

Abstract Submitted
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First-Principles Investigation of Mn and Co Doped Trilayer Graphene XUAN LUO, National Graphene Research and Development Center, North Springfield, VA 22151 — First-principles calculations were performed through ABINIT to investigate trilayer graphene for spintronics materials. We studied two stacking orders for trilayer graphene: Bernal (ABA) and rhombohedra (ABC) by using interstitial and substitution transition metal Mn and Co doped trilayer graphene. We found that the ABC stacking order exhibits larger band gap than that of ABA, the Co doped ABC trilayer graphene possesses a band gap and is ferromagnetic. This results show that interstitial Co doped ABC stacking trilayer graphene has potential applications in spintronics.

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