

Electron transfer processes in lanthanide doped materials: Insights from multiconfigurational calculations

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Lanthanide ions are notorious for their ability to change oxidation state. This manifests itself in the presence of low-lying excited states, so-called charge-transfer states (CTS), where an electron is transferred between the lanthanide dopant and another center in the luminescent material. Well-known are the ligand-to-metal charge transfer (LMCT) states of Eu^{3+} -doped materials in the near-UV that enable the use of these materials in e.g. fluorescent lamps thanks to their high absorbance for the 254 nm mercury emission [1].

In many other cases, electron transfer processes are held responsible for various phenomena, e.g. thermal quenching of luminescence, persistent luminescence, ... These assignments are not seldom done in the context of empirical energy levels schemes [2]. While this strategy allows a quick comparison between different materials and the exploitation of systematic behavior, important details unavoidably remain elusive in individual cases [3]. It is here where *ab initio* calculations are an indispensable complement to experimental studies.

In a general introduction to *ab initio* calculations, the choice for multiconfigurational techniques is motivated [4]. Subsequently, several examples of electron transfer processes between distinct lanthanide centers in crystalline solids are given. In all cases, diabatic electron transfer diagrams are constructed from first principles and used for the interpretation of experimental results [5].

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