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**Voltage controlled magnetocrystalline anisotropy at the Fe/MgO (001) interface** PAVEL LUKASHEV, University of Northern Iowa, EVGENY TSYMBAL, University of Nebraska - Lincoln — The effect of electric fields on magnetocrystalline anisotropy energy (MAE) is a promising way to control the magnetization orientation purely by voltage (rather than by current required for a spin transfer torque), which can potentially alleviate the energy dissipation bottleneck of the existing magnetic memory technology. Here we perform density-functional calculations to explore the voltage controlled magnetic anisotropy (VCMA) of a thin film Fe stacked along the [001] direction when an external electric field is applied across an adjacent epitaxial MgO layer. The results are analyzed by evaluating layer and orbital resolved contributions to MAE. We find that MAE is confined to a depth of few atomic layers near the interface, as determined by the metal screening length, indicating that the VCMA is an interface effect. The applied electric field leads to a nearly linear change in the interface MAE due to a change in the 3d-orbital occupancy of the interfacial Fe atoms and is enhanced, as compared to the clean Fe (001) surface, due a relatively large dielectric constant of MgO. In addition to the electric field screening, there is a notable effect of atomic displacements driven by an applied electric field, when atomic relaxations are taken into account.

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