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# First-Principle Studies of Ni/hBN/Ni nano-spin-valve-like Structure for Spin Electronics

Hexagonal boron nitride (hBN) sandwiched between magnetic nickel layers has been theoretically studied within the framework of generalized gradient approximations of density functional theory. Possible thirty-six stacking arrangements of nickel layers with respect to hBN were considered to determine the most stable stacking structure. Our results show that strong hybridization between hBN and nickel slabs occurred when nickel atoms of the first nickel layer placed on the top or below nitrogen atoms. The strong hybridization leads the N-top stacking arrangement as the most favored energy state. This result is an analog to previous theoretical studies of Ni/hBN interface which found that nitrogen atom on-top sites of nickel layer with boron atom on the hcp- or fcc-sites (second or third layer respectively) are the most energetically favored stacking arrangement[1]. Interestingly, hBN-nickel sandwich has an asymmetric stacking arrangement on the second and third nickel layer between upper and lower nickel slab as the most favored energy as shown in figure 1. This asymmetric stacking arrangement is in constrast with graphene-nickel sandwich that has a symmetric structural arrangement[2]. Furthermore, within the most stable structure, the anti-parallel spin configuration system has an energy lower than parallel spin configuration which is in agreement with previous experimental study[3]. Starting from this point, further calculation to explain the current path of Ni/2D/Ni nano-spin-valve system can be derived.

## References

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[2] Y. Wicaksono, S. Teranishi, K. Nishiguchi, K. Kusakabe, arXiv:1811.01308
[3] M. Z. Iqbal, S. Siddique, G. Hussain, Adv. Eng. Mater., 20 (2018) 1700692

## Figures

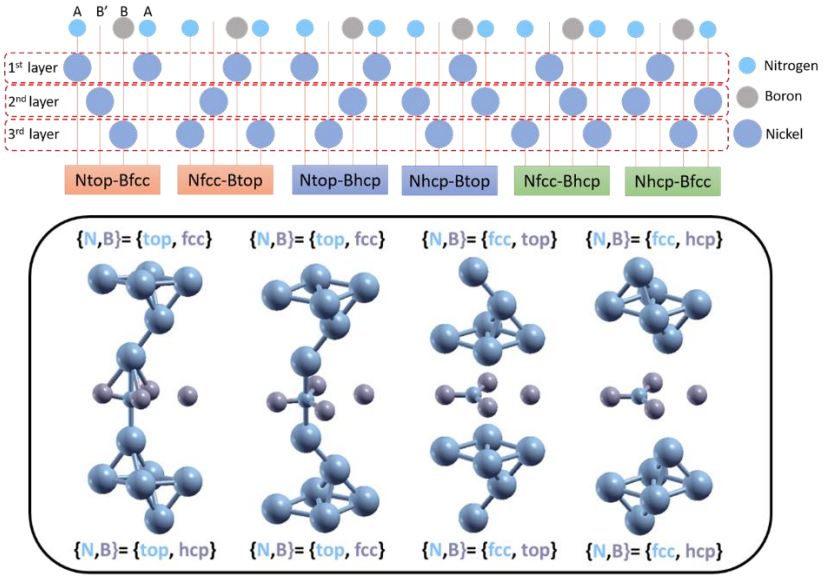


**Figure 1:** Various stacking arrangement on Ni/hBN interface (upper). Some representative figures as the results from thirty-six configurations. From left to right, the total energy increasing from the most stable to the unstable structure (lower). The combination of top-fcc on the top side and top-hcp on the bottom side are the most stable structure.