

Abstract Submitted
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First-principle studies of magnetic impurities in GaAs in the presence of spin-orbit interaction FHOKRUL ISLAM, CARLO CANALI, Kalmar University — We report on density-functional theory studies of substitutional transition-metal magnetic impurities (Mn, Fe, Co, Ni) in GaAs. Our calculations include the effect of spin-orbit interaction, which has not been considered in detail so far. For two interacting magnetic impurities in bulk, we calculate the effective exchange interaction constant defined as the difference between the ground state energies for the ferromagnetic and antiferromagnetic configuration of the magnetic moments. We find that for Mn and Co impurities, ferromagnetic alignment is energetically favourable, while Ni impurities tend to order antiferromagnetically. For Fe pairs both configurations are possible, depending on the pair orientation with respect to the GaAs crystal structure. In all cases, the exchange constant is strongly anisotropic, as a function of both the pair orientation and, due to the spin-orbit interaction, the direction of the magnetic moment. We comment also on the case where the magnetic impurities substitute Ga atoms on the (110) surface of GaAs, which recently has been investigated experimentally by novel STM techniques.

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