

Abstract Submitted
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The role of correlations on oxygen orbitals in late transition-metal oxides BAYO LAU, HUNG T. DANG, EMANUEL GULL, ANDREW J. MILLIS, Department of Physics, Columbia University, NY, NY — We investigate the effect on transition-metal oxide physics of including interactions on the oxygen sites as well as on the transition-metal site using a generalization of the single-site Dynamical Mean Field method. On-site repulsive and Hund's interactions in the full Slater-Kanamori form are treated using a numerically exact continuous-time quantum Monte-Carlo solver. We determine the metal-insulator and magnetic phase diagrams as a function of charge-transfer tendency and interaction strengths. The results are compared directly to models with no oxygen correlations, yielding insights about the role of oxygen-specific correlations.

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