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Dft-based evaluation of Li_2MnO_3 as a promising cathode coating material for lithium-ion batteries

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An ideal cathode coating material must exhibit excellent chemical stability, adequate electronic and ionic conductivity, a wide electrochemical stability window, and strong mechanical integrity to protect the electrode from degradation while ensuring efficient battery performance. Li_2MnO_3 has previously been used as a coating material due to its stabilizing effect on the core, but other beneficial properties it may offer as a coating material are still underexplored. In this study, these ideal coating properties of Li_2MnO_3 were investigated using Density Functional Theory (DFT). Given that the accuracy of DFT is highly dependent on the exchange-correlation functional, calculations were performed using meta-GGA, GGA+U, and GGA-PBE functionals to determine which provides the most accurate results compared to experimental data. To improve accuracy further, spin configurations were also considered. Among the tested methods, GGA+U combined with antiferromagnetic ordering produced results that were in closer agreement with experimental observations. The findings show that Li_2MnO_3 is thermodynamically stable, mechanically robust, and a semiconductor with a band gap of 2.17 eV. These results affirm Li_2MnO_3 as a promising cathode coating material, possessing the key attributes which are thermodynamic, electronic, and mechanical stability needed to enable durable, high-performance lithium-ion battery systems.

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