Development of simulation-experiment hybrid analysis technique for design of high-performance secondary batteries

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Objectives

Li-rich materials Li$_2$MnO$_3$-LiMO$_2$ (M = Co, Ni, Mn) have received a great deal of research attention due to their attractive properties of higher reversible capacity and energy density as lithium-ion battery (LIB) cathodes. For understanding the mechanism of charge and discharge irreversibility of this materials, we exhaustively examine the relationship between electrochemically stable Li/vacancy configurations and their corresponding voltage in the surface region of Li$_2$MnO$_3$ in the solid-state Li$_2$MnO$_3$-LiMO cathode material through high-throughput computing.

Outline of Results

By using our originally developed tool, we examine the relationship between electrochemically stable Li/vacancy configurations and their corresponding voltage in the surface region of Li$_2$MnO$_3$ in the solid-state Li$_2$MnO$_3$-LiMO cathode material through high-throughput computing. In this code, the calculations for the energy of each configuration are performed based on first-principle calculations. We found most stable configurations and corresponding voltage with reference of standard redox potential of Li (vs Li$^+$/Li) for several $x$’s ($x$: amounts of Li).