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Effect of structure, surface passivation, and doping on the electronic and optical properties of GaAs nanowires: A first principles study.[1]
S. V. KHARE, Dept. of Physics, V. GADE, Dept. of EECS, University of Toledo, N. SHI, R. RAMPRASAD, Dept. of Chemical, Materials, and Biomolecular Engineering, Univ. of Connecticut — We investigate the structural, energetic, electronic, and optical properties of hydrogen-passivated doped and undoped gallium arsenide nanowires along [001], [110], and [111] directions with diameter d up to 3 nm, using *ab initio* methods. A critical diameter $d_c \approx 2$ nm is found above which all wires have faceted cross sections determined by the symmetry of their axis. The wires possess several electronic properties relevant for sensing and other nanoelectronic applications: (i) Quantum confinement has a substantial effect on the electronic band structure and hence the band gap (E_g), which increases with decreasing diameter. (ii) Unlike Si or Ge wires, GaAs wires oriented along all axes are found to have a direct E_g.(iii) The electronic band structure shows a significant response to changes in surface passivation with hydrogen. (iv) Doping of wires with n and p type atoms produced a response in the band structure similar to that in a doped bulk crystal. (v) However, the dielectric function shows differences in absorption peaks with p type versus n type doping.

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