Abstract Submitted
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Redefining the metal/charge-transfer insulator paradigm in transition metal oxides[1] HUNG DANG, XINYUAN AI, Department of Physics, Columbia University, CHRIS MARIANETTI, Department of Applied Physics, Columbia University, ANDREW MILLIS, Department of Physics, Columbia University — The universality of the phase diagram in the variables of interaction strength and d-occupancy, shown for late transition metal oxides in Ref.[1], is examined for two series of early transition metal oxides: ($SrVO_3$, $SrCrO_3$, $SrMnO_3$) and ($LaTiO_3$, $LaVO_3$, $LaCrO_3$) using density functional theory (DFT), DFT+U and DFT+dynamical mean field theory methods. The interaction required to drive the metal-insulator transition is found to depend sensitively on the d-occupancy N_d, and beyond a threshold value of the d-occupancy an insulating state cannot be achieved for any practical value of the interaction. The critical N_d values are determined and compared to ab initio and experimental estimates where available. Additionally, the minimal model for the transition is determined and the crucial role played by the Hunds coupling is demonstrated.

[1] Xin Wang, M. J. Han, Luca de' Medici, C. A. Marianetti, and Andrew J. Millis (2011). arXiv:1110.2782

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