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Combining DFT and Many-body Methods to Understand Correlated Materials[1]

IGOR SOLOVYEV, National Institute for Materials Science, 1-2-1 Sengen, Tsukuba, Ibaraki 305-0047, Japan

Electronic and magnetic properties of strongly-correlated systems are typically controlled by a limited number of electronic states, located near the Fermi level and well isolated from the rest of the spectrum. This opens a formal way for combining the first-principles methods of electronic structure calculations, based on the density-functional theory (DFT), with model many- body methods, formulated in a restricted Hilbert space of states near the Fermi level. The core of this project is the construction of "*ab initio* model Hamiltonians", which would incorporate the physics of on-site Coulomb correlations and provide a transparent physical picture for the low-energy properties of strongly- correlated systems. First, I will describe a systematic procedure for constructing such an effective Hubbard-type model, which consists of three major steps, starting from the electronic structure in the local- density approximation.[1] (i) Construction of the kinetic-energy part using an exact version of the downfolding method;[1,2] (ii) Construction of the Wannier functions; (iii) Calculation of screened Coulomb interactions using a hybrid approach, which combines the random phase approximation with the constraint DFT.[1,3] Then, I will illustrate abilities of this method for resolving a number of controversial issues, related with the interplay of the experimental lattice distortion and magnetic properties of four narrow t_{2g} band perovskite oxides ($YTiO_3$, $LaTiO_3$, YVO_3, and $LaVO_3$), for which the obtained Hamiltonian was solved using a number of techniques, including the Hartree-Fock (HF) approximation,[4] the second-order perturbation theory and the t-matrix approach for the correlation energy,[4,5] and a variational superexchange theory, which takes into account the multiplet structure of the atomic states.[4] I will argue that the crystal distortion imposes a severe constraint on the form of the possible orbital states, which favors the formation of experimental magnetic structures in $YTiO_3$, YVO_3, and $LaVO_3$, even at the level of HF approximation. The correlation effects systematically improve the agreement with the experimental data and additionally stabilize the experimentally observed G- and C-type antiferromagnetic states in YVO_3 and $LaVO_3$. The role of relativistic spin-orbit interaction will be also discussed.

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