Supporting Information

Effect of oxygen vacancy electronic state on Ni migration in $Li_{0.5}(Ni_{0.8}Mn_{0.1}Co_{0.1})O_2$ cathode material: a first-principles study

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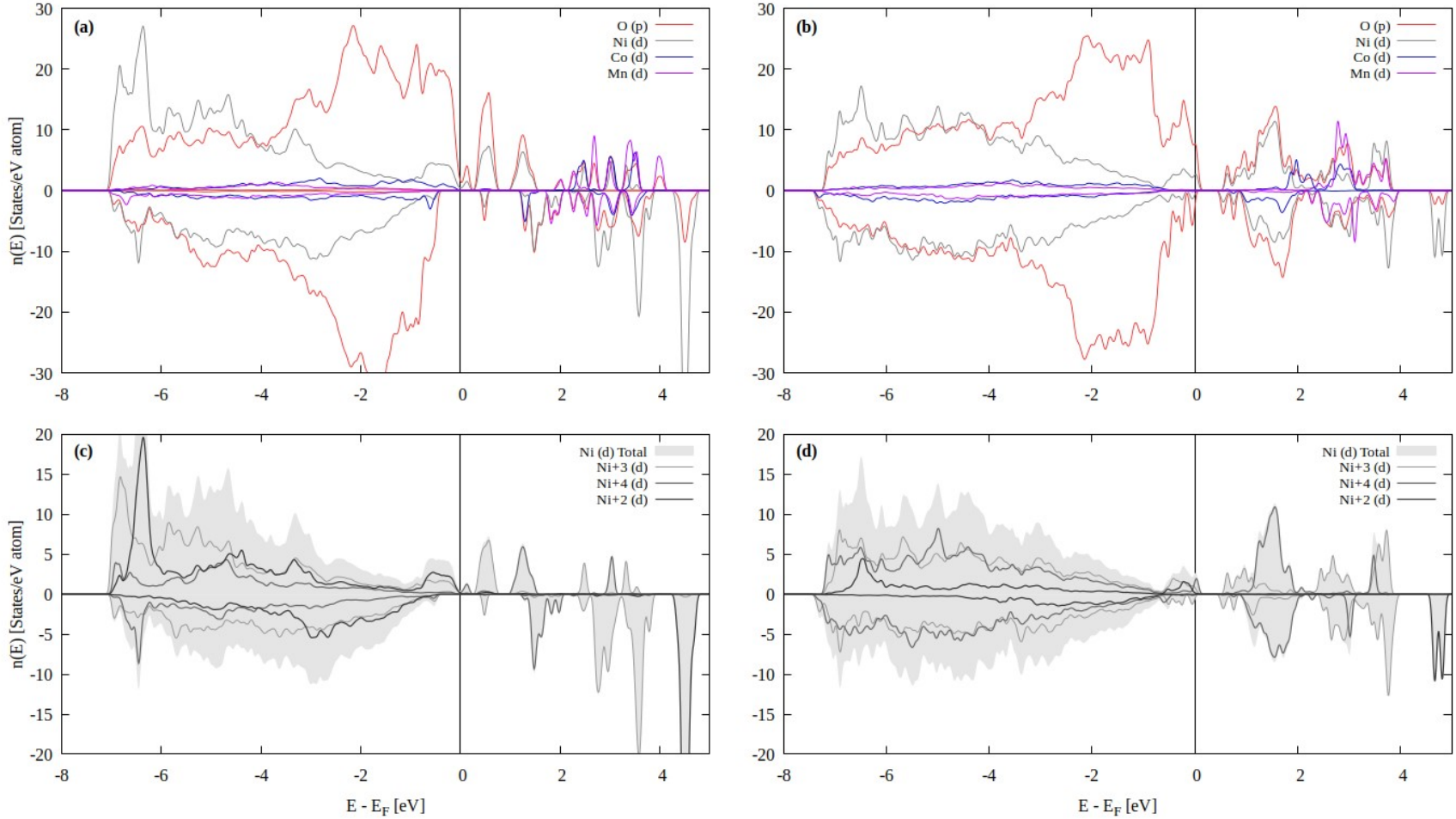

Figure S1. (a) and **(b)**, band-decomposed density of states profile of all atoms at 100% and 50% lithation respectively. **(c)** and **(d)** density of states of all Ni(*d*) decomposed to each oxidation state (+2, +3 and +4) at 100% and 50% lithation respectively.

