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

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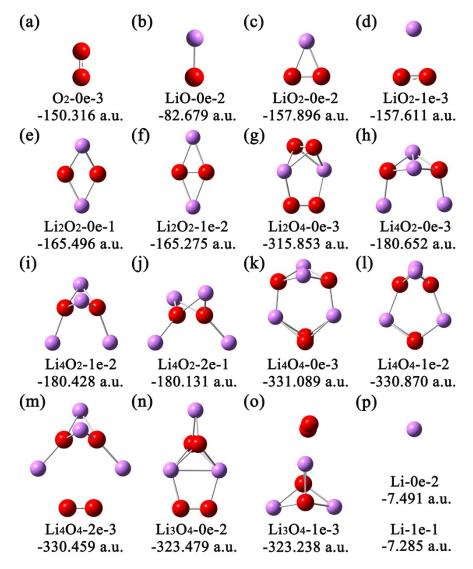


Fig. S-1 Structure and the corresponding total energy (in a.u.) of each non-Li₂O₂ cluster (Li_xO_y-ne-m). In Li_xO_y-ne-m, the first term represents the chemical formula, the second term n represents the number of lost electrons, and the third term m represents the spin multiplicity.

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