

Theoretical Study of the Impact of Surface Passivation and Functionalization on Electronic and Optical Properties of Pure Silicon and Germanium Nanocrystals [†]

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Abstract: Semiconductor nanocrystals with 2–10 nm are zero-dimensional materials, Quantum Dots (QDs). A scientifically and technologically useful feature is the ability to adjust their energy gap by a) modifying their dimensions [1–5], b) altering the surface passivation or surface reconstruction [6–9], and (c) by attaching surface organic functional groups [6-11]. Silicon and Germanium quantum dots offer diverse paths for property adjustment, have low toxicity, and can radiate to different regions of the visible spectrum [12–14, 16, 19]. This makes them superior to conventionally used markers such as organic dyes and fluorescent proteins and low production costs. They offer remarkable promise for their wider use in future bioimaging techniques, in targeted delivery of substances and drugs to cells, as well as in the research of processes of biological, biochemical, and biomedical interest [15, 17–20]. We performed a computational study within the time-dependent density functional theory framework employing the B3LYP functional [21, 22] using the Gaussian package [23]. We examined a) hydrogen passivated pure silicon nanocrystals [4, 5, 11], and (b) pure germanium nanocrystals with various forms of surface passivation [9, 10]. We selectively replaced hydrogen atoms with oxygen [8], nitrogen, and chlorine atoms, and judiciously chosen organic ligands [6]. The dots' energy gap dependence on their dimensions was investigated concerning the manifestation of quantum confinement [1–3]. The expected dependence of the gap is given by the equation [2]:

$$E_g = A + B \cdot D^{-n}$$

where, A, B, and n are fitting parameters, and D is the quantum dot diameter.

Keywords: quantum dots; zero-dimensional materials; nanocrystals; density functional theory; optical properties; optical gap; band gap; nanotechnology; bioimaging.

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Conflicts of Interest

The authors declare no conflict of interest.

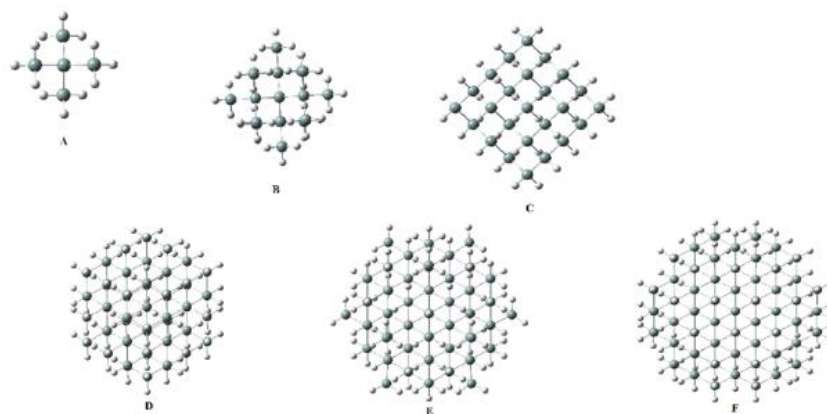


Figure 1. Hydrogen passivated Si_nH_m quantum dots for $n =$ a) 5, b) 17, c) 35, d) 71, e) 99, f) 147.

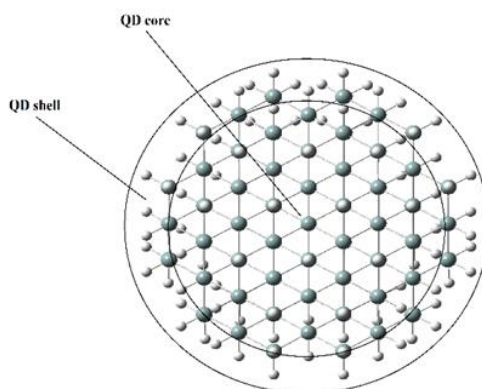


Figure 2. Core/shell representation of the quantum dots under study. Inner and outer domains are separated by circles. The outer shell is the region that we adjust the composition and add functional groups to examine their effect on electronic and optical properties.

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