

Exact Exchange Method Applied to Diluted Magnetic Semiconductors

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The exact exchange (EXX) method, which uses the exchange terms calculated on the Kohn-Sham orbitals, in the framework of the optimized effective potential method (OPM) provides us with one of ways going beyond LDA. Though EXX level calculation is only the first step of OPM, it gives unexpectedly good results when applied to semiconductors. The calculated band gaps of various semiconductors well reproduce the experimental observation: the accuracy is comparable with those obtained by far more sophisticated calculation based on the GW method. The main reason is that the self-interactions are crucial in determining the band gap and EXX is completely free from self-interactions.

One of big issues in the theory of diluted magnetic semiconductors (DMSs) is the nature of the magnetic coupling between magnetic ions in DMSs: whether it is long-ranged or not? This is important since it finally determines the magnetic transition temperature in the case of diluted systems. The position of the d-states energy of magnetic ions in DMS is essential for the above question. Expecting that EXX might give reasonable description on the position of the d-states energy as well as band gap of host semiconductors, we have performed the EXX calculations on various DMS systems.

The results show that the d-states are shifted considerably in the energy scale towards deeper positions compared with those obtained by LDA calculations. This means that the magnetic couplings become more long-ranged but, on the other hand, could be weakened. These results are consistent with the previous calculation using the self-interaction corrected (SIC) or pseudo-SIC LDA calculations and also the so-called LDA+U calculations. The present approach using EXX, however, has a big advantage that it is completely within the framework of density functional theory, and hence, first-principles.