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oxygen adsorption on (110) surfaces of Pyrolusite MnO_2 and Anatase TiO_2

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Recent studies have employed manganese dioxide (MnO_2) catalysts to improve the efficiency of Li-air batteries, while other studies have revealed that the Li/O_2 cell can be recharged with high efficiency without a catalyst using an appropriate porous carbon electrode. Interestingly, charge voltages of these cells are similar to those of the MnO_2 , while both of these exhibits higher charge voltages than the cobalt-catalyzed cells. However, it has been observed that in the absence of a catalyst the recharge occurs at about high voltage, a large hysteresis between charge and discharge voltages. Ab initio planewave pseudopotential method will be used to investigate the interaction of the oxygen molecule with the (110) surfaces of MnO_2 , in particular tendencies of oxygen reduction. Their surface and adsorption energies were determined together with the distances between O-O of the oxygen molecule, in the vertical and horizontal orientation, the metal and oxygen molecule before and after relaxation. We found that manganese dioxide is more effective and gave lowest adsorption energies, and reduces oxygen molecule better than titanium dioxide. However the horizontal orientation of the oxygen molecule is more favourable in terms of oxygen reduction than the vertical orientation.

Level (Hons, MSc, PhD, other)?

MSc

Consider for a student award (Yes / No)?

Yes

**Would you like to
 submit a short paper
 for the Conference
 Proceedings (Yes / No)?**

No

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