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Electric-field-induced modification to the magnetic and transport properties of Fe/MgO-based interfaces revisited: Exchange stiffness and Hall conductivities

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The electric field-induced modifications to the magnetocrystalline anisotropy, exchange stiffness and anomalous/spin Hall conductivities of Fe/MgO-based interfaces are systematically investigated by means of first principles calculations. We confirm that the magnetocrystalline anisotropy (MCA) is sensitive to an application of the electric field, showing an increase of MCA upon the positive field associated to the accumulation of negative charges at the Fe side. The modification of MCA energy due to electric field and the band-filling effects are consistent with previous studies [1]. Additionally, we find crucial roles of the modification of d_{xy} and d_{yz} bands of Fe, due to the modification of the Fe-O atomic distance, to the changes of exchange stiffness and Hall conductivities upon the application of electric field. In the first place, while the exchange stiffness constants are positive (ferromagnetic) in the considered systems, there are negative energy orbital contributions to the exchange stiffness preferring antiferromagnetic alignment. The different contributions turn out to be strongly related to the symmetry breaking of d_{xy} and d_{yz} bands arising from spin canting on neighboring atoms. These orbital contributions are further enhanced on the positive field due to the modification of the Fe-O atomic distance, explaining the increase of exchange stiffness on going from negative to positive field. Secondly, the Hall conductivities are also shown to be increased upon the application of positive electric field. The mapping of the Hall conductivities within the two-dimensional Brillouin zone shows that the electric-field-induced modification is related to the modification of the band structures of the atoms at the interface with the MgO substrate. Inspecting further the band characters reveals that this modification is also mainly driven by the changes in the d_{xz} and d_{yz} bands. The focus of our presentation will be on the mechanisms of the electric-field-induced modifications to these latter properties: exchange stiffness constants and anomalous (as well as spin) Hall conductivities.

[1] K. Nakamura, et.al. PRL 102, 187201 (2009)