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Density Functional Theory Study of spinel LiMn2O4: Towards the Order-N DFT method implemented in the ONETEP code.

The search for the next affordable, environmentally friendly, and high-energy-density cathode material is an integral part of the betterment of lithium-ion batteries, in a quest to address the grievous challenges confronting energy storage systems. Density Functional Theory (DFT) has made significant progress in this search, however, it is found wanting at unravelling the electronic structure of the exciting area of nanostructured materials that consist of a substantial amount of structural features key to battery performance. Since traditional DFT scales cubical with system size which limits the number of atoms to be studied to a few hundred, leading to the birth of linear-scaling DFT methods. In this current work, we employ the traditional DFT implemented in CASTEP and the linear scaling DFT implemented in ONETEP to determine optimal settings essential for running the ONETEP code, especially at the centre for high-performance computing (CHPC). DFT calculations were performed under the generalized gradient approximation (GGA) method on both simulation codes (CASTEP and ONETEP). The changes in the electronic structure of the promising Li-battery cathode material Li-Mn-O spinel during Li-intercalation (discharge process) was captured through the density of states (DoS). The ONETEP and CASTEP simulation codes successfully deduced the metallic behaviour of spinel LiMn2O4. The open cell voltages (OCV) were also calculated and a good agreement between the two codes was observed. Strong and weak scaling tests were also performed at the CHPC on processors ranging from 0 to 216. The efficient kernel cutoff required to achieve better linear scaling whilst persevering accuracy for the Li-Mn-O spinel was found to be between 40 – 200 Bohr. The findings of this study guides exploration of the electronic structure exploration of nanostructured Li-Mn-O spinel (>3.3 nm) incorporating crucial structural properties observed experimentally with linear scaling DFT implemented in the ONETEP code.

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