Activator – Ligand Interactions in Luminescent Materials for LEDs

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For Luminescence Conversion LEDs high brightness blue light emitting diodes based on Group III-nitride materials can be used [1]. The light source works as an efficient pump exciting a luminescent material which returns to its ground state by emitting green, yellow, or red light. The principle of this down conversion is well-founded in the pronounced Stokes Shift between absorption and emission of electromagnetic radiation.

Suitable luminescent materials for such color conversion in LEDs must show the following properties: (a) high absorption of the blue pump light, (b) high quantum efficiency, (c) short emission decay time, (d) high quenching temperature of emission, and (e) high thermal and (photo)chemical stability. The most promising activators to fulfill these requirements are Ce^{3+} and Eu^{2+}, both showing 5d --> 4f broad band emission. For example, the most efficient phosphor currently used in white LEDs is yellow emitting $Y_{3-x}Gd_xAl_{5-y}Ga_yO_{12}:Ce^{3+}$ [2]. Alternatively, a combination of green emitting $SrGa_2S_4:Eu^{2+}$ and orange emitting $SrS:Eu^{2+}$ can be used for a trichromatic design with improved efficiency and color rendering [3].

Since the spectral position of the 5d --> 4f transition of Ce^{3+} and Eu^{2+} is strongly host lattice dependent, the excitation and emission characteristics of these activators are determined by the chemical nature and symmetry of their surroundings. Fig. 1 shows a simplified representation of the orbital interactions between the activator M and the ligands L. The energy difference between the f block levels and the low lying d block levels correlates with the absorption properties of the activator.

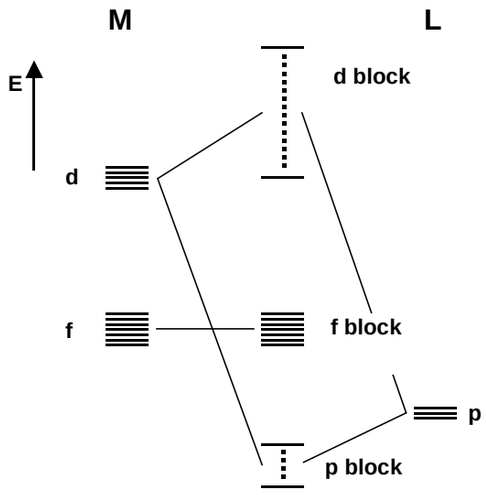

Fig. 1: Schematic representation of the orbital interaction between the activator metal (M) d- and f-orbitals and ligand (L) p-orbitals

In order to study the relationships between the electronic and crystal structures of the host lattice and the resulting luminescence properties of the activator in more detail, electronic structure calculations were carried out for various Eu^{2+} doped host lattices within the tight binding approximation. For this purpose anionic model complexes based on known crystal structures were used including the second coordination sphere of the activator ion.

In this presentation we will discuss the results of our electronic structure calculations of the activator – ligand interactions and elucidate the parameters that determine the luminescence properties of a given Eu^{2+} or Ce^{3+} doped material useful for Luminescence Conversion LEDs.

[1] S. Nakamura et al., *Appl. Phys. Lett.* **67** (1995) 1868
[2] Y. Shimizu et al. US Patent 5998925 (1999)
[3] R. Mueller-Mach, G.O. Mueller, in *Proc. SPIE, Light-Emitting Diodes: Research, Manufacturing, and Applications IV*, Vol. 3938, p.30

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