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A finite-size supercell correction scheme for charged defects in one-dimensional systems: Application to impurities in silicon nanowires

SUNGHYUN KIM, Dept. Physics, KAIST, Korea, JI-SANG PARK, National Renewable Energy Laboratory, K.J. CHANG, Dept. Physics, KAIST, Korea — The formation energies of defects in solids are important to determine their stability and charge transition levels. In first-principles calculations for charged defects, supercells subject to periodic boundary conditions are commonly used. However, this approach suffers from spurious interactions between the defect and its image charges. Due to the long-ranged Coulomb interaction, a very large supercell is inevitable to obtain the numerical convergence. To overcome this problem, several finite-size supercell corrections have been proposed for bulk solids and two-dimensional systems. In this work, we propose a new finite-size correction scheme for charged defects in one-dimensional systems, where the medium is surrounded by vacuum in radial directions. The energy correction is obtained by solving the Poisson equation with the macroscopic dielectric constant. We show that the macroscopic dielectric constant and the defect charge distribution can be derived from the electrostatic potential in first-principles calculations. We test our scheme for charged B and P impurities in silicon nanowires. We find that the corrected formation energies converge rapidly with either increasing of the wire length or increasing of the vacuum pad, providing reliable charge transition levels.

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