Theory on heavily co-doped silicon nanocrystals

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Silicon nanoparticles (Si NPs) heavily co-doped by boron and phosphorous are promising nanomaterials, as they exhibit advantageous features compared to their undoped counterparts[1]: their photoluminescent emission energies are lower (possibly below the band gap of bulk Si), and they show excellent chemical stability against oxidation in aqueous environments unlike pure Si NPs. They can be produced in large quantities and their size can be tuned by experimental parameters. These advantageous properties might be harnessed by applying them as in-vivo fluorescent biomarkers emitting in the near-infrared biological window. Despite their remarkable potential, the structure of heavily co-doped Si NPs is not well understood at an atomic level. We study 1-2.5 nm sized B and P co-doped Si NPs utilizing first principles computer simulation techniques, such as density functional theory (DFT) and time-dependent DFT, and compare our result to the experiments. We study the correlation between the atomic structure (e.g. the distribution of dopants within the Si NP) and electronic structure (formation energies and emission energies).[2] We also investigate the signature of characteristic atomic configurations in the Raman spectra and infrared vibration spectra, in order to provide a deep insight for the interpretation of the experimental results.

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[2] B. Somogyi, R. Derian, I. Štich, A. Gali, *J. Phys. Chem. C*, **2017**, *121* (49), pp 27741–2775