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Stability of DX center in semiconductor quantum dots JINGBO LI, SU-HUAI WEI, National Renewable Energy Laboratory, Golden, CO 80401, LIN-WANG WANG, Lawrence Berkeley National Laboratory, Berkeley, CA 94720 — Semiconductor quantum dot(QD) are of great current interest for applications because the physical properties of QD such as the band gap can be tailored by size or shape. On the other hand the application of semiconductors as novel electronic devices depend critically on its doping properties. Although defect properties have been extensively studied in the past for bulk, very few studies have been done for QD. For example, it is known that DX^- center in Si doped GaAs is unstable in bulk, however, it is not clear whether it is stable the case in GaAs QD. Using first principles band structure method, we study how the size of QD affects the stability and transition energy levels of DX center of GaAs:Si. We find that although Si DX center is unstable in bulk GaAs, when the dot size is small enough, it is stabilized. The critical size of QD is around 3nm of diameter. The stabilization is due to the strong quantum confinement effect, the conduction band edge of QD increases. The formation energy of the tetrahedral coordinated Si^-_{Ga} also increases because the occupied shallow defect level is mostly CBM-like. On the other hand, the DX^- defect level contains significant amount of non-CBM characters, so the increase of formation energy of the DX^- center is less than the shallow Si^-_{Ga} defect. Our studies show that defect in QD could be significantly different from the bulk.

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