First-principles study of single water interactions with the $LaMnO_3$ surface in the presence of defects, Sr substitution and varied surface morphologies

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Lanthanum manganite ($LaMnO_3$) has been shown to have tremendous catalytic activity for the oxygen reduction reaction (OER) and oxygen evolution reaction (ORR) and is cheaper than other catalytic materials (Suntivich, Jin et al. 2011 Nature Chemistry 3, 546). Previous work studying ORR and OER indicates that water plays an important role in the intermediate reactions, however very little research has been done on the interaction between water and the $LaMnO_3$ surface (Wang Yan, et al. 2013. Journal Phys Chem C 5, 2106). Using Density Functional Theory calculations, we examine the details of water adsorption and dissociation on a perfect and defective $LaMnO_3$ surfaces. We find that oxygen vacancies cause a strong preference for water dissociation on the surface but that the interaction is largely robust in the presence of strontium (Sr) substitutions. We also explore the dependence of interaction on structural parameters with a few different surface morphologies. Our results provide insights to the catalytic function of $LaMnO_3$ in both ORR and OER applications.

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