_1/amd$	-1.9388
$LiNiO_2$	$Imma$	-1.9154
$LiNiO_2$	$Imm2$	-1.7062
$LiNiO_2$	$P\bar{1}$	-1.9478
$LiNiO_2$	$P6/mmm$	-1.1215
$LiNiO_2$	$R\bar{3}m$	-1.9568

Table 1 *(Continued)*

Phase	Crystal structure	E_f (eV)
$LiNiO_3$	$Pm\bar{3}m$	-1.0715
LiNi	$P4/mmm$	-0.2499
LiNi	$P6_3mc$	-0.1692
LiNi	$R\bar{3}m$	-0.2329
LiO_2	$Fm\bar{3}m$	-0.4565
LiO_2	$Pnnm$	-1.3949
LiO_3	$Imm2$	-1.15017
Mn	$I\bar{4}3m$	0.0000
$Mn_{15}NiO_{32}$	$R\bar{3}m$	-1.9258
$Mn_{15}O_{32}$	$C2/m$	-1.8206
$Mn_{21}O_{40}$	$I\bar{4}$	-2.0050
$Mn_2Ni_2O_5$	$P4/mmm$	-1.8520
Mn_2NiO_4	$Fd\bar{3}m$ - $I4_1/amd$	-2.1828
Mn_2NiO_4	$Imma$	-2.2293
Mn_2NiO_6	$Cmce$	-1.7458
Mn_2O_3	$Ia\bar{3}$	-2.3156
Mn_2O_3	$P4_12_12$	-2.2467
Mn_2O_3	$Pbca$	-2.3213
Mn_2O_3	$Pm\bar{3}m$	-1.8810
Mn_2O_3	$Pna2_1$	-2.2347
Mn_2O_3	$R\bar{3}c$	-2.2619
Mn_2O_5	$P4/mbm$	-1.1608
Mn_2O_7	$P2_1/c$	-0.9463
Mn_2O	$P4_2/mnm$	-1.3283
Mn_3Ni	$I4/mmm$ - $Fm\bar{3}m$	-0.1322

Table 1 *(Continued)*

Phase	Crystal structure	E_f (eV)
Mn_3NiO_4	$Cmmm$	-2.3133
Mn_3NiO_8	$P4_332$	-1.7918
Mn_3NiO_8	$R\bar{3}m$	-1.7904
Mn_3Ni	$P6_3/mmc$	-0.1154
Mn_3Ni	$Pm\bar{3}m$	-0.1056
Mn_3O_4	$Fd\bar{3}m$	-2.3781
Mn_3O_4	$I4_1/amd$	-2.3922
Mn_3O_4	$Pbcm$	-2.3469
Mn_3O_4	Pm	-2.1827
Mn_3O	$I4/mmm$	-0.4000
Mn_3O	$P6_3/mmc$	-1.0877
Mn_3O	$Pm\bar{3}m$	-0.2936
Mn_4NiO_8	$C2/m$	-2.0801
Mn_4O_5	$P4/mmm$	-2.0508
Mn_5NiO_{12}	$C2/m$	-1.8663
Mn_5O_8	$C2/m$	-2.2373
Mn_5O_8	$R\bar{3}m$	-2.1716
Mn_7O_{12}	$Im\bar{3}$	-2.1199
$MnNi_2O_4$	$I4_1/amd$	-1.9781
$MnNi_3$	$I4/mmm$	-0.4639
$MnNi_3O_4$	$Cmmm$	-2.1431
$MnNi_3$	$Pm\bar{3}m$	-0.2319
$MnNi_6O_8$	$Fm\bar{3}m$	-2.0796
$MnNiO_2$	$P4/mmm$	-2.2040
$MnNiO_3$	$Pm\bar{3}m$	-1.4496

Table 1 *(Continued)*

Phase	Crystal structure	E_f (eV)
$MnNiO_3$	$R\bar{3}$	-2.0820
MnNi	$P4/mmm$ - $Pmma$	-0.4592
MnNi	$P\bar{6}m2$	-0.4341
MnNi	$Pm\bar{3}m$	-0.4329
MnO_2	$C2/m$	-1.9825
MnO_2	$Fd\bar{3}m$	-1.9705
MnO_2	$I4/m$	-1.9998
MnO_2	$P3m1$	-1.9891
MnO_2	$P4_2/mnm$	-1.9624
MnO_2	$P6_3mc$	-1.9723
MnO_2	$Pnma$	-1.9933
MnO_2	$Pmmn$	-1.8387
MnO_2	$Pnnm$	-1.9666
MnO_2	$R\bar{3}m$	-1.9905
MnO_3	$Pm\bar{3}m$	-0.3700
MnO	$F\bar{4}3m$	-2.3557
MnO	$Fm\bar{3}m$	-2.4129
MnO	$P6_3mc$	-2.3765
MnO	$P\bar{6}m2$	-2.1934
MnO	$Pm\bar{3}m$	-1.8672
MnO	$Pmma$	-2.1223
Ni	$Fm\bar{3}m$	0.0000
$Ni_{15}O_{16}$	$Im\bar{3}m$	-2.0007
$Ni_{15}O_{16}$	$R\bar{3}m$	-1.9409
Ni_2O_3	$Pm\bar{3}m$	-0.0772

Table 1 *(Continued)*

Phase	Crystal structure	E_f (eV)
Ni_2O	$P4_2/mnm$	-1.1629
Ni_3O_4	$C2/m$	-1.7716
Ni_3O_4	$Cmmm$	-1.7983
Ni_3O	$P6_3/mmc$	-0.9037
Ni_4O_5	$P4/mmm$	-1.5422
Ni_5O_6	$C2/m$	-1.8756
Ni_6O_7	$P\bar{1}$	-1.9007
Ni_9O_{10}	$P\bar{1}$	-1.9534
NiO_2	$Fd\bar{3}m$	-1.2921
NiO_2	$Immm$	-0.9426
NiO_2	$P3m1$	-1.3008
NiO_2	$R\bar{3}m$ - $C2m$	-1.3026
NiO_3	$I4/mmm$	-0.2432
NiO	$F\bar{4}3m$	-1.3802
NiO	$P4/mmm$	-1.2036
NiO	$P6_3mc$	-1.3672
NiO	$P\bar{6}m2$	-1.6424
NiO	$Pmma$	-1.6355
NiO	$R\bar{3}m$ - $Fm\bar{3}m$	-2.0669
O_2	*dimer*	0.0000

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