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First Principle Study of Metal Oxide 110 β-MO₂ (M= Ti, Mn, V) Surfaces Stability and their Interaction with Li₂O₂

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Metal-air batteries are viewed as the next generation energy storage devices due to their high energy density and environmental friendliness. However, they suffer from 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 metal oxide catalysts,(110) beta;-MO₂ surfaces. Electronic and structural stability of clean and Li-O adsorbed surfaces such as elastic constants, phonon dispersions, density of states and band structures are investigated. The phonon dispersion curves show that clean beta;-TiO₂ surface is the most stable structure since it does not display vibrations in the negative frequencies along the Gamma; region in Brillouin zone. The electronic band structures calculated indicate the absence of gap at fermi level of all the surfaces that are adsorbed with lithium and oxygen, thus they are all metallic. These findings are important in improving the cycling performance of Li-air battery and give insight on the reactivity of (110) beta;-MO₂ surfaces with lithium and oxygen.

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Yes

Level for award
 (Hons, MSc,
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Hons

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