Silicon nanocrystals with enhanced functionalities: DFT study

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In semiconductor nanocrystals (NCs), with decreasing core diameter, surface to volume ratio increases and larger fraction of the constituent atoms resides directly on the surface. For example, in a 2 nm Silicon NCs (SiNCs), 50% of the Si atoms are at the surface. This offers an additional degree of freedom to manipulate the properties of such a NC. Also, Si surface bonding chemistry is covalent, hence electrons from attached elements or ligands play a key role in determining the electronic structure of the NCs. In the small NCs (~2 nm), quantised k-vector is not anymore a good quantum number defining the available states in the NC, as it was in the bulk crystal with a long range periodicity. Nevertheless, one can still plot so called "fuzzy band-structures" [1] and study the role of ligands on its properties. From our previous Tight Binding [2,3] and recent Density Functional Theory [4] approaches, we found that covalently bonded ligands strongly modify the band-gap, Fermi energy, oscillator strength/ radiative rate and the overall density of states in the "bands". Because novel functionalities contributing to more efficient light emission or absorption in Si are in high demand for photovoltaics and optoelectronics, we will discuss whether it is possible to achieve a "direct bandgap" in SiNCs and whether the absorption cross section can be tuned by the ligands.

References:

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