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DFT+U study of Li adsorption on (110) β-MnO_2 surface

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Abstract :

Lithium-air batteries are actively being developed worldwide because of their potential to deliver ultra-high energy density. Currently, the li-ion batteries are being used in electric vehicle however; their energy is much lower than that of Li-air batteries. Density Functional Theory is used to investigate lithium adsorbed manganese dioxide surfaces in the context of lithium-air battery development. In this study, we calculate the surface energies of low Miller index planes and the most stable surface orientation was found to be the (110). It was observed that the triply-coordinated lithium, bonded to two bridging and one in-plane oxygen atoms (bbp) has lowest adsorption energy which is the favorable site. Surface oxidation becomes favorable when concentration of lithium adsorbets increases at the surface of which bridging-peroxo is most stable.

Award :

No

Level :

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Paper :

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