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Developments in electronic structure theory
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Density functional theory study of perovskite oxide interfaces: Effects of exchange-correlation functional and thin film thickness on geometry, interface electronic structure, and magnetic order KEVIN J. MAY, ALEXIE M. KOLPAK, Massachustts Institute of Technology —Perovskite oxides have attracted significant attention in many diverse research fields such as electrocatalysis, oxide electronics and physics, owing to the variety of electronic and magnetic properties attainable in this family of materials. Thin films are of interest since their properties can differ drastically from those of the bulk[1]. Density functional theory drastically underestimates the band gap of many materials, and often inadequately describes the electron-electron interactions in strongly correlated materials. Previous work has shown that the choice of exchange-correlation (E_{xc}) functional can change the calculated magnetic ground state and structural properties of the bulk oxide. Moreover, the optimal E_{xc} can differ among different compounds[2,3]. This work aims to describe the structural, electronic and magnetic properties of $LaMO_3$ (M = V, Cr, Mn, Fe, Co, Ni) thin films on a $SrTiO_3$ substrate, as a function of the film thickness (1-4 unit cells) at a preliminary GGA level. Changes in the predicted magnetic ground state, octahedral rotation, and electronic reconstruction (such as two-dimensional electron gases) at the interface will be compared among different film thicknesses and reference bulk calculations.

1. Rondinelli, J. M. & Spaldin, N. A. *Adv. Mater.* **23,** 3363–81 (2011).
2. He, J. & Franchini, C. *Phys. Rev. B* **86,** 235117 (2012).
3. Yang, Z., Huang, Z., Ye, L. & Xie, X. *Phys. Rev. B* **60,** 15674–15682 (1999).