Di-cyclo nonatetraenyl Europium (II) [(η9-C_9H_9)$_2$]Eu Complexes: Structural Properties, Electronic Structure and Photoluminescence

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The electronic structure calculation of Eu complexes is a tremendous interest, as nowadays Eu^{2+} ion is becoming more and more crucial, for instance in lighting technologies. For this, the ligand-field density-functional theory (LFDFT) [1-3] method that is recently available in the Amsterdam Modelling Suite was applied. In this work, we present the theoretical study of the molecular Eu(η$_9$-C_9H_9)$_2$ complex and its underlying photoluminescence properties with respect to the Eu *4f – 5d* electron transitions. We model the excitation and emission spectra with good agreement with the experiments, opening up the possibility of modeling lanthanides in complex environment like nanomaterials by means of LFDFT at much-reduced computational resources and cost. The LFDFT method provides good photoluminescence results of Eu^{2+}-compounds. Purely based on a structural input, the Eu *4f – 5d* excitation and *5d – 4f* emission spectra are calculated with good agreement with the experiments. The geometries of the D9d and D9h structures are investigated and related to a thermodynamic quasi-equilibrium of the two structures.[4]

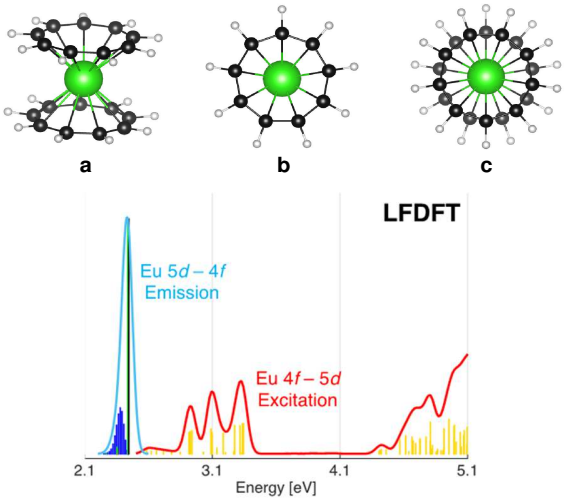

Fig.1. Graphical representations of the calculated excitation spectra of the molecular Eu(η$_9$-C_9H_9)^2 complex as function of the photon energy (in eV). Ball-and-stick model of the molecular Eu complex **(a)** showing the structures that belong to the D_9h (b) and D_9d (c) point groups from the top view. Color code: Eu (in green), C (in black) and H (in grey).

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