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Dopant binding energies in P-doped Ge[110] nanowires using a real-space pseudopotential approach[1] ALEX J. LEE, JAMES R. CHELIKOWSKY, University of Texas at Austin, TZU-LIANG CHAN, Hong Kong Baptist University — We apply a real-space pseudopotential formalism for charged one-dimensional periodic systems to examine the binding energies of P dopants in Ge[110] nanowires with varying periodicities and diameters. Binding energies calculated by density functional quasiparticle energies of the neutral dopant are severely underestimated whereas those calculated by quasiparticle energies of the ionized defect are overestimated. We found the best method for determining binding energies is to adopt a composite approach that evaluates the total energy difference between charged and neutral systems for the ionization energy of the P dopant, but uses the quasiparticle energy for the electron affinity of the pure Ge nanowire. Our formalism offers a simple density functional method for calculating dopant binding energies of small nanowire systems without the use of computationally intensive many-body perturbation theory calculations.

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