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TÉMA

Surface engineering of indirect bandgap semiconductor nanoparticles for enhanced optical properties

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IV-group bulk crystalline semiconductors, Diamond (C), Silicon and Germanium, all possess diamond structure and indirect bandgaps. The latter property results in very poor emission and band-edge absorption, limiting their use in optoelectronic and photonic applications. In nanocrystal form, oscillator strength is enhanced via the spatial confinement of carriers, which leads to relaxation of the k-selection rule and band-mixing. However, very important (and often undervalued) are also effects resulting from surface chemistry and structural relaxation; both strongly pronounced due to the covalent chemistry of these materials. Structural relaxation leads to reduction in the crystalline core and amorphisation of the interface layer. In such a case various defects are generated that can act as color centers, non-radiative traps, self-trapping sites or dangling bonds, etc. Various surface chemistries can lead to additional strains and charge transfer. These effects critically contribute to modifications of the electronic structure and are not often included in theoretical models of nanocrystals emitting in visible and infrared spectral ranges (core sizes over 1.5 nm). Due to the covalent chemistry, it is also very difficult to develop well-defined and reproducible chemical synthesis of these materials and each known production technique offers slightly different result with respect to the core crystallinity, shape and size and surface capping.

Weak emission/absorption, lack of well-defined samples and applicable models makes the interpretation of experimental results very challenging. One needs to combine available models, many different experimental spectroscopy techniques on both ensemble and single quantum dot-levels and various samples to deduce the origin of emission and absorption for each particular case. In our work, we focus on the experimental properties of chemically synthesized Si-, C- and Ge-nanocrystals. Wet chemical synthesis offers convenient low-cost and up-scalable production, as well as versatile surface passivation and functionalization. Unfortunately, most available wet-chemically synthesized nanocrystals (Si-, Ge-, C-) are not yet very well characterized and many questions remain over their properties. In our work, we suggested several novel effects that can arise from surface charge transfer, such as the formation of direct bandgap and full spectral tunability in C-capped Si-nanocrystals [1-4]. In our current work we also focus on effects of defects, charge transfer and strain in C-capped Ge nanocrystals, C-dots and Ge/Si core-shell systems.

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