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A theoretical study of Si and Ge nanowires. A. FAZZIO, J. T. ARANTES, CEDRIC ROCHA LEÃO, ANTÔNIO J. R. DA SILVA, Instituto de Física, Universidade de São Paulo — We have performed a systematical *ab initio* study of the electronic and structural properties of pure Ge and Si nanowires (NWs), as well as Ge nanowires doped with Mn atoms. All our results are obtained via total energy Density Functional Theory (DFT) calculations within the generalized gradient approximation and pseudopotentials. The growth directions for all wires were considered to be along the (110) direction, and they present a hexagonal cross section formed by the intersection of $\{111\}$ and $\{001\}$ planes, with all the dangling bonds saturated with H atoms. We have considered three different diameters of SiNW's of similar shapes: 2.01 nm, 2.67 nm e 3.61 nm. In particular, we analyze how their properties, such as dispersion relations, band gaps and structural properties, like nearest neighbor distances, vary with the diameter. Similar calculations were also performed for the Ge NWs. In this latter case we have also investigated Mn doping. We focused on tetrahedral interstitial and substitutional sites, and conclude that the most stable position for Mn is substitutional at the surface of the nanowire.

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