

## **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**

**Harry Ramanantoanina<sup>a\*</sup>, Mohammed Sahnoun<sup>b</sup>, Andrea Barbiero<sup>a</sup>, Marilena Ferbinteanu<sup>c</sup>  
and Fanica Cimpoesu<sup>d\*</sup>**

<sup>a</sup> *Department of Chemistry of the University of Fribourg (Switzerland), Chemin du Musée 9, 1700 Fribourg, Switzerland, Fax: +41 26 300 9738; Tel: +41 26 300 8700; E-mail: harry.ra@hotmail.com*

<sup>b</sup> *Laboratoire de physique de la matière et modélisation mathématique, LPQ3M, Université de Mascara, Algeria*

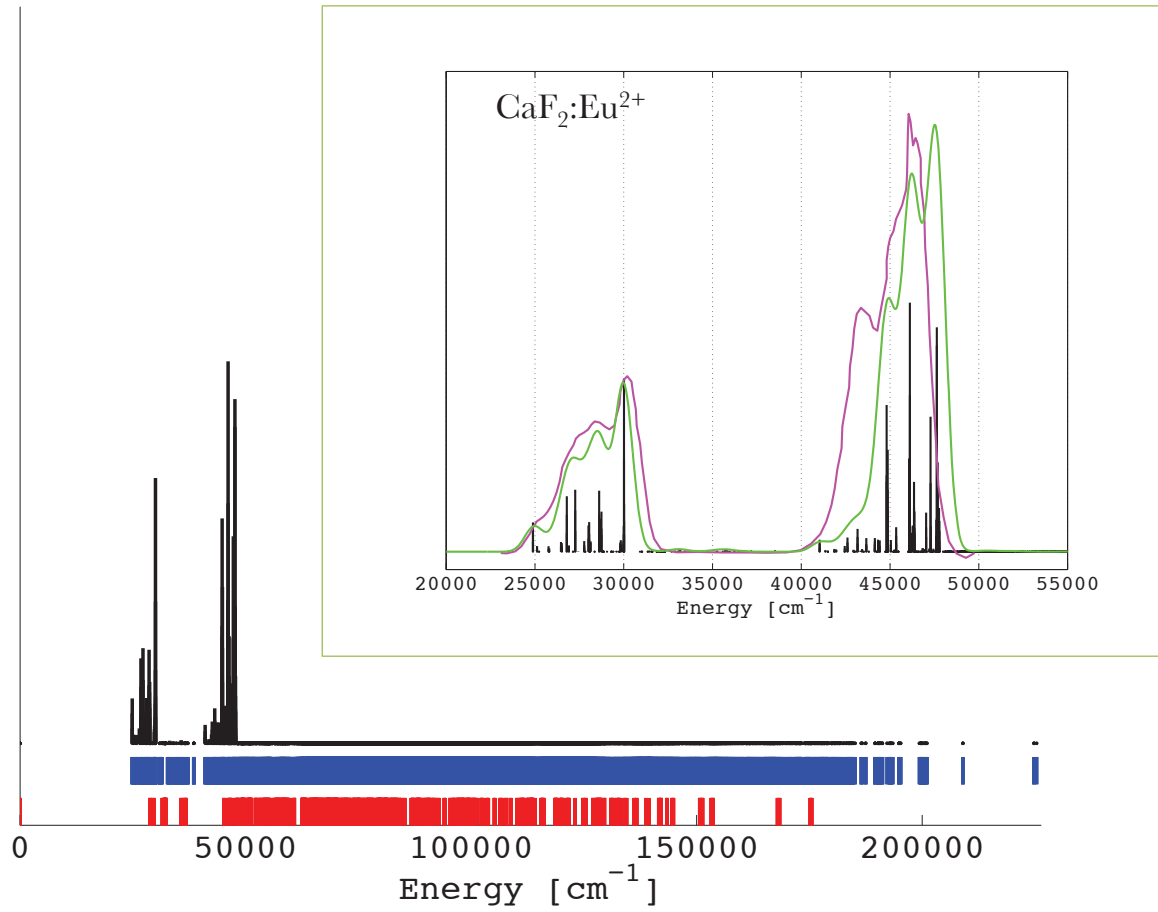
<sup>c</sup> *Faculty of Chemistry, Inorganic Chemistry Department, University of Bucharest, Dumbrova Rosie 23, Bucharest 0206462, Romania*

