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Optimization of the surface stability of the $LiMn_2O_4$ spinel by employing DFT calculations ALTAF KARIM, KRISTIN PERSSON, Lawrence Berkeley National Laboratory — One of the most important materials for the lithium batteries electrodes is LiMn2O4. We used GGA+U method to calculate the bulk and surface properties of LiMn2O4. Our calculations show that the both correct AFM and electron localization (GGA+U) are necessary to obtain the semiconducting, Jahn-Teller distorted electronic ground state of LiMn2O4. Further we calculated energies of different surfaces such as (100), (110), and (111) to study their stability. Our calculations show that (111) surface has the lowest energy which makes it more stable than other surfaces and it also confirms the experimental results, whereas (101) and (001) similar energies. Absolute surface energies change with +U value, but the ratios between the energies are very similar. Based on these calculations we constructed the equilibrium (Wulff) shape of LiMn2O4 particle, which is similar to the cubo-octahedral shape with predominant {1 1 1} facets as it was found in experiments. Our density of states calculations show that the bulk and (100) are semiconducting, whereas (110) and (111) surfaces exhibit metallic behavior. We also calculated the LiMn2O4 bulk and surface potentials as a function of lithium concentration.

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