Supporting Information for *Acta Phys. -Chim. Sin.* 2017, *33* (9), 1781−1788
doi: 10.3866/PKU.WHXB201705041

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

鄢慧君　　李　彪　　蒋　宁　　夏定国*

(北京大学工学院，先进电池材料理论与技术北京市重点实验室，北京 100871)

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

YAN Hui-Jun　　LI Biao　　JIANG Ning　　XIA Ding-Guo*

(*Beijing Key Laboratory of Theory and Technology for Advanced Batteries Materials, College of Engineering, Peking University, Beijing 100871, P. R. China*)

*Corresponding authors. Email: dgxia@pku.edu.cn; Tel: +86-10-62767962.

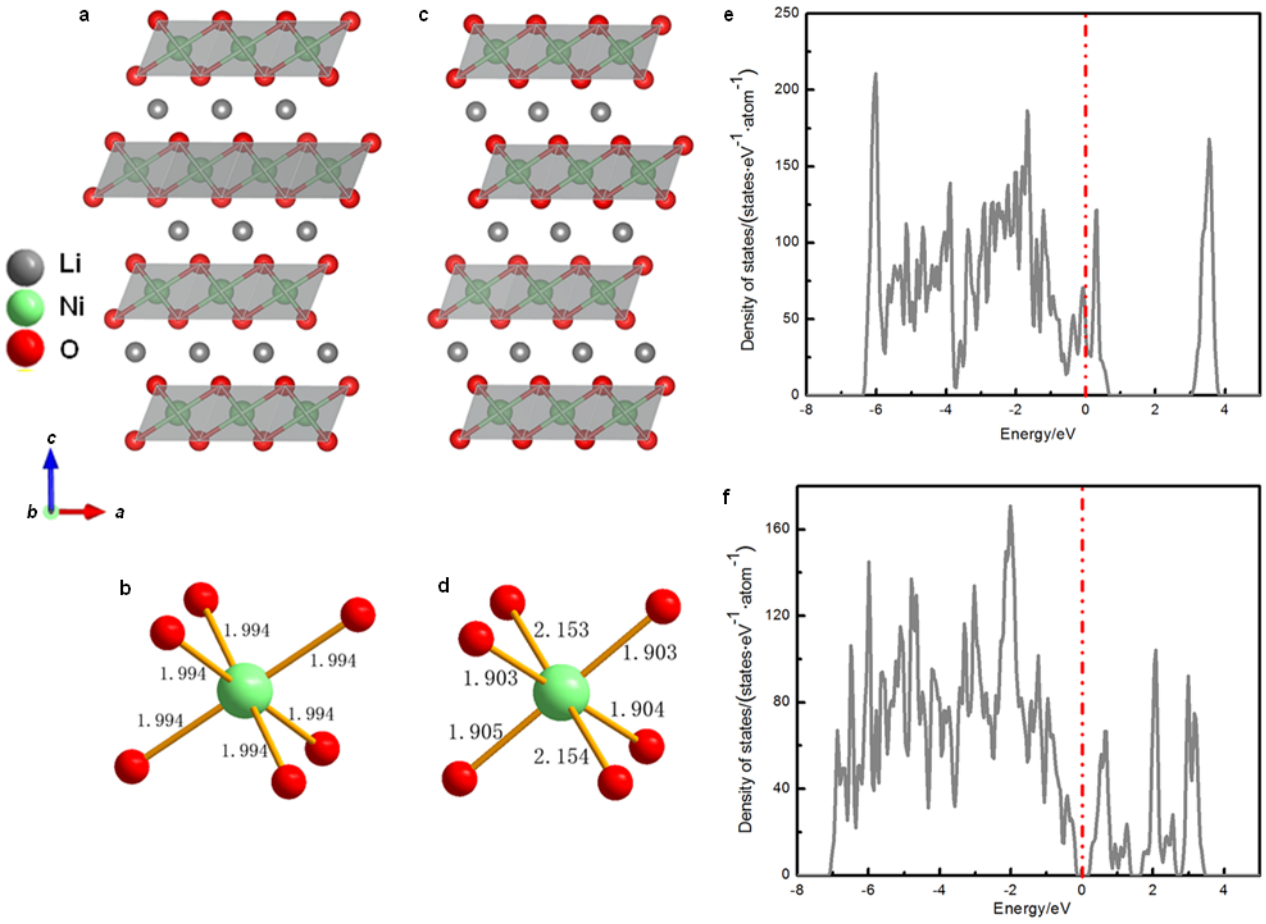

