Adsorption of Water Clusters on the $LaMnO_3$ Surface

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Lanthanum manganite ($LaMnO_3$) has been shown to have tremendous catalytic activity for the oxygen reduction reaction (ORR) and oxygen evolution reaction (OER) and is cheaper than other catalytic materials (Suntivich, Jin et al. 2011 Nature Chemistry 3, 546). Recently, experiments have also found that $LaMnO_3$ is an effective pseudocapacitor by allowing intercalation of anions into the surface (Mefford, J. Tyler et al. 2014 Nature Materials 13, 726). The structure of water at the interface between $LaMnO_3$ and the aqueous solution can play a large role in both of these applications, as the structure can facilitate or hinder surface reactions and intercalation. Using density functional theory, we perform calculations of water clusters on the $LaMnO_3$ surface. Adsorption of a water dimer and trimer on the surface show a balance between water-water interactions and water-surface interactions, where water-surface interactions dominate and water-water bonding contributes additional stability. These results provide insight into the physics of water's interaction with a complex transition metal oxide.

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