Orthorhombic phase of $La_{0.5}Bi_{0.5}NiO_3$ studied by first principles

J. Kaczkowski,[1] M. Pugaczowa-Michalska,[1] and A. Jezierski[1]

[1] *Institute of Molecular Physics Polish Academy of Sciences, Smoluchowskiego 17, 60-179 Poznań, Poland*

The electronic density of states near the Fermi level is an important physical quantity for understanding metal-insulator transition, charge transfer induced negative thermal expansion in perovskite $BiNiO_3$. The aim of presented first principles study of $La_{0.5}Bi_{0.5}NiO_3$ is to investigate electronic structure of orthorhombic phase *Pbnm*. The calculations show that metallicity and magnetism of the system are strongly related with hybridization between Ni *3d* and O *2p*. To improve the quality of the electronic structure description of the system, especially the treatment of correlation for the Ni *3d*, we employ GGA, LDA, and GGA + *U*, LDA + *U*. The LSDA results give good agreement with experiment [1]. Thus, the screening effects originating from the hybridized *3d* and O *2p* electrons are sufficiently strong that they reduce the electronic correlations in the $La_{0.5}Bi_{0.5}NiO_3$, making it a weakly correlated metal. The charge disproportionation of Bi ions into Bi^{3+} and Bi^{5+} is suppresed by La ions [2].

References:

[1] S. Ishiwata et al., Physica B 329-333 (2003) 813.

[2] M.Pugaczowa-Michalska, J. Kaczkowski, Comp. Mater. Sci. 126 (2017) 407.