Electronic structure and peculiarities of the single-ion magnetic anisotropy of rare-earth ions in the iron oxypnictides RFeAsO (R = Ce, Pr, Nd, Sm, Gd)

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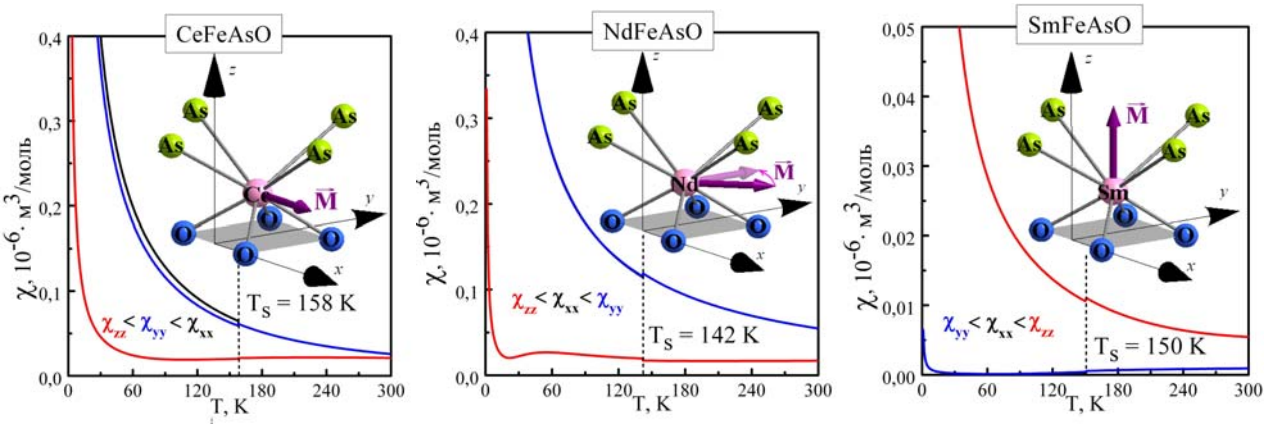
At present, the problem of the interaction between a rare-earth metal and magnetic subsystems in the iron-based high-temperature superconductors $R\mathrm{FeAsO}_{1-x}\mathrm{F}_x$ (R – rare-earth elements) has not been solved and requires further investigations. In particular, the substitution of La ions with Ce, Pr, Nd, and other ions leads to twice as much increase of the superconducting transition temperature. This observation is usually associated with a purely geometrical factor, namely, with the difference in the radii of the rare-earth ions and significant modification of the distance between iron ions and surrounding ligand ions. However, one can suppose that this effect can be connected with a strongly anisotropic interaction between rare-earth and iron subsystems since the rare-earth magnetic subsystem is usually highly anisotropic, and constants of the anisotropic exchange between iron and rare-earth subsystems are large enough [1]. Therefore, one can expect that fluctuations of the iron magnetic moments are allowed in a certain direction and suppressed in others. In this report we study anisotropic magnetic properties of R^{3+} ions in the RFeAsO matrix.

Energy levels of the R^{3+} ions, *g*-factor values, temperature dependences of magnetic susceptibility components and *fourth*-order anisotropy constants have been calculated using the modified crystal field theory (MCFT) [2]. The iron-subsystem effect on magnetic properties of R^{3+} ions was theoretically studied for both crystallographic phases observed experimentally. On the base of our calculations some conclusions about the nature of the magnetic anisotropy of R^{3+} ions have been made (see figure): (a) in tetragonal and orthorhombic phases the "easy" direction of the cerium-ion magnetic moment is the [110] axis; (b) the "easy" direction of the Nd^{3+} magnetic moment in NdFeAsO changes after the structural transition, namely, in the tetragonal phase it prefers the [010] axis, whereas in the orthorhombic phase it is the [110] direction; the magnetic moment of Sm^{3+} ion preserves the [001] direction in both phases.



[1] H. Maeter *et al*, *Phys Rew B*, **80**, 094524 (2009).
[2] K. V. Lamonova *et al*, *J. Phys. Chem. A.* **115**, 13596 (2011).