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Tight-Binding Theoretical Study of Monolayer h-BN on Ni (111) Surface

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Abstract. We present here a tight-binding calculation of the band structure of monolayer hexagonal boron nitride (h-BN) on NI (111) substrate taking into account of electron hoppings upto third nearest neighbour. Here h-BN is placed over a single layer of ferromagnetic ordered Ni in which the nitrogen atom of the honeycomb lattice of h-BN layer lies on the Ni atom of the bottom layer. Due to close matching of the lattice constants between h-BN and Ni, the hybridization between $2p_z$ orbital of N and $3d_{z^2}$ orbital of Ni is expected to be relative stronger. Further the ferromagnetism in Ni arising due to spin dependent electrostatic exchange interaction is also taken into account. All these above effects are incorporated in the tight-binding Hamiltonian. The magnetization in Ni layer is computed self-consistently. Finally the band structure of the system is calculated and the results are discussed to interpret the experimental data.

Keywords: h-BN-Nickel (111) system, Green's function, Magnetization, Tight-binding method
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