Fig.S1 The structures of $LiNiO_2$ with space group $R\bar{3}m$ (a) and *C2/m* (c); the local octahedral environment in $LiNiO_2$ with space group $R\bar{3}m$ (b) and *C2/m* (d), the length of Ni-O bonds measured in angstrom are labeled; the total density of states for the $LiNiO_2$ with space group $R\bar{3}m$ (e) and *C2/m* (f).

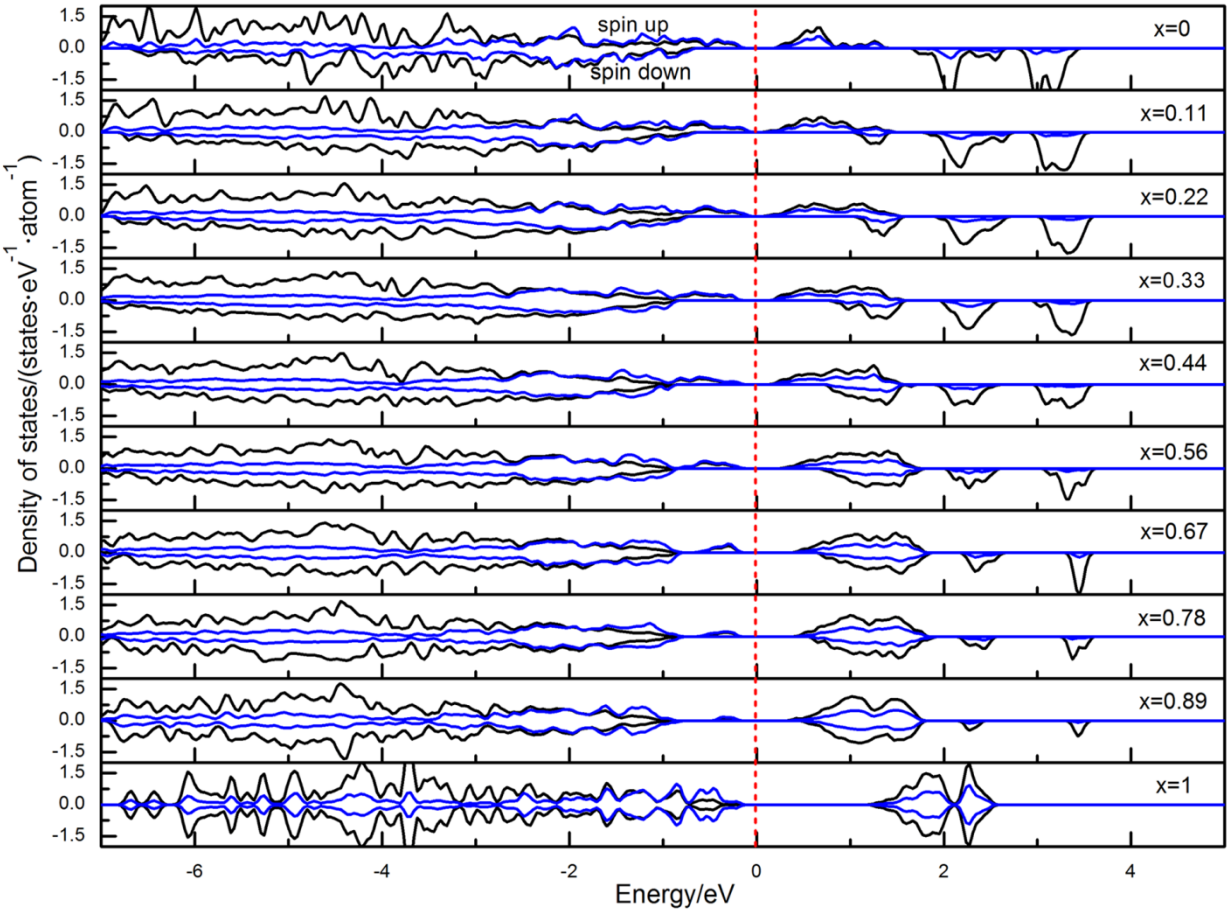

Fig.S2 The evolution of the average projected density of states (PDOS) evolution during the charge process in $Li_{1-x}NiO_2$ (with *C2/m* space group). The black and blue lines represent the nickel and oxygen atom, respectively.

