

Abstract Submitted
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Multiferroicity of BiMnO₃ reexamined from first principles. TATSUYA SHISHIDOU, TAMIO OGUCHI, ADSM, Hiroshima University — BiMnO₃ is believed to show both ferromagnetic and ferroelectric orders. In contrast to its robustly confirmed ferromagnetism, only one experimental group has succeeded in observing ferroelectric hysteresis loop[1]. Another group has reported small magnetocapacitance effect around the ferromagnetic Curie temperature[2]. Using first-principles scalar-relativistic full-potential linear augmented plane wave (FLAPW) method and adopting the experimental lattice data, we have given several significant insights on physical properties of BiMnO₃[3]. Further extended results will be shown in this talk. With including spin-orbit interaction, possible directional coupling between the polarization and magnetization will be discussed together with magnetocrystalline anisotropy. Results of structural optimization based on the first-principles atomic forces will be presented to verify its ferroelectricity. Possible doping effect will also be explored. [1] A. Moreira dos Santos *et al.*, Solid State Commun. **122** 49 (2002). [2] T. Kimura *et al.*, Phys. Rev. B **67** 180401(R) (2003). [3] T. Shishidou, N. Mikamo, Y. Uratani, F. Ishii, and T. Oguchi, J. Phys.: Condens. Matter **16** S5677 (2004).

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