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First principles investigation of magnetocrystalline anisotropy at Full Heusler / MgO interfaces RAJASEKARAKUMAR VADAPOO, ALI HALLAL, MAIRBEK CHSHIEV, SPINTEC, CEA/CNRS/UJF-Grenoble-INP, INAC, 38054 Grenoble, France — Magnetic tunnel junctions with perpendicular magnetic anisotropy (PMA) have the potential for realizing next generation high density non-volatile memories and logic devices [1]. The origin of high PMA in these interfaces has been explained by orbital hybridizations at interface along with spin-orbit interactions [2]. Here we present a systematic study of PMA in Heusler alloy [X_2YZ]/ MgO interfaces using first principle methods with X=Co, YZ=FeAl, MnGe and MnSi. Among the interfaces studied, we found that Co terminated interface of Co_2FeAl/MgO gives rise to PMA value of 1.2erg/cm^2 in agreement with recent experimental observations [3]. On the contrary, FeAl terminated interfaces of the same structure shows in-plane magnetic anisotropy (IMA). We also found that the most of PMA contribution originates from d_{yz} and d_z^2 orbitals of Co atoms at the interface. Finally, Co_2MnGe and Co_2MnSi structures tend to favor IMA for any termination.

[1] S. Iked et al., Nature materials 9, 721 (2010)
[2] H. X. Yang et al., Physical Review B 84, 054401 (2011).
[3] M. Belmeguenai et al., Cond-mat.mtrl-sci, may 2013, arXiv:1305.0714.

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