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Ferroelectric control of magnetocrystalline anisotropy and orbital magnetism in thin-film Fe/BaTiO₃ heterostructures PAVEL LUKASHEV, J.D. BURTON, SITARAM JASWAL, EVGENY TSYMBAL, University of Nebraska - Lincoln — Correlations between magnetocrystalline anisotropy energy (MAE), ferroelectric (FE) polarization, and orbital magnetic moment are studied for ferroelectric/ferromagnetic heterostructures consisting of barium titanate (BaTiO₃) and thin-film iron (Fe). Using first-principles calculations we investigated different geometries of the BaTiO₃/Fe system, in particular with 1, 3, and 5 monolayers of Fe with either a free vacuum surface or Cu as a capping layer. We show that there is a large MAE change ($\sim 20\%$) upon switching of the polarization sign in the case of a vacuum layer, while the presence of Cu effectively removes the difference in MAE for opposite FE polarization directions in BaTiO₃. This is explained by analyzing the correlation between MAE and orbital magnetic moments for different geometries and opposite polarization directions, as well as the film thickness. We show that the magnetoelectric coupling between MAE and FE polarization is directly linked to the degree of the magnetoelectric coupling between orbital moment and FE polarization.

Prefer Oral Session
 Prefer Poster Session

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