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Induced magnetization in ferroelectric-antiperovskite heterostructure PAVEL LUKASHEV, RENAT SABIRIANOV, University of Nebraska, Omaha — We theoretically predict the linear magnetoelectric effect (ME) in ferroelectric-antiperovskite $PbTiO_3/Mn_3GaN$ heterostructure. The effect is caused by the recently reported piezomagnetic nature of the Mn_3GaN. Elastic deformations in the Mn_3GaN are due to the surface strain and the soft mode atomic displacements from ferroelectric to the antiperovskite (AP) phase. Both mechanisms lower the symmetry of the AP component, which results in the induced magnetization. Reversal of the polarization direction in the ferroelectric phase results in the magnetization reversal in Mn_3GaN, thus the observed effect is linear. We study few interface geometries to account for the electrostatic complementarity at the surface. Those interfaces, which are electrostatically incompatible exhibit strong tetragonal distortion of the cell. The induced magnetization depends on the termination of the components of the heterostructure, and ranges from 0.25 μ_B to 0.6 μ_B per unit cell of Mn_3GaN. All calculations were performed by projector augmented wave method.

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