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Ideal structure for tunneling magnetoresistance and spin injection into semiconductros: Ni(111)/BN/Co(111)

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Abstract

Using the Vienna ab initio simulation package (VASP) incorporating van der Waals interaction, we have explored structural, adsorption, and magnetic properties of Ni(111)/BN/Co(111) systems. We have found that both Ni(111) and Co(111) layers shows half metallic state, while the spacer BN layer becomes weak metal for one monolayer (ML) thickness and an insulating barrier for two ML thickness. The half metallic states in both Ni(111) and Co(111) layers are robust because it is unchanged independently on the magnetic coupling of Ni(111) and Co(111). This finding suggests that the Ni(111)/BN/Co(111) systems can be utilized for perfect tunneling magnetoresistance system. Moreover, it can be applied for potential spin injecting into semiconductor in FM/semiconductor system due to the fact that the half metallic state in FM layers at the interface will be unchanged.