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TÉMA

Surface engineering in silicon- and germanium-based nanocrystals

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The two possibilities to control and enhance the optical properties of the nanocrystals made from indirect band-gap semiconductors are presented by quantum confinement and surface engineering. The quantum confinement effect can lead to the relaxation of the momentum conservation rules for small nanocrystal sizes while the surface engineering offers the possibility to manipulate the eigenstates of confined carriers in the reciprocal space due to the valley mixing effects. Here, we present the theoretical sp3d5s* empirical tight-binding study of the silicon nanocrystals coated by electronegative ligands [1]. We demonstrate the strong modification of the ground conduction band states with the admixture of the G valley and the emergence of direct-like G - G radiative transitions. These results might be relevant to the fast photoluminescence observed in alkyl-coated silicon nanocrystals [2,3].

Another potentially interesting system is presented by core-shell Si/Ge nanocrystals structures where one might expect excitons indirect in both real and reciprocal space. We study theoretically the optical transitions in Si/Ge nanocrystals using a combination of sp3d5s* tight-binding method to compute the electron states and optical transitions in the system and the valence force field method to compute the strain inside the nanocrystal. Electron ground state in Si nanocrystal is located in the X valley while the ground state for the nanocrystals with large Ge core is formed by the states from the L valley. Using the original algorithm based on the Fourier transform we analyze the valley structure of the electron states and find a critical core radius where the X-L crossover takes place. Characteristic times of optical transitions are also calculated, unambiguously indicating strong enhancement of the optical transitions in the nanocystals with large Ge core.

References:

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