COMPUTATIONAL MODELLING OF Eu^{III}-BASED DOWN-SHIFTING SPECTRAL CONVERTERS FOR NOVEL SOLAR CELL TECHNOLOGIES

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Photovoltaic (PV) devices that directly convert sunlight into electricity are a key factor in the transition to a green economy. The main problem in the massive use of PV devices is their low efficiency due to the mismatch between the incoming solar spectrum and the absorption profile of the cell. PV cells performance can be improved by using spectral converters, materials that absorb the solar radiation and reemit it as photons with a wavelength in the range of maximal absorption by the PV cells. Due to their intense emission in the silicon bandgap region, Eu^{III} complexes (Fig. 1) have been proposed as down-shifting spectral converters to absorb the high-energy part of the solar spectrum and convert it to a wavelength range for optimal absorption in silicon-based PV cells.

Eu^{III} complexes have relatively low absorption coefficients in the spectral region of interest for photovoltaic applications, but their performance can be improved using the so-called antenna ligands that can act as sensitizers. The luminescence process in a Eu^{III} complex (Fig. 2) occurs in four different stages: 1) high-energy photon absorption by the antenna ligand, 2) efficient energy conversion from the lowest excited singlet state S_1 to the lowest triplet T_1 of the ligand (inter-system crossing), 3) energy transfer from T_1 to the emitting excited state of the Eu^{III} cation, and finally, 4) reemission of photons by the cation in the desired wavelength.

In this presentation we will discuss our results for a family of Eu^{III} complexes with different ligands.[1] Using different levels of theory for the calculations, including Time-Dependent Density Functional Theory (*TD-DFT)*, semiempirical methods, and the Sparkle model implemented in the *Lanthanide Luminescence* software (LUMPAC), we studied the antenna effect to characterize the photophysical processes involved in the conversion process and unravel the key factors for the design of novel spectral converters with enhanced efficiencies. [2]

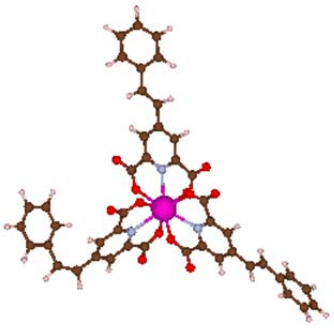

Figure 1. Example of a tridentate Eu^{III} complex studied in this work.

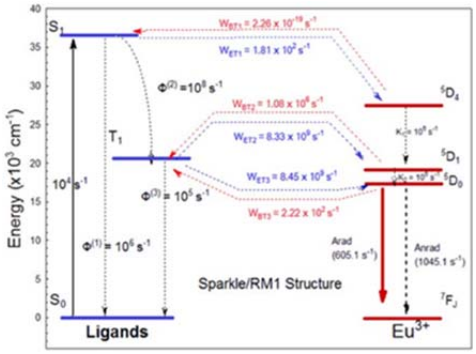

Figure 2. Jablonski diagram with the principal photophysical properties of an Eu^{III} complex with organic ligands. Figure taken from ref. [2]

[1] M. Latva, H. Takalo, et al. *J. Lumin*. **1997**, 75, 149-169.

[2] Dutra L.D.L, Thiago, T.D.B; Freire R. *J. Comp. Chem*, **2014**, 35, 772-775.