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Structure and magnetism of $Mn_{0.5}Ni_{0.5}$/Ni(001) system BOTHINA HAMAD, Physics Department, University of Jordan — The dependence of the magnetic structure on the geometry of materials is well-established for decades. Most of the theoretical and experimental investigations have focused on transition metals adsorbed on (001) noble metal surfaces. These systems can be considered as two-dimensional magnets with negligible influence of the substrate. Several experimental investigations have reported a c(2×2) ordered alloy structure for MnCu/Cu(001) and MnNi/Ni(001) systems. In this work, I present a theoretical study of the magnetic structure for the c(2×2) ordered $Mn_{0.5}Ni_{0.5}$/Ni(001) alloyed system. The calculations were performed using the density functional theory (DFT) and the exchange-correlation potential was treated by the generalized gradient approximation (GGA). In this study, an in-plane ferromagnetic structure was obtained, which is more stable than the antiferromagnetic by 398 meV. The Mn and Ni atoms exhibit local magnetic moments of $3.998\mu_B$ and 0.250 μ_B, respectively. I obtained relaxations of +1.5% and -1.05% for Mn and Ni surface atoms, respectively.

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