Modeling energy transfer-driven lanthanide-based luminescent thermometers

Albano N. Carneiro Neto,[1,*] Carlos D.S. Brites,[1] L. D. Carlos,[1]
[1] Department of Physics and CICECO – Aveiro Institute of Materials, University of Aveiro, 3810-193 Aveiro, Portugal
e-mail: albanoneto@ua.pt

Luminescent thermometers using trivalent lanthanide ions (Ln^{3+}) have gained significant interest for their applications in electronics and medicine, specifically for measuring local temperature [1]. While the thermometric properties can be well-characterized through measurements [2], these properties are typically determined after the synthesis of the material. To overcome this trial-and-error approach, theoretical calculations can offer a smarter design for new luminescent Ln-based thermometers. One such theoretical framework is the application of Boltzmann statistics in thermally coupled levels, which enables the development of single ion thermometers [3].

Regarding thermometric properties of dual-emitting centers, recent advancements in the theoretical modeling of Ln^{3+} intensities as they relate to temperature will be presented. Additionally, it will be discussed how the energy transfer involving Ln^{3+} ions (ligand-to-Ln^{3+} and Ln^{3+}-to-Ln^{3+}) can describe thermometric parameters Δ and the relative thermal sensitivity $S_r = \Delta^{-1}\left|\frac{\partial \Delta}{\partial T}\right|$ (where Δ represents the ratio between two different Ln^{3+} intensities) in energy transfer-driven lanthanide-based thermometers. These parameters can be determined with great accuracy and alignment to experimental results (Fig. 1) [4].

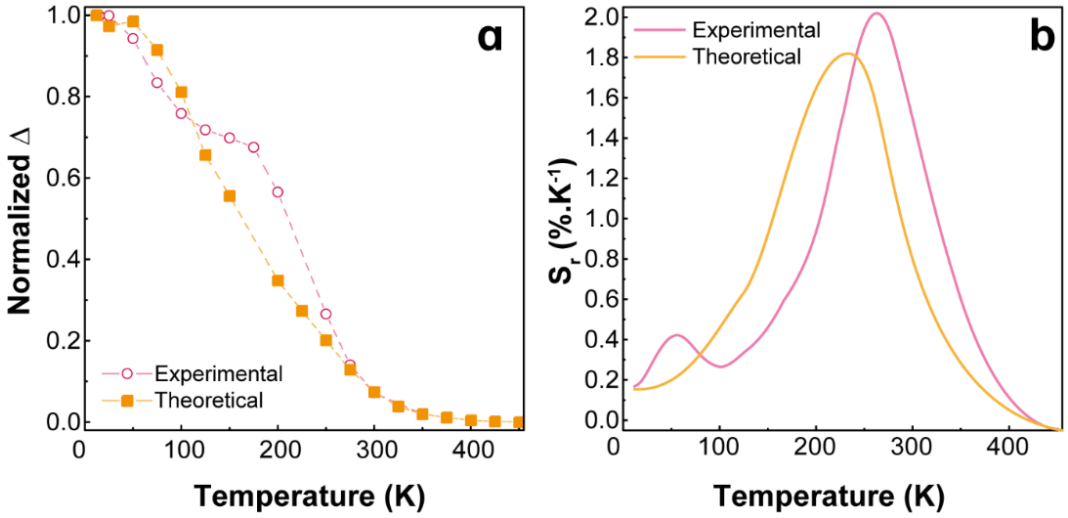

Fig. 1. Temperature dependence of the (a) thermometric parameters and (b) relative thermal sensitivity as a function of the temperature for $[Tb_{0.94}Eu_{0.06}(bpy)_2(NO_3)_3]$ (bpy = 2,2'-bipydine) complex [4].

References

[1] A. Bednarkiewicz, L. Marciniak, L.D. Carlos, D. Jaque, *Nanoscale* **12** (2020) 14405.
[2] C.D.S. Brites, A. Millán, L.D. Carlos, *in: J.-C.G. Bünzli, V.K. Pecharsky (Eds.), Handb. Phys. Chem. Rare Earths, Vol. 49, Elsevier*, **2016**.
[3] M. Suta, A. Meijerink, *Adv. Theory Simulations*. **3** (2020) 2000176.
[4] A.N. Carneiro Neto, E. Mamontova, A.M.P. Botas, C.D.S. Brites, R.A.S. Ferreira, J. Rouquette, Y. Guari, J. Larionova, J. Long, L.D. Carlos, *Adv. Opt. Mater.* **10** (2022) 2101870.