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First Principles Study on Ni(111)/hBN/Co(0001): Toward Realization of hBN-based Spin-Valve Nanostructure as Cross-Correlation Materials

A comprehensive and systematic first-principles study on 2D materials-based spin-valve nanostructure has successfully revealed a unique spintronics functionality of 2D materials-based spin-valve1,2. 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 rugged hBN plane and the controllable BN polarization2. Controlling the BN polarization lead to the ability to move the N and B atoms toward upper or lower Ni(111) slab. An induced magnetic moment at an N site appears when N is moved closer to one of the Ni atoms. Interestingly, the moment direction is switched by the position of the N layer in the resulting bi-stable state with electrical polarization when APC is chosen. The transmission probability calculation of Ni/hBN/Ni having the determined interface structure at the center of the junction exhibits a spin-filtering effect where the spin-polarized current is controlled by the electric field when a field-induced reversal of the polarization is realized. However, the asymmetric stacking arrangement between upper and lower Ni(111) slabs of the most stable stacking arrangements make the fabrication of the materials become difficult to control. In this study, we propose a hybrid spin-valve nanostructure where hBN growth on the top of Ni(111) slab but covered by Co(0001). We undertook an ab-initio study to explore the cross-correlations functionality of Ni(111)/hBN/Co(0001). A maximum of two pd-hybridization bonds stabilized the structure, with APC proving to be the most favorable magnetic alignment. We proposed four stacking arrangements with 2pd-hybridizations, namely $Ni_{top\text{-}hcp}$(111)/hBN/$Co_{top\text{-}hollow}$(0001), $Ni_{top\text{-}fcc}$(111)/hBN/$Co_{top\text{-}hollow}$(0001), $Ni_{top\text{-}hcp}$(111)/hBN/$Co_{top\text{-}hcp}$(0001), and $Ni_{top\text{-}fcc}$(111)/hBN/$Co_{top\text{-}hcp}$(0001). All those stacking arrangements show the rugged BN-plane and lead to bi-stable states which lead to the easier fabrication. The rugged of BN-plane is ~0.27 Å which is higher than that of Ni(111)/hBN/Ni(111) which the rugged is ~0.25 Å. Spin-charge density mapping was done to understand the magnetic properties of the system. Opposite with the case of Ni(111)/hBN/Ni(111), where induced magnetic moment direction of N atom changes between two bi-stable state, the B atom magnetic moment changes between two bi-stable state as shown in figure 1. The further transmission probability calculation to be expected to understand different transport properties.

References

[1] Y. Wicaksono, S. Teranishi, K. Nishiguchi, and K. Kusakabe, Carbon 143 (2019) 828-836.
[2] H. Harfah, Y. Wicaksono, M. A. Majidi, and K. Kusakabe, arXiv:1905.12252 (submitted to ACS Applied Materials and Interfaces)

Figures

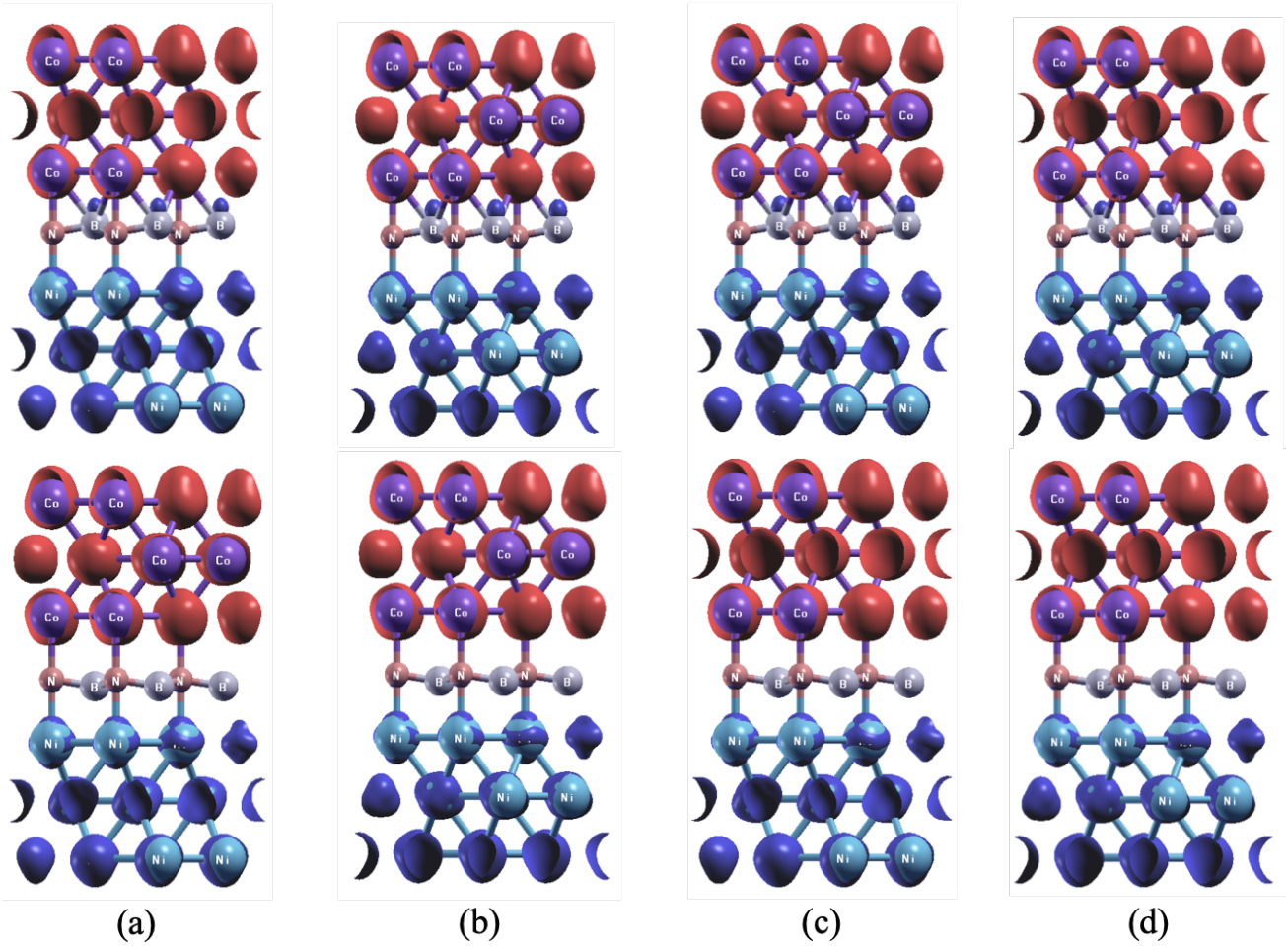

Figure 1: Spin charge density mapping of the bi-stability state of (a) $Ni_{top\text{-}fcc}(111)/hBN/Co_{top\text{-}hcp}(0001)$, (b) $Ni_{top\text{-}hcp}(111)/hBN/Co_{top\text{-}hcp}(0001)$, (c) $Ni_{top\text{-}fcc}(111)/hBN/Co_{top\text{-}hollow}(0001)$, and (d) $Ni_{top\text{-}hcp}(111)/hBN/Co_{top\text{-}hollow}(0001)$. The charge density in red represents spin-up electron density and that in blue represents spin-down electron density.