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Exploring compatibility and accuracy of functionals on structural and electronic properties of manganese oxide cathode materials: A dft and dft+u study

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Lithium manganese oxides (LMO) have gained significant interest as positive electrode materials for lithium-ion batteries, owing to their high capacity and suitability for achieving remarkable energy densities thus positioning them as promising candidates for advancing LIB technology. Among these materials, Li_2MnO_3 and LiMnO_2 exhibit unique structural and electronic properties that are crucial for their performance in LIBs. This study aims to assess the structural and electronic characteristics of layered lithium manganese oxide cathode materials for lithium-ion batteries using DFT-based computational simulations. Through comparison with experimental data, our findings demonstrate the reliability of computational predictions, with calculated lattice parameters showing excellent agreement with measured values (within 0.5% for Li_2MnO_3 and 3.5% for LiMnO_2). Band structure analysis reveals a moderate direct band-gap of approximately 1.439 eV for Li_2MnO_3 , matching the experimental value of 1.64 eV, and 1.379 eV for LiMnO_2 , aligning closely with the experimental value of 1.58 eV. These findings shows the reliability of computational simulations in predicting the properties of manganese oxide cathode materials for lithium-ion batteries, paving the way for their future implementation as shells in a core-shell design.