Understanding the adsorption phenomena of intermediates for Li-air battery electrocatalysts using density functional theory

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Li-air batteries are recently regarded as a promising electrical energy storage device. This intense interest is attributed to their high theoretical energy density. However, one of the biggest challenges is the development of electrocatalysts with high activity and stability. Many catalysts have been investigated to improve oxygen reduction reaction (ORR) or oxygen evolution reaction (OER). Nevertheless, Li-air batteries are still facing a lot of problems because of their sluggish kinetics. In this research, therefore, we note that two types of the electrocatalysts expected to be prospective cathode materials using density functional theory (DFT) calculations: PdFe catalysts with an atomically ordered structure and $LaB_xB'_{1-x}O_3$ (B, B' = Mn, Fe, Co, and Ni) perovskite catalysts. First, our results showed that adsorption strength of LiO_2, which is an intermediate molecule in ORR or OER, on the PdFe surfaces could be a simple descriptor of the overpotentials both for ORR and OER. In addition, based on this results, we easily predicted the potential candidate $LaB_xB'_{1-x}O_3$ perovskite catalysts. We expect that these database will provide useful information for designing the new Li-air battery electrocatalysts.