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Electronic properties of Li/MO₂ (M= Ti, V, Mn) surfaces in Li-air batteries

Lithium-air batteries, based on their high theoretical specific energy, are a particularly attractive technology for electrical energy storage that promises a long-range electric vehicle extensively affordable. However, they suffer from the production of unstable discharge products which leads to capacity fading of the battery. Several catalysts have been used to improve Oxygen Reduction Reaction (ORR) and Oxygen Evolution Reaction (OER) which will yield stable discharge product. In this study, Density functional theory (DFT) is employed to investigate the relative stability of electronic properties of oxygen adsorption on Li/MO2 (110) surfaces. Electronic properties such as band structures and density of states (DOS) are investigated on different configurations (dissociated, peroxo on Li, peroxo on Li-M, and peroxo on M) as oxygen is adsorbed on Li/MO2. The electronic band structures were calculated to check the conductivity of the systems. The DOS was calculated to check the stability of the system by comparing how each system behaves towards the Fermi level. The electronic properties calculations were running in parallel on 24 of 2400 cores using CHPC with memory usage of 2048 MB. These findings are important in improving the cycling performance of Li-air batteries and give insight into the reactivity of Li/MO2 (110) surfaces.

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