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Magnetoelectric effects in SrRuO₃/BaTiO₃ heterostructures: A First Principles Study M.K. NIRANJAN, J.D. BURTON, S.S. JASWAL, E.Y. TSYMBAL, University of Nebraska, Lincoln, USA, J.P. VELEV, University of Puerto Rico, San Juan, USA — Ferroelectric materials in combination with ferromagnets have emerged as structures in which strong magnetoelectric coupling may exist originating from unconventional physical mechanisms. The use of oxides such as SrRuO₃ as a metal electrode has been found to be of fundamental importance for the realization of ferroelectric films with critical thicknesses down to three unit cells. Here we present a study of SrRuO₃/BaTiO₃ heterostructures within the framework of density functional theory. This heterostructure is interesting since SrRuO₃ is a weak ferromagnetic oxide metal and hence, when used as an electrode on BaTiO₃, presents the possibility of coupling between electric and magnetic order parameters. In particular we study the magnetoelectric (ME) effect at the interface of SrRuO₃/BaTiO₃ by treating SrRuO₃ as spin polarized metal. We find that magnetic properties at the interface are affected as the ferroelectric polarization in the BaTiO₃ is reversed. We discuss the origins of ME effect and compare them with previously proposed ME coupling mechanisms in Fe/BaTiO₃, Fe₃O₄/BaTiO₃, and SrRuO₃/SrTiO₃ heterostructures^{1,2}. ¹Niranjan et al., Phys. Rev. B, **78**, 140405 (2008); ²Rondinelli et al., Nat. Nanotechnology, **3**, 46, (2008)

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