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Half-metallic ferromagnetism on surfaces of insulating and antiferromagnetic LaFeO₃ thin films ROHAN MISHRA, Washington University in St. Louis, YOUNG-MIN KIM, Korea Basic Science Institute, QIAN HE, Oak Ridge National Laboratory, SEONG-KEUN KIM, Korea Institute of Science Technology, SEOHYOUNG CHANG, ANAND BHATTACHARYA, Argonne National Laboratory, SOKRATES T. PANTELIDES, Vanderbilt University, Oak Ridge National Laboratory, ALBINA BORISEVICH, Oak Ridge National Laboratory — The surfaces of perovskite transition metal oxides having correlated electrons show novel electronic and magnetic phenomena. In this work, we combine scanning transmission electron microscopy imaging and electron energy loss spectroscopy (EELS) with density functional theory (DFT) calculations to study the surface of $(LaFeO_3)_m/(SrFeO_3)_n$ heterostructure thin films. Using EELS, we observe a reduction in the oxidation state of Fe on moving from the bulk to the surface over a length of ~5 unit cells. Simultaneously acquired STEM images allow us to map the associated changes in their structure, such as cation displacements and changes in oxygen polyhedral tilts. DFT calculations coupled with the STEM results show that by reducing the surface layer of a $LaFeO_3$ film such that the surface is terminated with FeO_4 tetrahedra instead of the FeO_6 octahedra as present in the bulk, it is possible to stabilize an exotic phase where the surface layer displays a half-metallic ferromagnetic behavior, while the bulk remains antiferromagnetic and insulating, similar to the class of topological insulators. The calculations also predict that the magnetism and conductivity at the surface can be controlled by the partial pressure of oxygen.

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