<sup>d</sup> *Institute of Physical Chemistry, Splaiul Independentei 202, Bucharest 060021, Romania; E-mail: cfanica@yahoo.com*

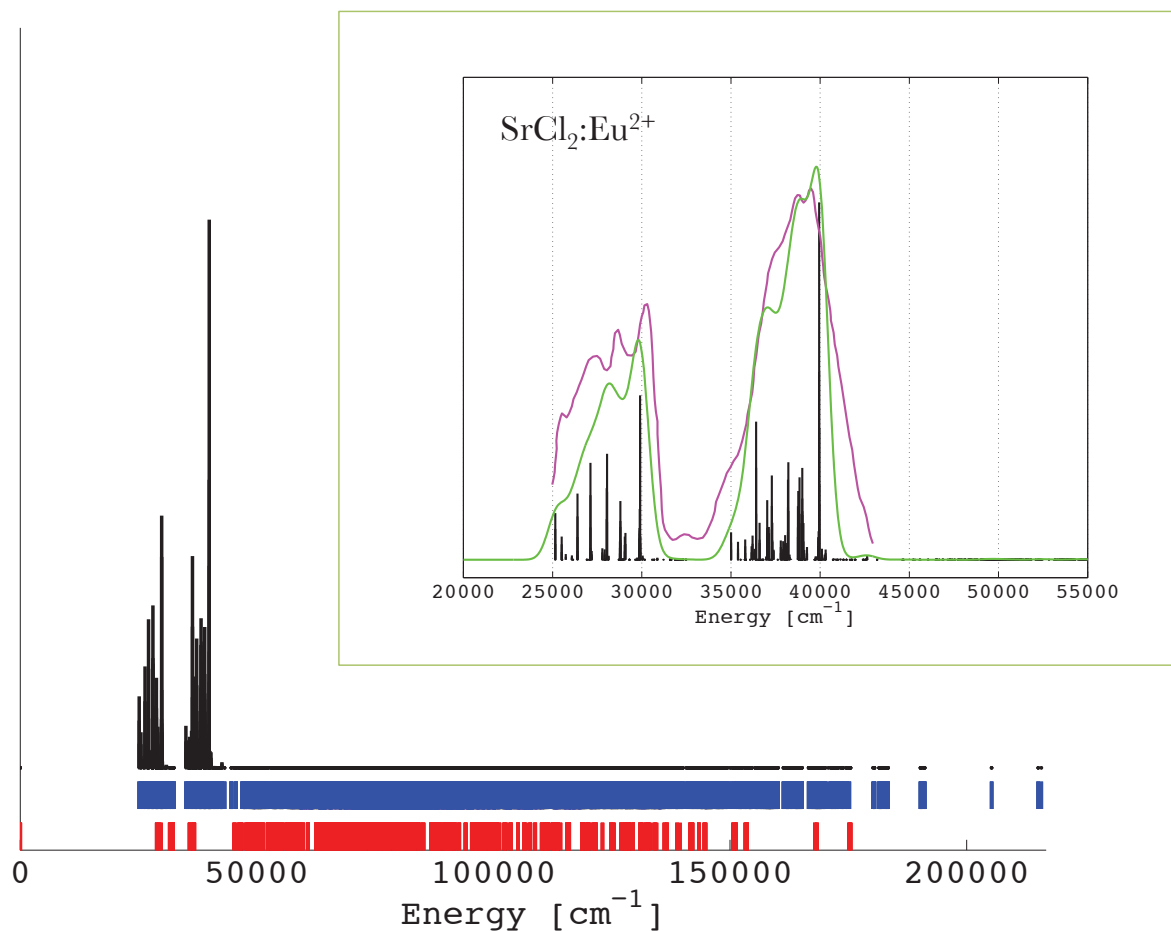
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**Electronic Supplementary Information (ESI): 3 pages.**

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**Fig. S1** Calculated multiplet energy levels of the  $4f^7$  (in red) and the  $4f^65d^1$  (in blue) electron configurations of  $\text{Eu}^{2+}$  doped into  $\text{CaF}_2$ , 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  $500 \text{ cm}^{-1}$  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  $\text{Eu}^{2+}$  doped into  $\text{SrCl}_2$ , 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  $500\text{ cm}^{-1}$  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.]