Modeling energy transfer rates between lanthanides and transition metal ions in luminescent bimetallic complexes

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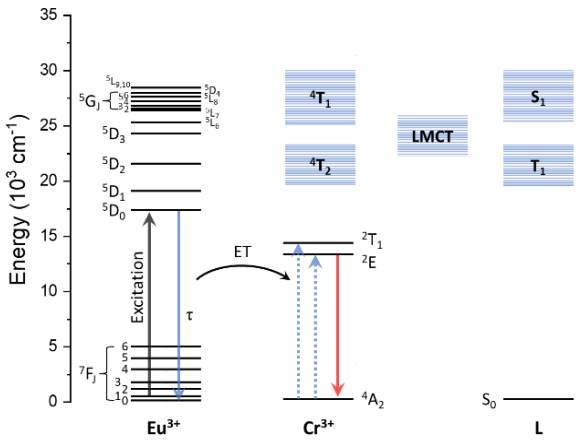
Luminescent lanthanide compounds have many applications as long as they have chromophores that absorb at longer wavelengths and present the necessary requirements to act as good sensitizers.Transition metals (M) are relevant chromophores because of their spectral features. Thus, many bimetallic complexes M-Ln^{3+} have been synthesized and investigated. However, despite the importance of theoretical models for developing more efficient M-Ln^{3+} complexes, few works have devoted efforts to elucidating the energy transfer process (ET) between M and Ln^{3+} ions. In this context in this seminar I will present the first efforts toward calculating the theoretical rates of energy transfer between M and Ln^{3+} ions, in heterometallic complexes, based on an adaptation of the energy transfer models previuosly developed for the case of lanthanide materials. As a case study the proposed model can estimate ET rates between Eu^{3+} and Cr^{3+} ions in the $[CrEuL_3]^{6+}$ complex (where L = 2-{6-[N,N-diethylcarboxamido]pyridin-2-yl}-1,1'-dimethyl-5,5'-methylene-2'-(5-methylpyridin-2-yl)bis[1H-benzimidazole]). The calculated rates (930 –1200 s^{-1}) are in excellent agreement with the experimental available data (750 – 1200 s^{-1}). This agreement is achieved by considering the pioneering treatment of phonon-assisted ET processes based on the Miyakawa-Dexter model. In this way the present model gets a more general character, and may be useful in describing photophysical properties driven by energy transfer between Ln^{3+} and transition metal ions.



Schematic energy levels diagram illustrating the Eu^{3+}, Cr^{3+} and the Ligand levels for the $[CrEuL_3]^{6+}$ complex and the energy transfer (ET) pathway.