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Water Adsorption on the LaMnO₃ Surface CHRIS BILLMAN, Physics Department and Quantum Theory Project, University of Florida, YAN WANG, Materials Science and Engineering, Massachusetts Institute of Technology, HAI-PING CHENG, Dept. of Physics and Quantum Theory Project, University of Florida — Studying the adsorption of water on the metallic LaMnO₃ surface can provide insight into this complicated surface-adsorbate interaction. Using density functional theory, we investigated the adsorption of a water monomer, dimer, trimer and a monolayer on the surface. The electronic structure of ground state configurations is explored using analysis of density of states, charge density, and crystal orbital overlap populations. We found that the interaction between the surface and water molecules is stronger than hydrogen bonding between molecules, which facilitates wetting of the surface. Adsorbed water molecules form very strong hydrogen bonds, with substantially shifted OH stretch modes. For the monolayer of adsorbed water, a hint of a bilayer is observed with a height separation of only 0.2 Å. However, simulated scanning tunneling microscopy (STM) images and vibrational spectra suggest a significant difference between the two layers due to intermolecular bonding and interaction with the substrate.

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