ATOM SPECIES ENERGY DEPENDENCE ON MAGNETIC CONFIGURATIONS IN THE PEROVSKITE YTTRIUM ORTHOFERRITE

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I. INTRODUCTION

Multiferroics are materials which combine (ferro)magnetic and ferroelectric ordering. These materials are very interesting both for radioelectronic applications and new scientific directions, such as straintronics. Early we described the ground states for the different magnetic orderings in the perovskite $YFeO_3$, and the dependence of the structural properties on them were established [1]. The difference total energy and structural parameters of the various magnetic configurations of the $YFeO_3$ appears due to interaction of iron d-shell electrons in magnetic sublattice, formed by iron ions, and interaction between iron ions and neighboring yttrium and oxygen ions which change electron density distribution and energy in the material. Unfortunately, contribution dependence for each atom species in various magnetic configurations of the $YFeO_3$ are unknown. Changes d-shell electron energy of Fe ions for these states of the $YFeO_3$ are unknown also. This information can be powerful for engineering magnetic properties of a multiferroics with perovskite structure for physical and technical applications. Thereby in this work we study energy dependence for each atom species and changes spin-resolved energy iron d-shell electrons of magnetic configurations of the $YFeO_3$ by ab-initio method.

II. METHOD

We performed our ab-initio calculations within the generalized gradient approximation (GGA) and the Perdew – Burke – Ernzerhof exchange-correlation functional with spin polarization as implemented in the OpenMX code [2-4]. We used pseudopotentials with the following valence states configuration: Y – 4s, 4p, 4d, and 5s states; Fe – 3p, 3d, and 4s states; O – 2s and 2p states. We selected the basis sets with 2

pseudoatomic orbital (PAO) functions for each electronic state and 1 adding PAO function as polarized. The integration over the 4×3×5 regular Γ-centered k-points mesh were performed. Calculation of the total and orbitally decomposed energy were performed after finding a total energy minimum point for each magnetic configuration through structure relaxation.

III. RESULTS AND DISCUSSION

Each atom species and Fe t_{2g}- and e_g-orbitals contribution dependence to the total energy on different magnetic configurations of the $YFeO_3$ multiferroic are given on Fig. 1. For all cases, the zero energy is a relative value. The total energy of the $YFeO_3$ is monotonously decreasing from ferromagnetic (FM) to antiferromagnetic (AFM) state with close energies between neighboring magnetic configurations. Decomposition of the total energy on atoms species show that energy states decreasing in a series FM → A-AFM → C-AFM due to the yttrium ions, and only G-AFM state related with the Fe and O ions contribution due to inversion their energy behavior.
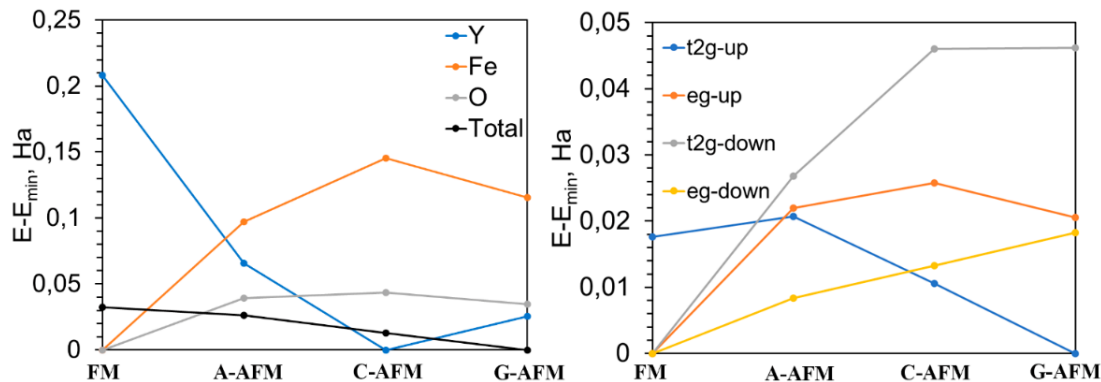

Figure 1. Energy dependence in different magnetic configurations of $YFeO_3$: left panel – each atoms species contributions; right panel – Fe t_{2g}- and e_g-orbitals contribution

The lowest energy state for iron d-electrons corresponds to ferromagnetic ordering, but not for t_{2g} spin up states, which has lowest energy in G-AFM ordering. In general, increasing of d-electrons energy at FM – AFM transition and decreasing of total energy due to yttrium ions stabilize G-AFM phase of $YFeO_3$.

IV. CONCLUSIONS

Thus, in this work we studied energy contribution dependence for each atom species for various magnetic states in the $YFeO_3$ perovskite multiferroic by ab-initio methods. It was shown, that stabilization of the experimentally observed G-AFM ordering in the $YFeO_3$ take place due to interaction between d-electrons in magnetic sublattice, formed by iron ions, with combination of decreasing total energy of system due to yttrium ions. We suppose that substitution yttrium ions by magnetic ions, for example 4f-elements ions, can change main magnetic configuration from G-AFM to another AFM or FM ordering. It also can vary the energy gap between neighboring magnetic states, which is of interest for magnetic memory devices and other straintronics applications.

REFERENCES

[1] L. Khoroshko, A. Baglov, "Magnetic configurations in $YFeO_3$ multiferroic", Proceedings of VI International conference "Applied Problems of Optics, Informatics, Radiophysics and Condensed Matter Physics", pp. 251–253, 2021.

[2] T. Ozaki "Variationally optimized atomic orbitals for large-scale electronic structures", Phys. Rev. B, Vol. 67, 155108-1–155108-5, 2003.

[3] T. Ozaki, H. Kino "Numerical atomic basis orbitals from H to Kr", Phys. Rev. B, Vol. 69, pp. 195113-1–195113-19, 2004.

[4] T. Ozaki, H. Kino "Efficient projector expansion for the ab initio LCAO method", Phys. Rev. B, Vol. 72, pp. 045121-1–045121-8, 2005.