Combining DFT and many-body methods to understand correlated materials

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Electronic and magnetic properties of strongly-correlated systems are typically controlled by a limited number of 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 the model many-body techniques, formulated in a restricted Hilbert space of states near the Fermi level. The core of this project is the construction of "*ab initio* low-energy models", which incorporate the physics of Coulomb correlations and provide a transparent picture for the low-energy properties. First, I will describe how such models can be constructed. The procedure 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]

The abilities of this method will be illustrated on two examples.

The first one is the narrow t_{2g} band perovskite oxides: $YTiO_3$, YVO_3, and $LaVO_3$. Recently, they have attracted much attention due to the large variety of the magnetic structures, which can be realised in these compounds. These magnetic properties are controlled by tiny distortions in the perovskite structure, which are amplified by Coulomb correlations. For example, YVO_3 can be found in two distinct antiferromagnetic configurations, the existence of which is closely related with the orthorhombic-monoclinic structural phase transition at T=77K. We could not only reproduce this behaviour, but also present a transparent physical picture, explaining how the lattice distortion changes the distribution of electron densities around the V sites and controls the form of interatomic magnetic interactions (Fig. 1).[4]

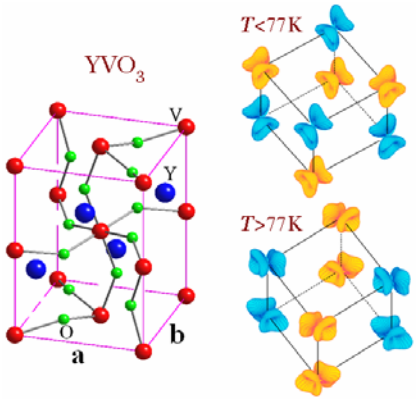

Fig. 1 Distorted perovskite structure and the shape of electron densities around V sites in orthorhombic (top) and monoclinic (bottom) phases of YVO_3. Different magnetic sublattices are shown by different colours.

Another example is the alkali hyperoxide, KO_2. This system can be regarded as a molecular analogue of correlated electron systems, comprising of orbitally degenerate magnetic O_2^- ions. Using first-principles electronic structure calculations, we set up an effective spin-orbital model for the low-energy *molecular* bands of KO_2 and argue that many anomalous properties of this compound replicate the status of its orbital system in different temperature regimes.[5]

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[5]I. V. Solovyev, cond-mat/0612475.