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Why MnO_2 is used as a catalyst in Li-air batteries and not TiO_2

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Abstract content (Max 300 words) Formatting & Special chars

The Li-air batteries, also known as Li-O_2 , promise to transform energy use this century as lightweight methods for storing electricity. Such batteries could be used to fuel electric automobiles and store the electricity generated by solar panels and wind turbines. A catalyst play an important role here; it has been shown that nanostructured MnO_2 in different polymorphic states are able to catalyse the formation and decomposition of Li_2O_2 in the cathode, thus decreasing the overpotentials required for the operation of the Li-air cell. The adsorption and co-adsorption of lithium and oxygen at the surface of rutile-like manganese dioxide ($\beta\text{-MnO}_2$) and ($\beta\text{-TiO}_2$) which are important in the context of Li-air batteries are investigated using density functional theory. In the absence of lithium, the most stable surface of $\beta\text{-MnO}_2$ and $\beta\text{-TiO}_2$, the (110), adsorbs oxygen in the form of peroxy groups bridging and mononuclear respectively. Conversely, in the absence of excess oxygen, lithium atoms adsorb on the (110) surface at two different sites, which are both tri-coordinated to surface oxygen anions. Surface (110) $\beta\text{-MnO}_2$ is energetically more stable than $\beta\text{-TiO}_2$ looking at surface free energy.

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