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First-principles study of the effects on ferromagnetic coupling in Mn/GaAs digital ferromagnetic heterostructure by free holes Injection and Be co-dopant MEICHUN QIAN, WARREN PICKETT, C.Y. FONG, Department of Physics, Univ. of California Davis — We use density functional theory to study the effect of free holes injection and Be co-dopant on the ferromagnetic coupling in Mn/GaAs digital ferromagnetic heterostructure (DFH). The injection of free holes is simulated by assigning a range of concentrations of missing electrons in unit cell. The δ-layer doping of Mn atoms in GaAs introduces three spin-polarized hole bands which are the consequence of hybridization between the d-states of the Mn atoms and the p-states of the nearest neighboring As atoms. The distribution of hole charge density shows that these spin-polarized holes are confined to the vicinity of the Mn δ-layer. After the injection of free holes, the Fermi energy E_F is lowered, then the number of spin-polarized holes in the layer of MnAs is increased monotonously. We characterize the ferromagnetic coupling by the total energy difference between the ferromagnetic and the antiferromagnetic phases , E_{FA}, per one pair of Mn atoms. The results of E_{FA}, E_F, and the projected spin-polarized holes at Mn and the nearest neighboring As atoms are shown as a function of concentration of the injected free holes. We demonstrate the enhancement of the ferromagnetic coupling, which is in agreement with the experimental results of Nazmul et al.[1]. In contract, after the Be co-dopant in Mn/GaAs-DFH, the ferromagnetic coupling is deteriorated. We will give the explanation. [1] A. M. Nazmul et at. Phys. Rev. B67, 241308(R) (2003).

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