Influence of Stacking Arrangement of the 2D Materials-Based Spin Valve on Magnetoresistance Performance: A First Principles Study of Ni/hBN/Ni Spin Valve

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Ni/hBN/Ni spin valve is a hexagonal boron nitride sandwiched by nickel slabs as a ferromagnetic material with current-perpendicular-to-plane given to the system which is of great importance in the development of a spintronic device to achieve a high potential application as a logic gate device based on a spin configuration. To enable successful design and application by understanding comprehensively the nature of the properties of this new type devices, a careful study using generalized gradient approximations of density functional theory has been performed. The exhaustive calculations of thirty-six possible structures were considered. Our results show that strong p-d hybridization between hBN and nickel slabs occurred when nickel atoms of the first nickel layer placed on the top or below nitrogen atoms. A detailed analysis shows that the anti-parallel spin configuration system has energy lower than parallel spin configuration which is in agreement with previous experimental study[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. Nevertheless, this asymmetric stacking arrangement is in contrast with graphene-nickel sandwich that has a symmetric structural arrangement[2]. Spin charge density mapping and band structure calculations were done to support our understanding on the magnetic properties of the system. Furthermore, this study successfully extracts the rules of the significant influence of nitrogen atom in the stacking arrangement of the hBN-nickel sandwich which the calculation of the magnetoresistance affected by the classified group of the stacking arrangement is demanding for further investigation.

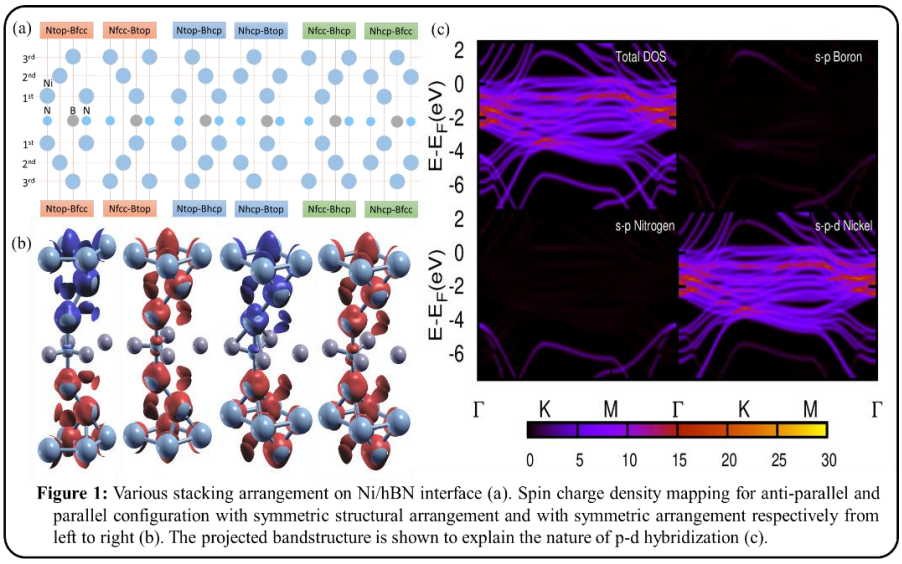

Figure 1: Various stacking arrangement on Ni/hBN interface (a). Spin charge density mapping for anti-parallel and parallel configuration with symmetric structural arrangement and with symmetric arrangement respectively from left to right (b). The projected bandstructure is shown to explain the nature of p-d hybridization (c).

References:

[1] M. Z. Iqbal et. al., Adv. Eng. Mater., 20 (2018) 1700692.

[2] Y. Wicaksono et. al., Carbon 143 (2019) 828-836.