Screened Coulomb and Exchange Parameters of Localized Electrons in the Self-Consistent Constrained RPA

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Screened Coulomb and exchange interactions play an important role in studying the structural and electronic properties of strongly correlated materials. The strong Coulomb interaction between localized electrons have prompted the theoretical electronic-structure method beyond the traditional density functional theory approximation method. For these strongly correlated systems, it has been recognized that the localized electrons are better described in the local basis where their Coulomb interactions are generally parameterized. Evaluating these parameters from *ab initio* approaches can provide better understanding for the strong-correlation effects.

We have developed a self-consistent first-principles approach [1] to evaluate the screened Coulomb and exchange parameters using the constrained random phase approximation [2] (cRPA). In the implementation, the localized electrons are described in terms of the maximally localized Wannier functions and the screening is evaluated by direct calculation of the dielectric function. We present a comprehensive study of the self-consistent cRPA approach and the calculated parameters for the 3d electrons in the transition metals and transition metal oxides. An extended application of the cRPA approach is to evaluate the screened Coulomb interactions for localized defect states. Preliminary results for defects systems are also presented.

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[2] F. Aryasetiawan, M. Imada, A. Georges, G. Kotliar, S. Biermann, and A. I. Lichtenstein, Phys. Rev. B **70**, 195104 (2004).

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