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**First-principles study of electric field and structural strain impact on perpendicular magnetic anisotropy of Fe/MgO interfaces** FATIMA IBRAHIM, HONGXIN YANG, BERNARD DIENY, MAIRBEK CHSHIEV, SPINTEC, CEA/CNRS/UJF-Grenoble-INP, INAC, 38054 Grenoble, France — Electric-field (EF) control of magnetic anisotropy is promising in the context of establishing low-energy consumption memory devices [1] since it allows EF-assisted switching of magnetization in magnetic tunnel junctions with perpendicular magnetic anisotropy (PMA) [2]. Using first-principles calculations, we demonstrate that both the EF and structural strain induce changes of the PMA in Fe/MgO interfaces which originally exhibit strong PMA [3]. Namely, we find that the PMA change in response to strain is much larger than that induced by applied EF. This suggests that the EF control of PMA is caused not only by charge accumulation and depletion mechanism but rather mediated by structural modifications occurring at the interface in agreement with recent experimental reports [4,5]. In addition, using atomic and orbital-resolved analysis of PMA, we elucidate the effect of both the EF and structural strain on PMA showing in particular that it extends beyond the interfacial layer.

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[2] W.-G. Wang et al., Nat. Mater. 11, 64 (2012).

[3] H. X. Yang et al., Phys. Rev. B 84, 054401 (2011).

[4] V. B. Naik et al., Appl. Phys. Lett. 105, 052403 (2014).

[5] F. Bonell et al., Appl. Phys. Lett. 102, 152401 (2013).

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