Effect of composition and chemical architecture of core-shell nanocrystal phosphors, doped with Er^{3+} and Yb^{3+} lanthanide ions, on the efficiency of resonant non-radiative FRET energy transfer to an organic energy acceptor

Resonance energy transfer process has been known for around 70 years and nowadays is widely used in biology and medicine for applications such as visualizing biological processes in bio-assays, through Fluorescence Lifetime Imaging FLIM. Förster Resonance Energy Transfer (FRET or RET) is a non-radiative energy transfer mechanism between two molecules - donor (*D*) and acceptor (*A*) and is widely used to study their distance dependent interaction and to visualize biological processes, such as antibody-antigen reaction, DNA hybridization, proteins folding etc. To observe RET, strict requirements should be satisfied, such as short distance (in the range of 1 – 10 nm) between *D* and *A* and their spectral overlap (between *D* emission and *A* absorption). The most often used fluorophores in FRET mechanism are organic dyes (as *D* and *A*). However they have some disadvantages, for instance photobleaching, short luminescence lifetimes, and broad poorly separated absorption and emission bands. Thus other optically active species, such as lanthanide ions in nanocrystalline matrices (upconverting nanoparticles - UCNPs), seem to be ideal to circumvent issues found in organic dyes. Distribution of distances and concentration of Ln^{3+} in core-shell architecture of nanocrystals have a high impact on distances between ions and organic dyes.

Nanocrystals doped with Ln^{3+} ions may be of great importance as an optically active material to refine new materials that can serve as fluorescent labels for RET. Theoretical and experimental identification of the best distribution would allow for improved sensitivity of measurements and determination of energy transfer efficiencies on emission spectra and luminescence lifetimes. In order to indicate the nanocrystal architecture with the highest RET efficiency (including distribution and concentration) for the best potential donors for RET experiments, it is planned to experimentally verify the spectroscopic properties only for the best donors.

Energy transfer processes, which can occur in lanthanide ions, can be described by differential equations, but it gives only averaged results. In contrast, Monte Carlo (MC) analysis of energy transfers between ions will allow for the description of processes occurring between optically active ions based on the distances between ions. MC will enable the identification of the potentially best architecture of UCNPs, with the highest resonant energy transfer efficiency in fluorescent labels, which has a great potential in developing new materials for research. By quantitatively describing energy transfers and migration through MC calculations, it will provide a more comprehensive view of the effect of distance distribution on RET performance.