Underlying Phenomena Ruling Quantum Yield in Upconversion Nanoparticles

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Upconversion (UC) energy transfer offers an interesting excitation scheme for lanthanide-doped nanoparticles (NPs), since it allows access to the visible and ultraviolet emitting energy states of lanthanides through excitation in the near infrared. Such excitation strategy is finding applicability in a wide range of fields, from displays to bioimaging and theragnostics. For this reason, a great deal of work has been done to improve synthesis techniques in order to obtain upconverting nanoparticles with better properties. However, little attention is paid to the physical processes that modify UC quantum yield, which is expected to be limited, in the case of nanoparticles, by quenching associated to molecules present in the environment.

In this work we present a systematic study on the absolute quantum yield of upconverting nanoparticles. We chose $NaGdF_4$:Er^{3+}, Yb^{3+} as standard material to analyze, both quantitatively and qualitatively, the effect of the crystal phase, size and shape of the nanoparticles on quantum yield. The obtained results are discussed aiming to create a basis to understand the underlying causes that modify the outcome emission intensity. It is observed that the surface/volume ratio of the nanoparticles strongly affects the resulting quantum yield, making different morphologies also different in terms of upconversion efficiency. Moreover, it is demonstrated that the environment (solvent, capping agents) and the host material properties (mainly lattice distortions) strongly affect the final intensity output, since they trigger modifications in energy transfer probabilities between lanthanide ions and from the lanthanides to external quenchers.