Screened Coulomb interactions between localized electrons in solids

Bi-Ching Shih and Peihong Zhang

Department of Physics,University at Buffalo, The State University of New York

Buffalo, New York, USA

The screened Coulomb interaction, commonly referred to as on-site Coulomb or Hubbard U, is an important parameter for constructing effective low energy model for strongly correlated materials. It is also an essential input parameter for theoretical methods such as LDA+U and DMFT. We have developed a first-principles approach to evaluate the screened Coulomb (U) and exchange (J) energies between localized electrons within the pseudopotential planewave formalism. The localized electrons are represented by the maximally localized Wannier orbitals and the dielectric screening is calculated within the (constrained) random phase approximation. We have applied this newly developed method to calculate the U and J parameters for several transition-metal oxides.

This work is supported by National Science Foundation under Grant No. DMR-0946404 and by the Department of Energy under Grant No. DE-SC0002623.