

Existence of crystal-field states in superconducting $\text{CeFeAsO}_{1-x}\text{F}_x$

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There is going on a debate about the existence and the role played by the crystal field (CEF) in compounds containing 3d/4f/5f atoms/ions both in ionic and intermetallic compounds. The uniqueness of $\text{CeFeAsO}_{1-x}\text{F}_x$ relies in a fact that in the superconducting state (T_{sc} of 41 K for $x = 0.16$) well-defined crystal-field states have been found at 18.7 and 57 meV (Phys. Rev. Lett **101** (2008) 217002).

We have derived CEF parameters of the orthorhombic symmetry of the Ce^{3+} site and evaluated the low-energy electronic structure. We have calculated the single-ion properties of the Ce^{3+} ions and their contribution to properties of the whole compound. In particular, we have described the temperature dependence of the heat capacity with the λ -type peak at 4 K associated with the ordering of Ce ions. Very good reproduction of the temperature dependence allows for evaluation of the influence of the magnetic order within the Fe sublattice on the Ce states. Namely, the Ce ion experiences the energy splitting of the ground-state doublet by about 1 meV due to the Fe magnetism.