A Comparison of Theoretical Estimate of the Energy Barrier between Bi-stable state of hBN-based Magnetic Tunnel Junction

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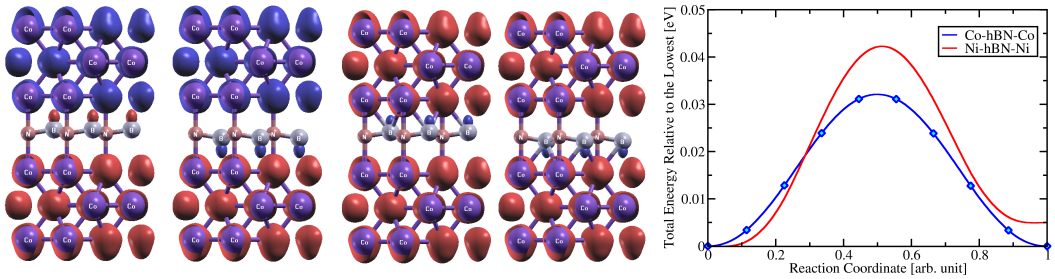
A comprehensive and systematic first-principles study on 2D materials-based spin-valve nanostructure has successfully revealed a lot of unique spintronics functionality of 2D materials-based spin-valve[1,2]. Our recent study on hexagonal boron nitride (hBN) sandwiched by Ni(111) slabs suggests that the most stable stacking arrangement among 36 possible stacking arrangements shows the cross-correlation functionality which comes from the bi-stable state of a rugged hBN plane and the controllable BN polarization[2]. Controlling the BN polarization lead to the ability to move the N and B atoms toward upper or lower Ni(111) slab. However, the small total energy difference between asymmetric (the most stable structure) and symmetric (the second most stable structure) of 2pd-hybridizations stacking arrangements (~33 meV) lead both of stacking arrangements could appear in the fabrication method. Controlling the symmetry of the upper and lower Ni(111) slabs to have an asymmetric arrangement in the fabrication process is a huge challenge to realizing hBN-based cross-correlation materials. To overcome the problem, we performed an ab-initio study on Co(0001)/hBN/Co(0001). Having a higher number of unpaired electrons compare to Ni, the charge polarization of the BN layer increases due to the higher number of electrons that are transferred from Co (0001) slabs to N atom. We proposed two most stable stacking arrangement of Co(0001)/hBN/Co(0001), asymmetric and symmetric stacking arrangement with the 2pd-hybridizations. Our results show a rugged hBN plane for both stacking arrangements not only in anti-parallel configuration but also in a parallel configuration. Furthermore, nudged elastic band (NEB) calculation was done to compare the theoretical estimation of energy barrier of bi-stable state. The result shows Co-hBN-Co has lower energy barrier compare to Ni-hBN-Ni leading to small required external electric field for switching between bi-stable state.



(a) (b) (c)

Figure 1: Spin charge density mapping of the bi-stability state of 2pd-hybridizations arrangements in (a) anti-parallel configuration and (b) parallel configuration. (c) The theoretical estimate of the energy barrier of Ni-hBN-Ni and Co-hBN-Co.

References

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[2] H. Harfah, Y. Wicaksono, M. A. Majidi, and K. Kusakabe, arXiv:1905.12252.