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Electronic structures and optical properties of colloidal quantum dots[1]

LIN-WANG WANG, Lawrence Berkeley National Laboratory

Colloidal quantum dots can be synthesized by relatively cheap wet chemistry approaches with large quantity. Despite of their simple synthetic methods, they can have high optical qualities, e.g., with close to 100% photoluminescence (PL) quantum efficiency. Their optical properties can be tuned by changing the size, shape, hetero structure and composition of the quantum dots. The surface ligand passivation of the quantum dot also plays an important role in determining the electronic and optical properties of the quantum dots. In this talk, we will present the calculations of the electronic structures and optical properties of colloidal nanocrystals. Charge patching method is used to construct the Hamiltonian of a colloidal quantum dot, followed by the calculation of its electronic structure and optical properties. Limited configuration interaction formalism can be used to study the fine structures of the exciton or multiexciton behavior, as well as the Auger effects in such systems. For a heterostructure nanocrystal, when its size becomes large (e.g., 10 nm in size), the internal strain might play an important role. The exciton might be localized in particular region of a quantum dot. The optical gap and PL intensity can also be altered by external stress on the nanocrystal. The surface chemistry of the colloidal quantum dots, especially for Pb chalcogenide systems, will also be discussed. It will be shown that the electronic structure and optical properties of Pb chalcogenide systems are robust against defects and imperfection of surface passivation, explaining why these nanocrystals can have such high optical qualities. We will show how one can change the electronic and optical properties by using different surface ligand passivations.

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