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Donor-pair defects and doping efficiency in silicon nanowires

BYUNGKI RYU, Department of Physics, Korea Advanced Institute of Science and Technology, Daejeon, 305-701, CHANG-YOUN MOON, Department of Physics and IPAP, Yonsei University, Seoul 120-749, WOO-JIN LEE, KEE JOO CHANG, Department of Physics, Korea Advanced Institute of Science and Technology, Daejeon, 305-701 — We investigate the doping efficiency of dopants in Si nanowires through first-principles density-functional calculations. For hydrogen- passivated Si nanowires doped with group-V elements such as P, As, and Sb, we consider wire diameters in the range of 8 - 30 Å and axis orientations along the [111] and [110] directions. A single substitutional donor prefers to locate on the wire center and acts as a shallow donor. When wire diameters are below a critical value, a donor-pair defect which consists of two dopants at the first-nearest distance can be stabilized, in contrast to bulk Si. The stability of the donor-pair defect is attributed to the confinement effect in nanostructures, which results in the increase of the band gap and thereby the destabilization of the shallow donor level. As the donor- pair defect with a deep level in the band gap is electrically inactive, the doping efficiency is expected to be low in small-diameter nanowires. The formation of the donor-pair defect is found to be more favorable for the P dopants, which have a smaller atomic radius than the As and Sb dopants.

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