阴离子硫氧化还原与 Li_{1-x}NiO_{2-y}S_y 的结构稳定性：第一性原理研究

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First-Principles Study: the Structural Stability and Sulfur Anion Redox of Li_{1-x}NiO_{2-y}S_y

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Fig. S1  The structures of LiNiO$_2$ with space group $R\bar{3}m$ (a) and $C2/m$ (c); the local octahedral environment in LiNiO$_2$ with space group $R\bar{3}m$ (b) and $C2/m$ (d), the length of Ni-O bonds measured in angstrom are labeled; the total density of states for the LiNiO$_2$ with space group $R\bar{3}m$ (e) and $C2/m$ (f).
Fig.S2 The evolution of the average projected density of states (PDOS) evolution during the charge process in Li$_{1-x}$NiO$_2$ (with C2/m space group). The black and blue lines represent the nickel and oxygen atom, respectively.
Fig. S3  The evolution of the average projected density of states (PDOS) evolution during the charge process in Li$_{1.0}$NiO$_{1.89}$S$_{0.11}$. The black, blue and cyan lines represent the nickel, oxygen and sulfur atom, respectively.