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Ab Initio Study of Electronic and Magnetic Properties of Co-doped AlAs. VIVIANA DOVALE-FARELO, WILLIAM LOPEZ-PEREZ, ALVARO GONZALEZ-GARCIA, RAFAEL GONZALEZ-HERNANDEZ, Universidad del Norte — First principles calculations were performed to study the electronic and magnetic properties of cobalt doped AlAs within Density Functional Theory formalism. The study was done using a 6.25% Co concentration with a 222 supercell. Substitutions of Al or As by Co atoms were done, preferring to replace Al atoms. Total energy calculations for non-magnetic (NM), ferromagnetic (FM) and antiferromagnetic (AFM) states were performed. In the supercell two Al atoms were replaced by two Co atoms at different distances (4.051 Å, 5.729 Å, 7.016 Å, 8.102 Å and 9.922 Å) for five different possible configurations: C0-1, C0-2, C0-3, C0-4 and C0-5. C0-n indicates the configuration corresponding to one Co atom placed in the origin and another one placed in n position. For 6.25% Co-doped AlAs, configuration C0-1 results to be more stable in a FM state with a total magnetization of 4 μB. In this configuration, the impurities are separated by a distance of 3.960 Å, and the smallest distance between Co-As was of 2.356 Å. The dilute magnetic semiconductor prefers the FM state over the AFM by an energy difference of 25 meV.

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