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Surface Effects on the Electronic, Magnetic and Structural Properties of Free-standing InP nanowires TOME SCHMIDT, Universidade Federal de Uberlandia — Nanowires due to their large surface-to-volume ratio of particular interest is the understanding of the surface structure and the electronic effects due to surface states. In this work we investigate the structural and electronic properties of InP nanowires aligned along the [111] direction, in which the surface have been studied by passivating with hydrogens or OH radicals and also oxidized. The magnetic properties of Mn doped InP nanowires with different surface termination have been also investigated. Our *ab initio* density functional calculations show that hydrogen passivation removes the surface states, opening up the band gap. Our results for oxygen adsorbed on the hydrogen passivated InP nanowires, show that there are many configurations where the oxygens are chemisorbed processes. For Mn doped InP nanowires our results reveal that the surface of the nanocrystals play a fundamental role on the impurity stability and on the magnetic properties of InP nanowires. The formation energy of pairs of Mn impurities in unpassivated nanowires are lower than that of the bulk InP. Most of the Mn pair configurations present FM coupling and their prefer to be inside the nanowire and not on the surface.

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