

Abstract Submitted
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Screened Coulomb Interactions of Localized Electrons from First-Principles BI-CHING SHIH, PEIHONG ZHANG, Department of Physics, University at Buffalo, State University of New York — We present a recently developed, maximally localized Wannier function approach for calculating the screened Coulomb (U) and exchange (J) interactions of localized electrons in solids. The localized orbitals are constructed using the maximally localized Wannier function approach. The dielectric screening is calculated from first-principles within the random phase approximation. Results for several systems containing strongly localized d electrons will be presented.

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