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Comparison of concentration dependence of relative fluorescence quantum yield and brightness in first biological window of wavelengths for aqueous colloidal solutions of Nd^{3+}: LaF_3 and Nd^{3+}: KY_3F_{10} nanocrystals synthesized by microwave-hydrothermal treatment

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Abstract

We set simple criteria to choose crystal host for Nd^{3+} doping and a value of doping concentration for synthesis of aqueous colloidal solutions of the fluoride nanocrystals (NCs) to use them as fluorescence probes for bioimaging in the first biological window of wavelengths (750 – 950 nm). It is a large Ω_4/Ω_6 ratio of intensity parameters, used in Judd-Ofelt theory, which increases a fluorescence branching ratio β to the $^4F_{3/2} \rightarrow {}^4I_{9/2}$ transition lying in the first biological window; and a low value of intensity parameters Ω_6, which makes weaker the Nd-Nd fluorescence self-quenching and quenching by OH- molecular groups positioned in the volume of the NCs. Hypothesis is checked on the concentration series of highly dispersible aqueous colloidal solutions of the Nd^{3+}: LaF_3 and Nd^{3+}: KY_3F_{10} NCs synthesized by hydrothermal microwave (HTMW) treatment with PVP as biocompatible surfactant. To do this, the dependence of relative fluorescence quantum yield (FQY) and fluorescence brightness (FB) on Nd^{3+} concentration connected with nonradiative energy transfer to the quenching acceptors is found from the measured fluorescence kinetics. We observed smooth decrease in FQY and pronounced maximum in FB with increasing neodymium concentration in both systems. However, for Nd^{3+}: KY_3F_{10} NCs the fall of fluorescence brightness begins at a concentration four times lower than for Nd^{3+}: LaF_3, which is due to a stronger energy transfer to the quenching acceptors in the former. At the same time the fluorescence branching ratios to the first and the second biological windows are almost equal for the Nd^{3+}: LaF_3, while for Nd^{3+}: KY_3F_{10} it is higher to the second biological window. The results are in line with twice larger the Ω_4/Ω_6 ratio and three times smaller Ω_6 intensity parameter in Nd^{3+}: LaF_3. These criteria must be accounted together with a choice of a strategy for synthesis of the NPs with high crystallinity [ChemistrySelect 2 (2017) 4874 – 4881] and high water dispersibility during selection of a crystal host for Nd^{3+} doping to use it for bioimaging in the first biological window of wavelengths.

Keywords: Nd^{3+}: LaF_3; Nd^{3+}: KY_3F_{10}; colloids; HTMW treatment; NIR fluorescence quenching, first biological window.