DFT study on atomic structures of FeNi/2D materials

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ABSTRACT

The applications of two-dimensional materials as the spacer layer of magnetic tunnel junctions has attracted attention in recent reserch. In this work, we carried out the DFT calculation to clarify the atomic structures of the FeNi/2D materials interface. We considered the stability of Fe or Ni termination on bare FeNi surfaces by examining the formation energy to add a single atomic layer. From the comparison of the models with various composition ratios of the topmost metallic layer, we found that the surface with Ni concentration of 75% is the most stable. As the next step, we considered graphene covered FeNi interfaces (FeNi/graphene) [Fig. 1] ;three models were prepared with different arrangements of graphene. As a result, the top-hcp [Fig. 1(a)] and top [Fig. 1(b)] arrangements are relatively stable. Interestingly, the interface with Ni concentration of 0% is energetically the most stable, which differs from the bare FeNi surface. This mechanism originates from the attractive interaction between Fe and C atoms. The density of states of C(p_z) and Fe(d_{z^2}) indicates the transfer of electrons from the metal substrate to graphene and the orbital hybridization between Fe and C atoms.

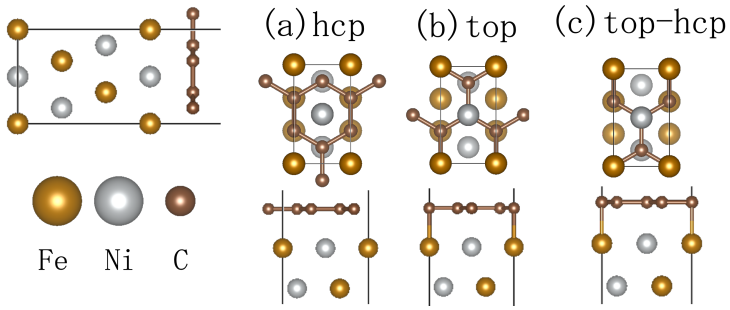

Figure 1: Computational models for FeNi/graphene.

References

[1] H. Naganuma *et al.* Appl. Phys. Lett. **116**, 173101 (2020).