Structural and Electronic Properties of Small Lithium Peroxide Clusters in View of Charge Process in Li-O₂ Batteries

Bipeng Hou, Xueling Lei, Zuoliang Gan, Shuying Zhong, Gang Liu, Chuying Ouyang

Department of Physics, Laboratory of Computational Materials Physics, Jiangxi Normal University, Nanchang, Jiangxi 330022, China

Fig. S-1 Structure and the corresponding total energy (in a.u.) of each non-Li₂O₂ cluster (LiₙOₙ-ne-m). In LiₙOₙ-ne-m, the first term represents the chemical formula, the second term n represents the number of lost electrons, and the third term m represents the spin multiplicity.

1 Corresponding author: Email: xueling@mail.ustc.edu.cn