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Quantum confinement in P-doped Si[110] nanowires[1] JIAXIN HAN, TZU-LIANG CHAN, JAMES CHELIKOWSKY, University of Texas at Austin — Recently, doped Si nanowires have been synthesized and demonstrated experimentally that they can be used as interconnects in electronic circuits or building blocks for semiconductor nanodevices. In order to understand how doping operates at the nanoscale, we used a real-space first-principles pseudopotential method to study P-doped Si[110] nanowires. We examined the size dependence of the electronic binding energy for the P donor level. We found the donor electron to be more strongly bound to the P atom with decreasing nanowire diameter owing to quantum confinement. We also examined the energetically favorable position of the P atom in Si nanowires. For nanowires with diameter less than 1 nm, the P atom is expelled to the surface owing to the stress introduced by the defect, which suggests that doping will be difficult for small-diameter Si nanowires. In addition, we calculated the core-level binding energy shift as the P atom moves from the surface towards the center of the nanowire. We will compare our results with experimental measurements.

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