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Ab-Initio Investigation of the Electronic Properties of Low Miller Index Surfaces in LiMn₂O₄ Spinel.

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Lithium manganese oxide (LiMn₂O₄) spinel attracted the most attention as a potential cathode material for lithium-ion batteries because of its three-dimensional crystal structure that allows a smooth diffusion of Li⁺ in and out of the material. However, its application as a cathode material is limited by irreversible capacity fading due to manganese dissolution, which is caused by the presence of the highly corrosive hydrofluoric acid (HF) continuously produced by degradation of the common LiPF6-based electrolytes. In this study, we employ the spin-polarized density functional theory calculations with on-site Coulomb interactions and long-range dispersion corrections [DFT+U–D3– (BJ)] to investigate the stability of (001), (011) and (111) surfaces. The surface energies show that the Li-terminated (001) facet is the most stable surface, which is in agreement with the reported literature. To mimic charge/discharge processes, delithiated facets were modeled from the most stable surfaces terminations, and their stabilities were evaluated by calculating the surface free energies. As compared to the surface energies of the pure pristine facets, we observed an increase in energy during delithiation process, which indicate the destabilization effect. Our findings on the LiMn₂O₄ low Miller index surfaces more essential when improving the electrochemical performance of secondary lithium-ion batteries.

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Yes

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 (Hons, MSc,
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MSc

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