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Mn doped InP nanowires: An ab initio study TOME SCHMIDT, Universidade Federal de Uberlandia, PEDRO VENEZUELA, Universidade Federal Fluminense, JEVERSON ARANTES, ADALBERTO FAZZIO, Universidade de Sao Paulo — We investigated the electronic and magnetic properties of Mn doped InP nanowires. Our study was based on total energy density functional calculations. The Mn dopants were placed substitutionally in In atom sites. We have found that the most energetically favorable position for the Mn atom is near the surface. However, a small amount of Mn atoms will be located at "bulk-like" positions in the wire. When the Mn atoms are in "bulk-like" positions, the Mn-3d majority-spin-orbitals appear in two different regions of the valence band (VB): about 2.0 eV below the top of the VB and resonant with the top of the VB. In these cases there is also an empty orbital in the gap whit p-character. The total valence spin-densities ($\rho_\uparrow - \rho_\downarrow$), for a single Mn atom in any of the configurations studied here, show a strong localized magnetic moment around the Mn atom site. In order to study the magnetic coupling we also did calculations with two Mn atoms in each cell. For several configurations studied, we concluded that if both Mn atoms are in "bulk-like" positions the system presents ferromagnetic ordering. On the other hand, if at least one of the Mn atoms is located near the surface, there is no magnetic ordering or the system is antiferromagnetic.

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