**Noncollinear Spin Torque Effect in Magnetic Heterojunctions: Combined First-Principles Calculation and TB-NEGF Method**

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Our theoretical researches focus on searching for novel nm-scale ferromagnetic/barrier/ferromagnetic (FM/B/FM) magnetic tunnel junctions (MTJs) with superior spin transport properties by choosing oxides [1] and organic molecules [2] as the central barriers. The relative orientation of two FM electrodes can be controlled by a spin-polarized current via the noncollinear spin torque effect. Recently, we have successfully employed the single-band tight-binding (SBTB) model to predict the noncollinear spin torque effect in FM/I/FM and FM/I/SF/I/FM [1] magnetic tunnel junctions, where I and SF represent insulting and spin-filter barriers, respectively. However, for real complex heterojunctions, the injected spin-polarized electrons from FM electrode can be strongly influenced by the complicated interfacial spin-polarized charge transfer, which is ignored in our previous SBTB model.

In this study, our newly developed “JunPy” [3] package successfully combined the self-consistent Hamiltonian by using the first-principles calculation, including multi-band dispersion relation and complicated interfacial coupling, with our newly derived TB model and non-equilibrium Green’s function (NEGF) method to investigate the noncollinear magnetotransport properties in nm-scale magnetic heterojunctions. This program is first testified for the spin-polarized currents and the noncollinear spin torque effect in conventional Fe/MgO/Fe MTJ. We further employed it to predict the giant field-like spin torque (FLST) effect in the amine-ended single-molecule magnetic junction [5], which may open a new avenue for multifunctional manipulation in next-generation organic FLST-MRAMs with lower power consumption. We believe that this newly developed calculation process not only can efficiently resolve current self-consistent difficulties in first-principles calculation for non-collinear case, but also may inspire future experimental explorations in novel magnetic heterojunctions for future spintronics applications. This work is supported by the Ministry of Science and Technology (MOST 106-2112-M-008-011- and 106-2633-M-008-002-) and the National Center for Theoretical Sciences, Republic of China.

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