

Electronic Supplementary Information (ESI)

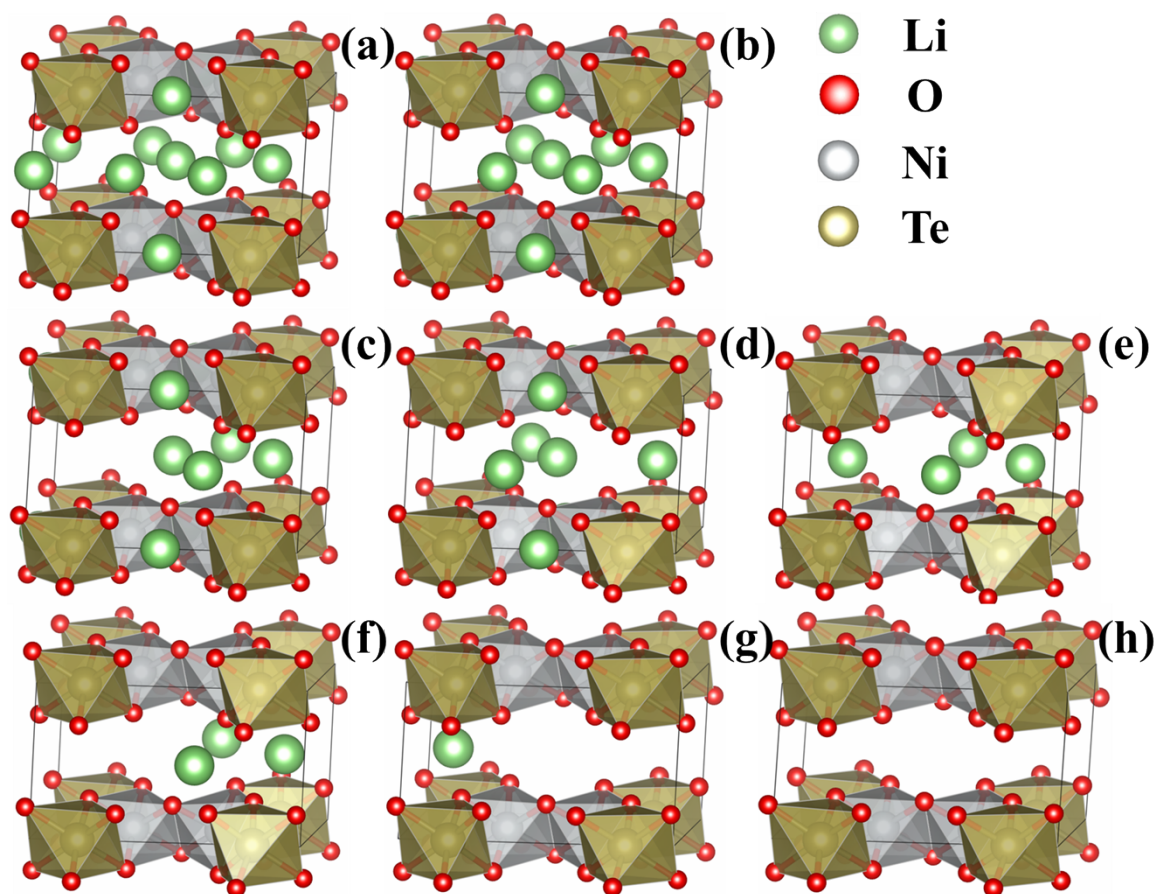
First-Principles Investigations on Delithiation of $\text{Li}_4\text{NiTeO}_6$

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ESI 1 Optimized configurations of $\text{Li}_x\text{NiTeO}_6$ ($x=3.5, 2, 1.5, 1\ldots$) from (a) to (h). Balls in green, red and octahedral in grey and brown are Li, O, Ni and Te, respectively. Note that not all geometrically identical Li atoms are depicted and the No. 18 Li atom is overshadowed on condition that the lattice is displayed with the same angle in Fig. 1. Whether this Li is extracted can be checked by summing up the shown Li atoms. With regard to (d), $\text{Li}_2\text{NiTeO}_6$, four Li atoms are shown; therefore, the No. 18 Li atom is removed from the lattice, which is the first one extracted from the LiNiTe layer. Also, note that the Li vacancies do not rearrange until the process from $\text{Li}_{2.5}\text{NiTeO}_6$ to $\text{Li}_2\text{NiTeO}_6$.

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