Development and applications of the LFDFT: the non-empirical calculation of ligand field and the simulation of the $f-d$ transitions by Density Functional Theory

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Fig. S1 Calculated multiplet energy levels of the 4f\(^7\) (in red) and the 4f\(^6\)5d\(^1\) (in blue) electron configurations of Eu\(^{2+}\) doped into CaF\(_2\), together with the calculated oscillator strength obtained for the transitions the 4f\(^7\) (5S\(_{7/2}\)) - 4f\(^6\)5d\(^1\) (in black). Inset: comparison between the theoretical results (i.e. zero phonon lines (in black) and the superposition of a Gaussian with a width of 500 cm\(^{-1}\) on the zero phonon lines (in green)) and the excitation spectrum (in magenta) reproduced from ref. [G. W. Burdick, A. Burdick, V. Deev, C.-K. Duan and M. F. Reid, *J. Lumin.*, 2005, 118, 205.]
Fig. S2 Calculated multiplet energy levels of the $4f^7$ (in red) and the $4f^6d^1$ (in blue) electron configurations of Eu$^{2+}$ doped into SrCl$_2$, together with the calculated oscillator strength obtained for the transitions the $4f^7 (^8S_7/2) - 4f^6d^1$ (in black). Inset: comparison between the theoretical results (i.e. zero phonon lines (in black) and the superposition of a Gaussian with a width of 500 cm$^{-1}$ on the zero phonon lines (in green)) and the excitation spectrum (in magenta) reproduced from ref. [Z. Pan, L. Ning, B.-M. Cheng and P. A. Tanner, Chem. Phys. Lett., 2006, 428, 78.]