Simulating photophysical properties of real-size nanoparticles containing lanthanide ions

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The understanding of the photophysical interactions underlying the luminescence phenomena for lanthanide-based materials is a tough task due to the complex energy transfer pathways and the challenge of determining lanthanide ion (Ln^{3+}) distribution within real-sized nanoparticles. In this lecture, the audience will be in contact with these issues and new methods for a computational framework development to simulate the doping process and map extensive interactions throughout complete real-size nanoparticle structures. By utilizing crystallographic data and custom computational codes for calculations of radiative and non-radiative rates, we can design accurate structural models of various geometries, including core-shell systems, to extract Ln^{3+}-Ln^{3+} distance distributions and its interactions. Furthermore, the dynamics of populations of 4f-levels are estimated and it enables the calculations of relative intensities and emission quantum yields. This new modeling protocol incorporates theories to calculate radiative and non-radiative rates, such as energy transfer and multiphonon relaxation [1,2]. These tools could provide reliable predictions to optimize the performance of Ln^{3+}-doped materials for applications in bioimaging, sensing, and photonics.

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[2] T. Miyakawa, D.L. Dexter, (1970) Phys. Rev. B, 1, 2961–2969.

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