

First-principles study on the factors that can affect oxygen-redox stability in Li-excess cathodes

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Oxygen redox in Li-excess oxide cathodes has been recently attracting great attention because it can provide the extra capacity in addition to the capacity from their transition metal (TM) redox. It is now understood that unhybridized O 2p states of O ions that are linearly coordinated by two lithium ions (Li-O-Li configuration) in the Li-excess structure are the source of electrons for the oxygen redox processes. However, it was found that the oxygen becomes less stable with oxidation and stabilizes with various forms: peroxo-like species formation, the hole localization on the O ions, and peroxide/superoxide/O₂ molecule formation. Understanding which factors that can affect the stabilization of oxidized oxygen is important as this would deepen our understanding of the stabilization of O redox against O loss which is detrimental to the cathode performance, yet there is no clear explanation at this point. In this talk, I will present the first-principles results on the distribution of excess Li and the effect of Li-excess level on the stability of oxidized oxygen in Li-excess cathode materials.