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Effect of quasiparticle excitations of strongly correlated d states on the electronic structure of the crystal CrAs

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A new class of half-metallic ferromagnets has been found in the zinc-blende crystal structure. The previously nonexistent zinc-blende CrAs thin films have been synthesized on GaAs (001) substrates by molecular-beam epitaxy, and show a ferromagnetic behavior at room temperature [1].

Here we present the results of the complex investigation of the electronic structure of zinc-blende CrAs that was carried out within the LDA+U and LDA+DMFT (for the first time) approaches. All the calculations have been done by means of ABINIT code [2]. The LDA+U approach describes interactions in the crystal with static mean field theory and the LDA+DMFT one describes correlation in solids beyond static mean field theory.

The spin-resolved partial and total densities of electronic states have been evaluated within the LDA+U theory. The spin-resolved spectral function was calculated by means of the Hubbard solver I, as implemented in the ABINIT code [2].

Let us compare briefly the results obtained in the LDA+U and LDA+DMFT approaches: $n(\varepsilon_F)$ for strongly correlated d electrons equal 0.55 and 0.25 st. / eV, respectively. The correlated states are extended to the energy values 4.3 and 6.5 eV below the Fermi level, respectively. The peak of DOS for correlated electrons with the spin down is located at 1.5 and 5.2 eV below Fermi energy, respectively. The Fermi energy values are 5.22 and 5.99 eV, respectively. So, we reach the conclusion that the crystal CrAs is an example of the strongly correlated system that should be described by means of the LDA+DMFT formalism.

1. *Akinaga H., Manago T., Shirai M.* Material Design of Half-Metallic Zinc-Blende CrAs and the Synthesis by Molecular-Beam Epitaxy // Jpn. J. Appl. Phys.-2000.-**39.**-L1118- L1120.
2. *Gonze X., Jollet F., Abreu Araujo F., Adams D., Amadon B.et al.* Recent developments in the ABINIT software package // Computer Phys. Comm.-2016.-**205.**-P. 106-131.