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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Electronic Supplementary Information (ESI): 3 pages.

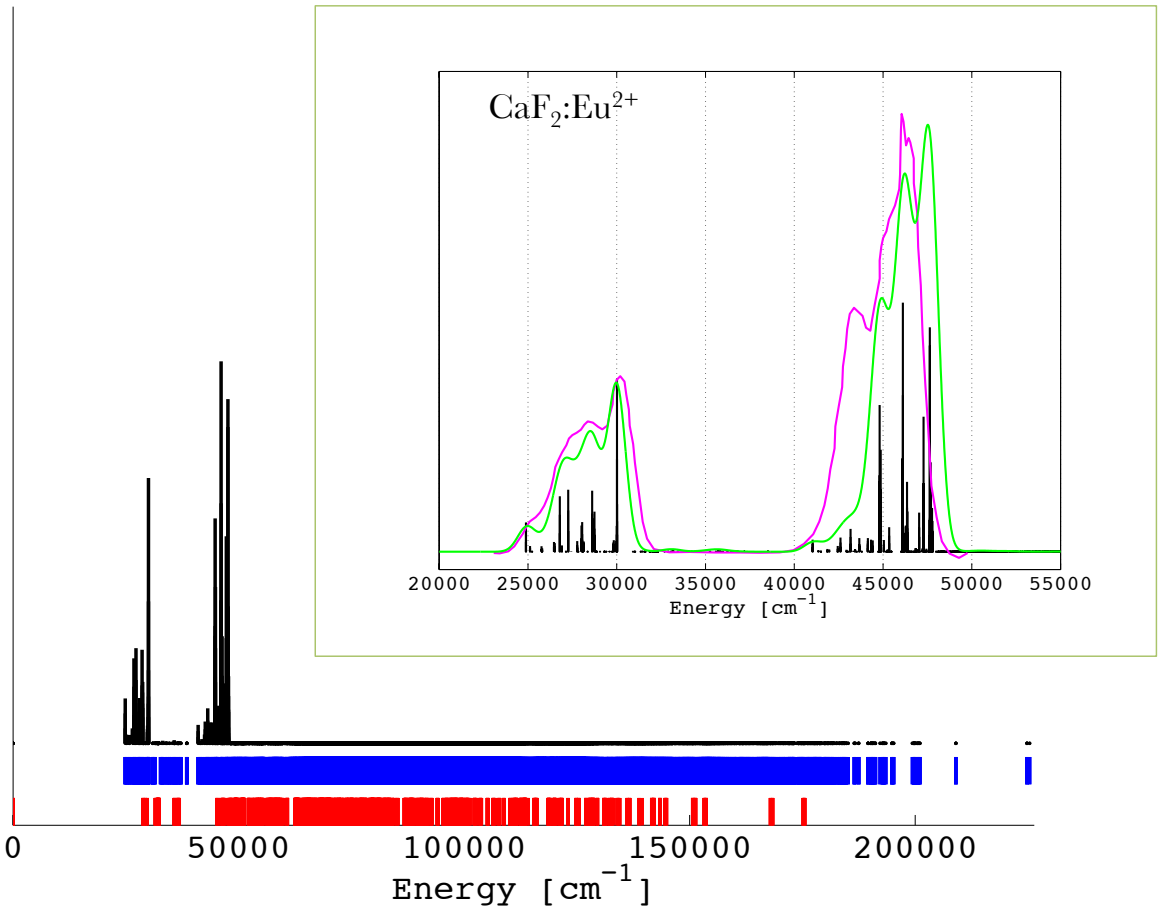

Fig. S1 Calculated multiplet energy levels of the $4f^7$ (in red) and the $4f^65d^1$ (in blue) electron configurations of Eu^{2+} doped into CaF_2, together with the calculated oscillator strength obtained for the transitions the $4f^7$ ($^8S_{7/2}$) - $4f^65d^1$ (in black). Inset: comparison between 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.]

