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On-site screened Coulomb interactions for localized electrons in transition metal oxides and defect systems BI-CHING SHIH, Department of Physics, University at Buffalo, State University of New York, PEIHONG ZHANG, Department of Physics, University at Buffalo, State University of New Your, DEPARTMENT OF PHYSICS TEAM — Electronic and structural properties of strongly correlated material systems are largely determined by the strength of the on-site Coulomb interaction. Theoretical models devised to capture the physics of strongly correlated materials usually involve screened Coulomb interactions as adjustable parameters. We present first-principles results for the screened on-site Coulomb and exchange energy for transition metal oxides. The dielectric screening is calculated within the random phase approximation and the localized electrons are represented by maximally localized Wannier functions. We further extend our study to calculate on-site Coulomb interactions for localized defect states in semiconductors. We acknowledge the computational support provided by the Center for Computational Research at the University at Buffalo, SUNY. This work is supported by the National Science Foundation under Grant No. DMR-0946404 and by the Department of Energy under Grant No. DE-SC0002623.

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