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Simulations of semiconductor nanoparticles[1]

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We review theoretical works concerning the optical properties of II-VI, III-V and group-IV semiconductor nanocrystals. We present simulations based on semi-empirical tight binding method. In the case of Si nanocrystals, we discuss why the time decay of the photoluminescence is characterized by stretched exponentials. The usual explanation is that excitations can migrate between neighbour nanocrystals but we discuss experimental results in which it cannot be the case. We show that stretched exponentials can be explained quantitatively by intrinsic recombination in an ensemble of isolated nanocrystals made of an indirect gap material. Optical properties of PbSe nanocrystals will be discussed in the second part of the talk. We show that the cubic lattice of the material leads to unusual properties compared to zinc-blende semiconductors. Interband and intraband optical transistions are calculated and compared to experiments. Finally we present results concerning the energy transfer between neighbor nanocrystals by Foerster-type transitions. Results for III-V and Si nanocrystals will be compared.

[1]This work is done in collaboration with G. Allan.