

Supplementary Information

Decomposition pathway and structural transformation of lithium nickel oxide under a high-delithiation state

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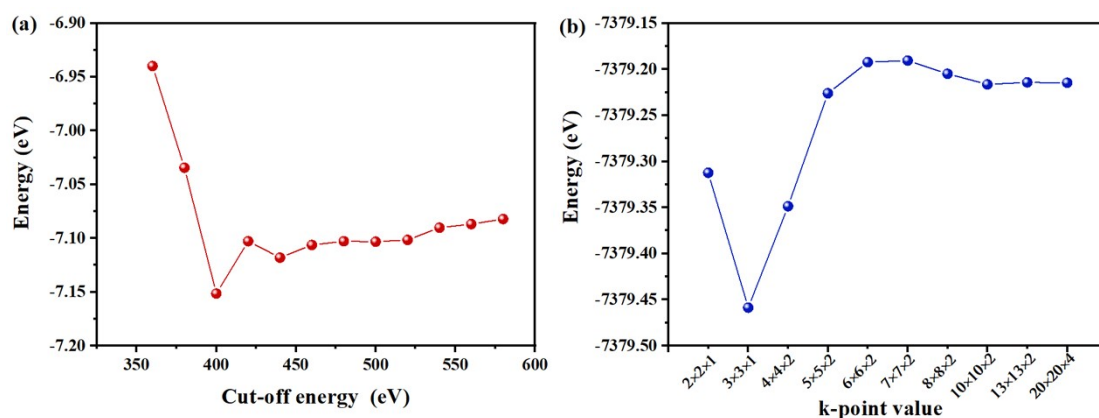


Figure S1. Convergence test with respect to (a) cut-off energy, and (b) k-point value

Table S1. Reaction energies of heterojunction 1 (a) and heterojunction 2 (b) for $\text{LiNi}_6\text{O}_{12}$

Chemical Reaction	Reaction Free Energy(eV)
Layered $\text{LiNi}_6\text{O}_{12}$ (003) $\rightarrow$ Layered LiNi_6O_6 (003)	7.8
Layered LiNi_6O_6 (003) $\rightarrow$ Rock Ni_6O_6 ($11\bar{1}$)	3.8
Layered $\text{LiNi}_6\text{O}_{12}$ (003) $\rightarrow$ Rock $\text{LiNi}_6\text{O}_{12}$ (003)	3.6
Rock $\text{LiNi}_6\text{O}_{12}$ (003) $\rightarrow$ Rock Ni_6O_6 ($11\bar{1}$)	7.9
Layered $\text{LiNi}_6\text{O}_{12}$ (010) $\rightarrow$ Layered LiNi_6O_6 (010)	7.6
Layered LiNi_6O_6 (010) $\rightarrow$ Rock Ni_6O_6 ($1\bar{1}2$)	-1.1
Layered $\text{LiNi}_6\text{O}_{12}$ (010) $\rightarrow$ Rock $\text{LiNi}_6\text{O}_{12}$ (010)	-1.7
Rock $\text{LiNi}_6\text{O}_{12}$ (010) $\rightarrow$ Rock Ni_6O_6 ($1\bar{1}2$)	8.2

Table S2. Reaction energies of heterojunction 1 (a) and heterojunction 2 (b) for $(\text{Li}_7\text{Ni})_{\text{Li}}(\text{Ni}_{47}\text{Li})_{\text{Ni}}\text{O}_{96}$

Chemical Reaction	Reaction Free Energy(eV)
Layered $(\text{Li}_7\text{Ni})_{\text{Li}}(\text{Ni}_{47}\text{Li})_{\text{Ni}}\text{O}_{96}$ (003) $\rightarrow$ Layered $(\text{Li}_7\text{Ni})_{\text{Li}}(\text{Ni}_{47}\text{Li})_{\text{Ni}}\text{O}_{48}$ (003)	9.3
Layered $(\text{Li}_7\text{Ni})_{\text{Li}}(\text{Ni}_{47}\text{Li})_{\text{Ni}}\text{O}_{48}$ (003) $\rightarrow$ Rock $(\text{Ni}_{47}\text{Li})_{\text{Ni}}\text{O}_{48}$ ($11\bar{1}$)	2.6
Layered $(\text{Li}_7\text{Ni})_{\text{Li}}(\text{Ni}_{47}\text{Li})_{\text{Ni}}\text{O}_{96}$ (003) $\rightarrow$ Rock $(\text{Li}_7\text{Ni})_{\text{Li}}(\text{Ni}_{47}\text{Li})_{\text{Ni}}\text{O}_{96}$ (003)	4.1
Rock $(\text{Li}_7\text{Ni})_{\text{Li}}(\text{Ni}_{47}\text{Li})_{\text{Ni}}\text{O}_{96}$ (003) $\rightarrow$ Rock $(\text{Ni}_{47}\text{Li})_{\text{Ni}}\text{O}_{48}$ ($11\bar{1}$)	7.8
Layered $(\text{Li}_7\text{Ni})_{\text{Li}}(\text{Ni}_{47}\text{Li})_{\text{Ni}}\text{O}_{96}$ (010) $\rightarrow$ Layered $(\text{Li}_7\text{Ni})_{\text{Li}}(\text{Ni}_{47}\text{Li})_{\text{Ni}}\text{O}_{48}$ (010)	7.9
Layered $(\text{Li}_7\text{Ni})_{\text{Li}}(\text{Ni}_{47}\text{Li})_{\text{Ni}}\text{O}_{48}$ (010) $\rightarrow$ Rock $(\text{Ni}_{47}\text{Li})_{\text{Ni}}\text{O}_{48}$ ($1\bar{1}2$)	0.6
Layered $(\text{Li}_7\text{Ni})_{\text{Li}}(\text{Ni}_{47}\text{Li})_{\text{Ni}}\text{O}_{96}$ (010) $\rightarrow$ Rock $(\text{Li}_7\text{Ni})_{\text{Li}}(\text{Ni}_{47}\text{Li})_{\text{Ni}}\text{O}_{96}$ (010)	-0.9
Rock $(\text{Li}_7\text{Ni})_{\text{Li}}(\text{Ni}_{47}\text{Li})_{\text{Ni}}\text{O}_{96}$ (010) $\rightarrow$ Rock $(\text{Ni}_{47}\text{Li})_{\text{Ni}}\text{O}_{48}$ ($1\bar{1}2$)	9.4