A New Approach for Calculating Excitonic Emission Characteristics of Hybrid "Spherical Semiconductor Quantum Dot+Spherical Metal Nanoparticle" Nanosystem

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In all existing theoretical models of the exciton-plasmon interaction in hybrid metal-semiconductor nanostructures with semiconductor quantum dots (QDs) and metal nanoparticles (NPs) the QDs are considered as point dipoles like atomic or molecular *fluorophores*. It is connected with the fact that electric scalar potential formed outside QD by the exciton state (the potential being a superposition of the dipole potential contributions of all crystal unit cells inside QD with corresponding weight coefficients in a form of the exciton envelope wave function) has a typical form of the (point) dipole potential $\varphi_i(\vec{r}) = ed_{exc}\vec{r}\cdot\vec{\alpha}_i/(\varepsilon_{eff}r^3)$, where d_{exc} is the excitonic dipole length which takes values in the range from a few tenths of Å to a few Å depending on a semiconductor, $\vec{\alpha}_i$ are the orts in the directions of corresponding dipole moments, indices i=1,2,3 correspond to three possible hole Bloch (site) wave functions of p-type. Such "point dipole" representation of QD is quite reasonable when considering direct Förster-type resonant energy transfer (FRET) from excitons in QD to plasmons in NP. However, by considering QD excitonic emission, when transverse electromagnetic field (EMF) is generated, the above representation of a QD becomes invalid.

In this work we have developed a new model of the excitonic emission in QD+NP nanosystem. The total EMF emitted by the exciton in QD has been calculated as a sum of the EMF contributions of all point (unit cell) dipoles emitting inside QD with corresponding weight coefficients. It turns out that the resulting EMF of QD contains only dipole and octupole components of electric type and quadrupole components of magnetic type in contrast to erroneous consideration of QD emission as that of a (point) dipole, when an infinite series of EMF multipole components is generated (these multipole components contribute to a substantial energy absorption in a metal NP and thus are responsible for a strong emission quenching at small interparticle separations).

The nanosystem, which is nonspherical as a whole, has been characterized by three spherical coordinate systems (orientation of the third one is determined by the crystal axes orientation in QD). Multiple scattering between spherical NP and spherical QD of the EM field has been accounted. Characteristic radiative and nonradiative times as well as excitonic radiation efficiency have been calculated as functions of the interparticle separation at different QD and NP sizes and temperatures T=4.2 K and T=300 K in the particular case of CdTe QD and silver and gold NP.