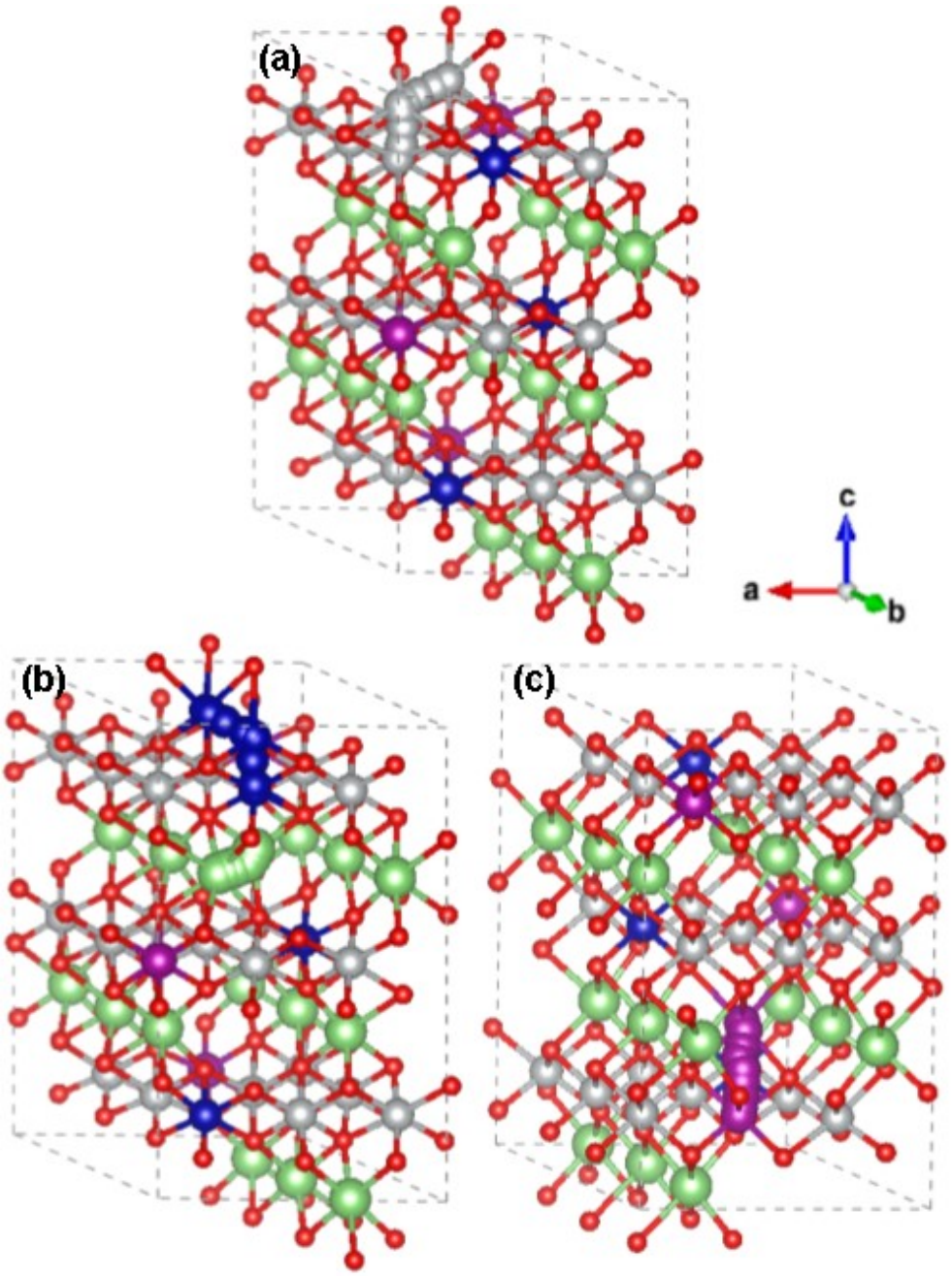

Figure S2. Minimum energy path of **(a)** Ni, **(b)** Co and **(c)** Mn calculated using CI-NEB. 3 images were employed for both Ni($O_{h,TM} \rightarrow T_d$) and Ni($T_d \rightarrow O_{h,Li}$). 5 images were employed for Co($O_{h,TM} \rightarrow T_d$) to account simultaneous Li diffusion to $T_{h,Li}$ and 3 images were employed for Co($T_d \rightarrow O_{h,Li}$). 7 images were employed for direct Mn($O_{h,TM} \rightarrow O_{h,Li}$) because T_d sites are found to be unstable for Mn to occupy.

