The p-n Doped Silicon Nanostructures

Jiangchao Chen, Andrew Schmitz, Dmitri S. Kilin

Department of Chemistry, University of South Dakota, Vermillion,

South Dakota 57069, United States

Crystalline silicon quantum dot (QD) doped with aluminum and phosphorous together has been modeled with a formula of $Si_{36}Al_1P_1H_{42}$. QD is elliptical, elongated in <111> direction, dopants are spread along this direction. Total energy, density of electronic states, and absorption spectra of the co-doped silicon quantum dot are simulated for various equilibrium and non-equilibrium modifications: ionized, photoexcited, and thermalized. All calculations are done by VASP software in the basis of plane waves, and valent electrons are treated explicitly while core electrons are described with pseudopotentials.[1] Our results show the features in the electronic structure of the QD in the bandap area near conduction band minimum and valence band maximum contributed by Al- and P-doping atoms, and transitions between those bands make contributions to absorption spectra. Thermal motion of ions leads to the deviation from an ideal crystal structure of silicon quantum dot and decreasing the bandgap after heating to 2000K. Interestingly, Al dopant was pushed out from the center to the surface of the QD upon thermalization.[2] This simulation can predict the charge transfer across p-n junction on atomistic scale, and our computation complements earlier works on QDs functionalized by a single doping atoms.[3]

1. (a) Kresse, G.; Furthmuller, J., Efficient iterative schemes for ab initio total-energy calculations using a plane-wave basis set. *Physical Review B* **1996,** *54* (16), 11169-11186; (b) Vanderbilt, D., Soft Self-Consistent Pseudopotentials in a Generalized Eigenvalue Formalizm. *Physical Review B* **1990,** *41* (11), 7892-7895.

2. Chen, J., Thermal motion of co-doped quantum dot. *YouTube* **2011**, http://youtu.be/ssg--BxVdPU.

3. (a) Mavros, M. G.; Micha, D. A.; Kilin, D. S., Optical Properties of Doped Silicon Quantum Dots with Crystalline and Amorphous Structures. *J. Phys. Chem. C* **2011,** *115* (40), 19529-19537; (b) Ochsenbein, S. T.; Feng, Y.; Whitaker, K. M.; Badaeva, E.; Liu, W. K.; Li, X.; Gamelin, D. R., Charge-controlled magnetism in colloidal doped semiconductor nanocrystals. *Nature Nanotechnology* **2009,** *4* (10), 681-687; (c) Fischer, S. A.; Prezhdo, O. V., Dopant Effects on Single and Multiple Excitons in Small Si Clusters: High-Level Ab Initio Calculations. *J. Phys. Chem. C* **2011,** *115* (20), 10006-10011.