Defects and charge carriers trapping in Lu_2O_3:Ln,M energy storage and persistent luminescence phosphors – an ab initio perspective

In a typical photoluminescence process, a particular specie (an atom or a molecule) is excited from its lowest-energy form – the ground state – to a form of higher energy, an excited state. Next, the specie minimizes its energy and returns to the ground state, while the spare energy is released in a form of photon. Another way to look at such process is that, on excitation, an electron is moved from its lowest energy level to some of the higher levels, and then goes back with a release of a photon. In a solid, the matter becomes more complicated, as there are enormous amounts of energy levels that form bands. Some of the bands (of lower energies) are filled with electrons, while some other (of higher energies) are empty. Group of those filled bands is called valence band, while the group of empty bands is called conduction band. As the states in valence band are filled, charge carriers cannot move freely among them. On contrary, an electron in conduction band has many free states to choose from. An electron excited to conduction band might travel a lot along the material until it relaxes back to valence band – and this is where the defects come in play.

Imagine an empty state in between valence and conduction band. An excited electron can relax to such a state, but it cannot move anymore, as there are no other states of similar energies. Such phenomenon is called carrier trapping. A trapped electron can be released by a portion of energy sufficient enough to excite it back to conduction band. Careful design of carrier traps using small portions of particular chemicals (dopants) can result in delay of the excited electrons in the trap states and, consequently, in very long luminescence lifetimes. Furthermore, some materials can be kept in an excited state as long as it is required – until a certain stimulation (e.g. laser light) is applied to release the carriers.

The essence of this project is analysis (using high quality quantum mechanical calculations) of different traps in lutetium oxide, Lu_2O_3 that can be created via addition of s-, d- and f-metals, such as Ca, Sr, Ti, Zr, Hf, V, Ta, Tb, Pr and other. The plan is to use faster and less precise calculations to optimize geometries of various structures with defects, and then use high-precision methods do analyze electronic structure. The purpose it to clarify, how particular defects and dopants are responsible for the trap states, and how deep the traps are. Such knowledge is required for better understatement of long-lasting (persistent) luminescence and energy storage, for improvement of phosphors and search for new materials and applications.