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Magnetic and electronic properties of complex oxide interfaces WEIDONG LUO, MARIA VARELA, STEPHEN J. PENNYCOOK, SOKRATES T. PANTELIDES, Vanderbilt University and Oak Ridge National Laboratory — Interfaces between two complex materials based on perovskite oxides can have novel physical properties. We studied the magnetic and electronic properties of $La_{0.67}Ca_{0.33}MnO_3/YBa_2Cu_3O_7$ (LCMO/YBCO) superlattices using first-principles density-functional theory (DFT). The energetics of several types of magnetic (spin) configurations of Mn ions near the LCMO/YBCO interface have been calculated using the DFT approach. Their magnetic and electronic properties have been explored and compared to the properties of bulk materials. These results are compared to recent experimental observation of suppressed magnetization at the LCMO/YBCO interface. We will also discuss the possibility of charge transfer across the interface, as suggested by recent experimental results from local electron energy-loss spectroscopy (EELS). This research was sponsored by the Office of Basic Energy Sciences, Division of Materials Sciences and Engineering, U.S. Department of Energy, under contract DE-AC05-00OR22725 with Oak Ridge National Laboratory, managed and operated by UT-Battelle, LLC, and by the McMinn Endowment at Vanderbilt University.

Weidong Luo
Vanderbilt Univ & ORNL

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