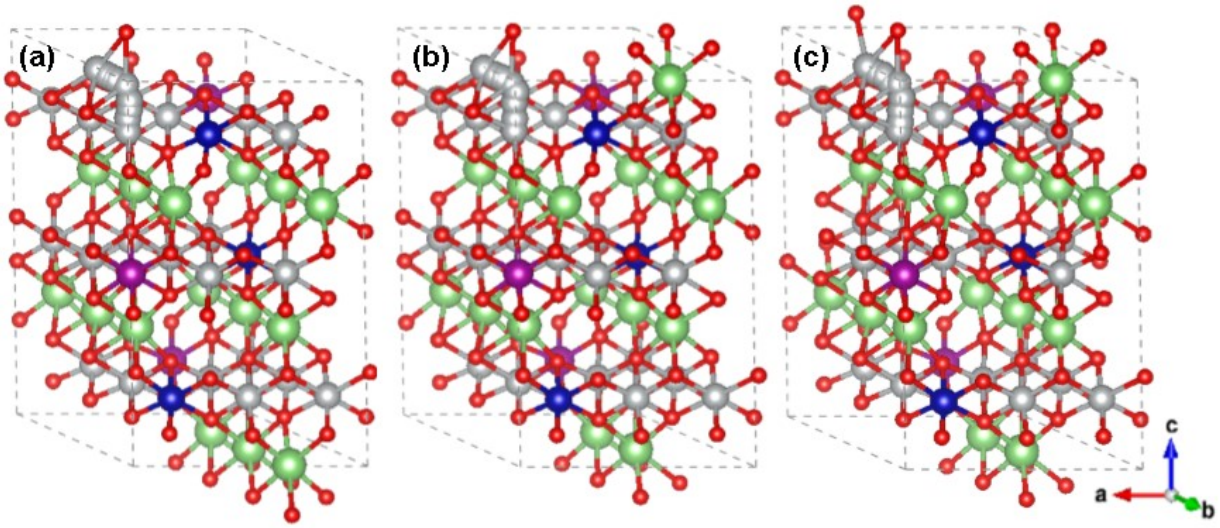

Figure S3. Minimum energy path of Ni diffusion next to a vacancy in shared plane of diffusion (O1) at **(a)** neutral, **(b)** (+1)- and **(c)** (+2)-charge states calculated using CI-NEB. 3 images were employed for both Ni($^{O_{h,TM}\rightarrow T_d}$) and Ni($^{T_d\rightarrow O_{h,Li}}$) at all charge states.

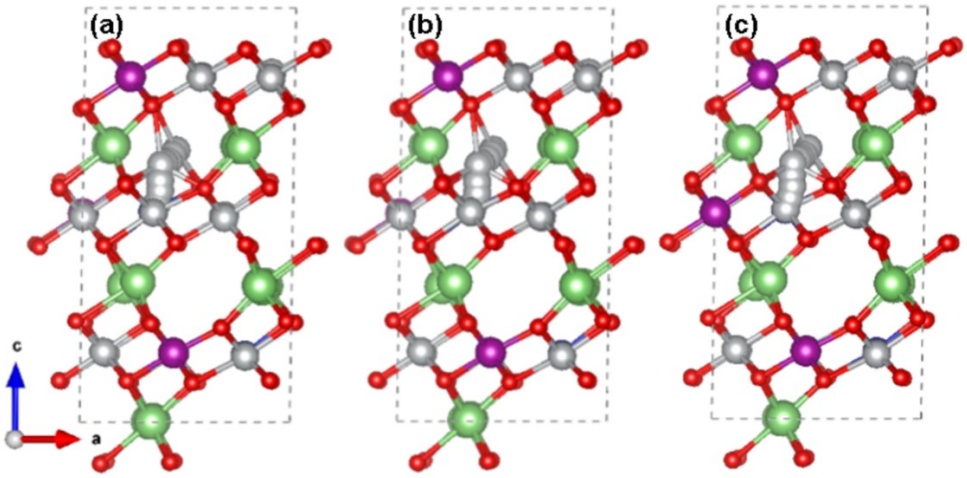

Figure S4. Minimum energy path of Ni diffusion next to a vacancy opposing the plane of diffusion (O2) at **(a)** neutral, **(b)** (+1)- and **(c)** (+2)-charge states calculated using CI-NEB. 3 images were employed for both Ni($^{O_{h,TM}\rightarrow T_d}$) and Ni($^{T_d\rightarrow O_{h,Li}}$) at all charge states.

Configuration	DFT+*U* (eV)		DFT+*U*+D3 (eV)	
	O1	O2	O1	O2
FS1	-0,527	-0,841	-0,334	-0,439
FS2	-0,019	-0,192	-0,490	-0,347

Table S1. Calculated Ni migration energy in neutral O_{vac}-contained $Li_{0.5}$NMC811 without and with dispersion correction. The 'O1' and 'O2' notation refer to the location of O_{vac} with respect the normal plane of the dislocated Ni (see **Figure 5** of the main manuscript). The values and notation of FS refers to the "Final State" (of DFT+*U* results) as tabulated in the **Figure 6** in the main manuscript.