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Optical properties of doping effects in Si quantum dots JINGBO LI, SU-HUAI WEI, National Renewable Energy Laboratory — Si quantum dots (QDs) have many applications such as in high-efficient solar cells and light emitting diodes. Understanding the doping properties in Si QDs are very important for both theory and experiment. Using first-principles methods, we have systematically calculated the defect formation energies and transition energy levels of group-III and group-V impurities doped in Si QDs as functions of the QD size. The general chemical trends found in the QDs are similar to those found in bulk Si. We show that defect formation energy and transition energy level increase when the size of the QD decreases, thus doping in small Si QDs becomes more difficult. We explain the general chemical trends and the variation as a function of QDs size in terms of the atomic eigenvalues and quantum confinement effects. We also calculate the absorption spectrum of size-dependent Si QDs and quantum rods by large-scale "charge patching method". We show that the band gap and optical transitions of Si nanocrystals can be tailored continuously by size or shape. These results provide guidelines for future device designs that require the knowledge of the size/shape-dependence of the nanocrystal's electronic and optical properties.

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