Abstract Submitted
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First-Principles Study of Enhanced Magnetoelectric Effects at the Fe/MgO(001) Interface M.K. NIRANJAN, S.S. JASWAL, E.Y. TSYMBAL, University of Nebraska, Lincoln, Nebraska, NE, C.-G DUAN, East China Normal University, Shanghai, China — The magnetoelectric effect allows affecting magnetic properties of materials by electric fields with potential for technological applications such as electrically controlled magnetic data storage. In this study we explore, using first-principles methods, the magnetoelectric effect at the Fe/MgO(001) interface,[1]. By explicitly introducing an electric field in our density-functional calculations we demonstrate that the magnetic moment of Fe atoms at the interface changes linearly as a function of the applied electric field with the surface magnetoelectric coefficient being strongly enhanced as compared to that for the clean Fe(001) surface.[1] The effect originates from the increased screening charge associated with a large dielectric constant of MgO. The influence of electric field on relative occupancy of the Fe-3d orbitals leads to significant change in the surface magnetocrystalline anisotropy. These results are compared with the available experimental work.[2] Our results indicate that using high-k dielectrics at the interface with ferromagnetic metals may be very effective in controlling the magnetic properties by electric fields thereby leading to interesting device applications. [1]C.-G. Duan et al., Phys. Rev. Lett. **101**, 137201 (2008). [2] T. Maruyama et al., Nat. Nanotech., **4**, 158 (2009).

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