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The Role of Silicon Oxide Layers in Luminescence of Ensembles of Silicon Quantum Dots

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Abstract: Based on the quantum confinement-luminescence center model, to ensembles of spherical silicon nanocrystals (nc-Si) containing two kinds of luminescence centers (LCs) in the SiO_x layers surrounding the nc-Si, the relationship between the photoluminescence (PL) and the thickness of the SiO_x layer is studied with the excitation energy flux density as a parameter. When there is no SiO_x layer surrounding the nc-Si, the electron-heavy hole pair can only recombine inside the nc-Si, then the PL blueshift with reducing particle sizes roughly accords with the rule predicted by the quantum confinement model of Canham. When there presences a SiO_x layer, some of the carriers may tunnel into it and recombine outside the nc-Si at the LCs to emit visible light. The thicker the SiO_x layer is, the higher the radiative recombination rate occurred outside the nc-Si will be. When the central scale of the nc-Si is much smaller than the critical scale, the radiative recombination rate outside the nc-Si dominates, and visible PL will be possible for some nc-Si samples with big average radius, greater than 4 nm, for example. When there is only one kind of LC in the SiO_x layer, the PL peak position does not shift with reducing particle sizes. All these conclusions are in accord with the experimental results. When there are two or more kinds of LCs in the SiO_x layer, the PL peak position energy and intensity swing with reducing particle sizes.

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Key words: silicon oxide layer, quantum dot, luminescence

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