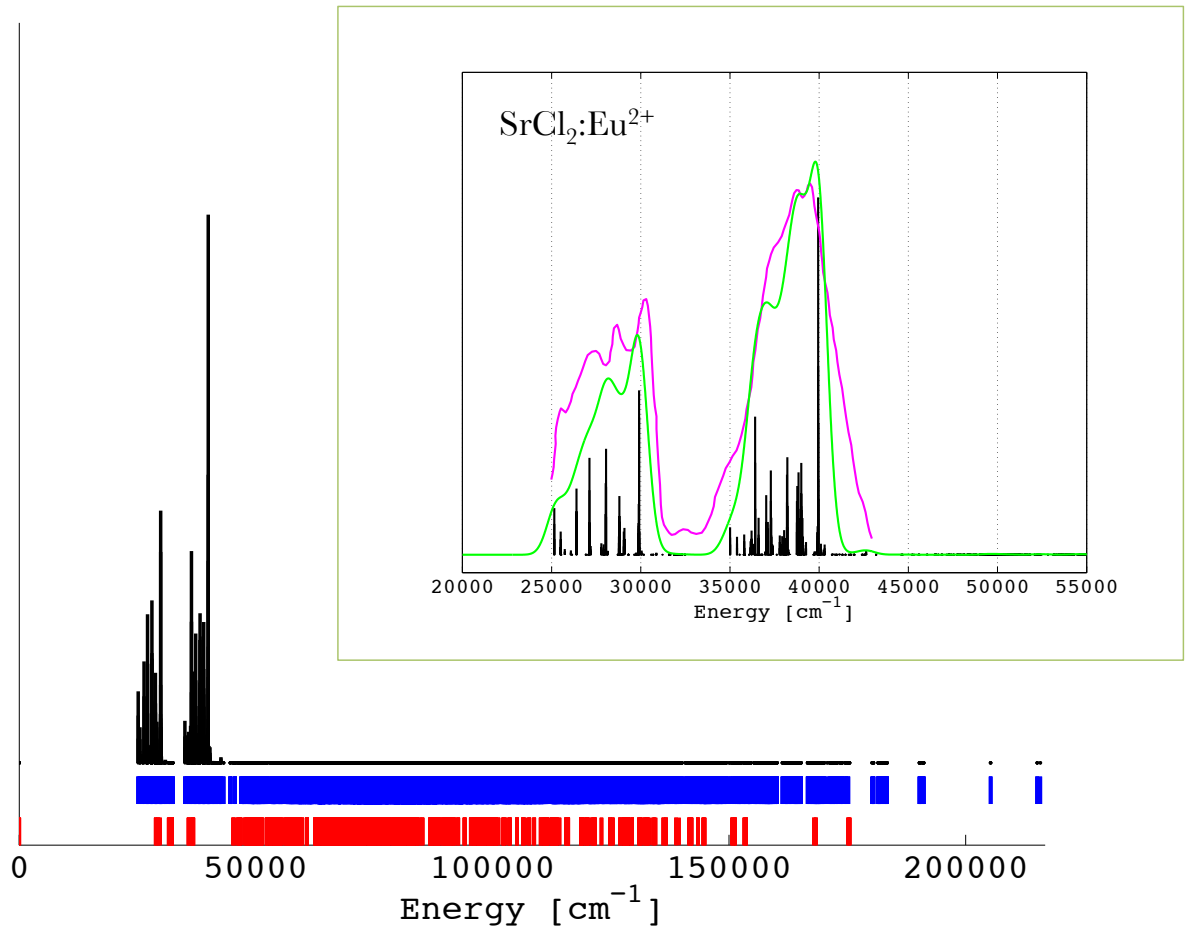

Fig. S2 Calculated multiplet energy levels of the $4f^7$ (in red) and the $4f^65d^1$ (in blue) electron configurations of Eu^{2+} doped into $SrCl_2$, together with the calculated oscillator strength obtained for the transitions the $4f^7$ ($^8S_{7/2}$) - $4f^65d^1$ (in black). Inset: comparison between 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.]