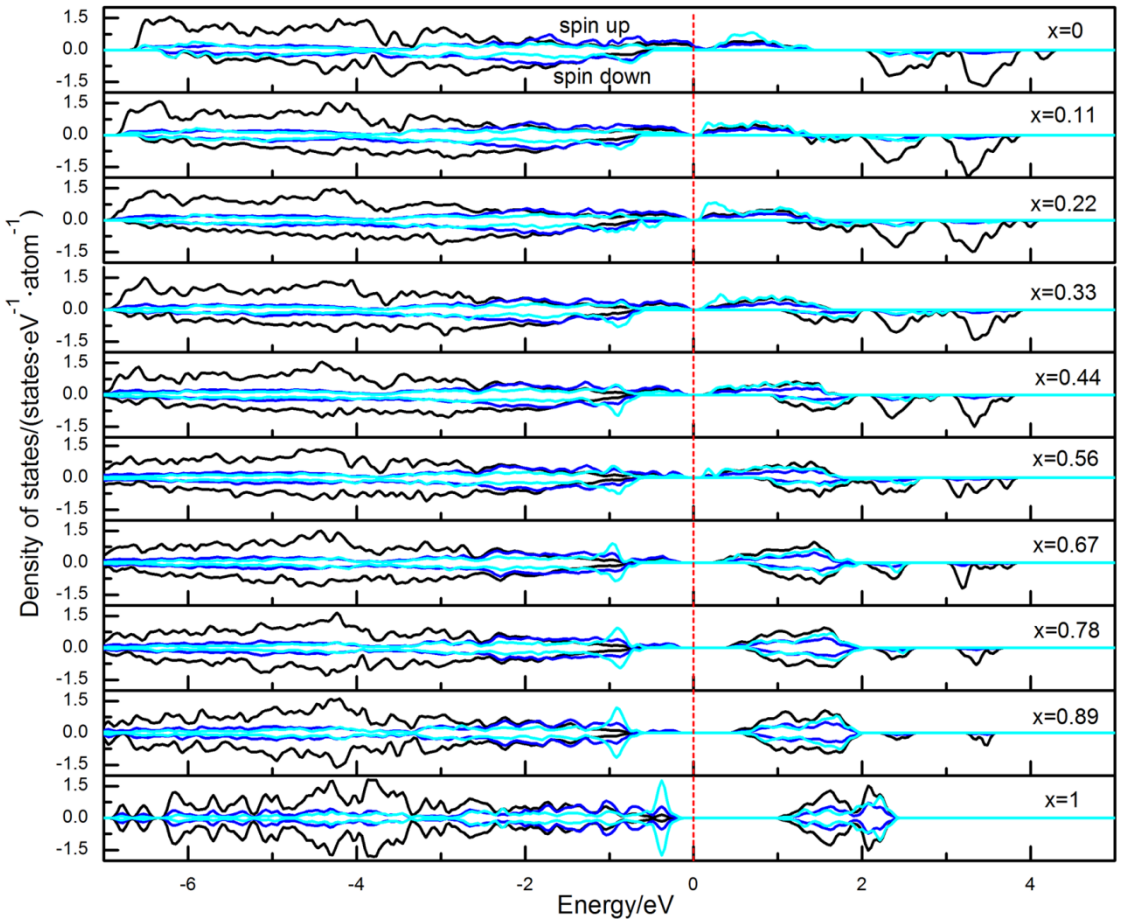

Fig.S3 The evolution of the average projected density of states (PDOS) evolution during the charge process in $Li_{1-x}NiO_{1.89}S_{0.11}$. The black, blue and cyan lines represent the nickel, oxygen and sulfur atom, respectively.