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Hybrid density functional theory applied and the role of electron correlations in LCMO TIMOTHY PENNYCOOK, WEIDONG LUO, SOKRATES PANTELIDES, Vanderbilt University — Transition metal oxides (TMOs) are generally considered too complex for density functional theory (DFT) in the local density approximation (LDA or GGA) because of the 3d electrons. It is widely believed that a Hubbard U is needed to account for strong correlations. A prominent example is that GGA underestimates the Jahn-Teller distortions in LaMnO3 (LMO) causing it to predict the wrong magnetic ordering; GGA+U predicts both the structure and magnetic ordering correctly for LMO, but for the rest of the $La_xCa_{1-x}MnO_3$ series it was recently demonstrated that the opposite is true (PRL 99, 036402). Recently, new exchange-correlation functionals have become available that do very well in correcting the well-known band gap problem of semiconductors and insulators. We have performed calculations using the parameter-free HSE06 hybrid density functional for LMO and find that it accurately reproduces both the magnetic ordering and the Jahn-Teller distortions seen experimentally. We will present results using the HSE06 functional from across the LCMO series. This work was supported in part by DOE grant DE-FG02-09ER46554.

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