

Energy level modeling of lanthanide defects in SrAl₂O₄

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Lanthanide ions form an important class of optical dopants in a wide variety of materials used in modern photonic devices. Everyday examples are the Ce³⁺ and Eu²⁺ based conversion phosphors used to build white LEDs and Er³⁺ based infrared lasers for telecommunication [1].

Energy level schemes offer a natural connection between the electronic structure of materials and their spectroscopic properties. During the last decades, empirical methods and relationships were devised for constructing energy level schemes of lanthanide defects in wide band gap solids [2].

These simple techniques allow to locate the charge-state transition levels as well as the excited 5d levels of all 14 lanthanide ions with respect to the host's valence and conduction bands with only limited experimental input. These energy level schemes offer a lot of information on optical and electronic properties. The features in the absorption and excitation spectra of the luminescent materials can be determined from location of absorption bands, both originating from interconfigurational 4f^N-4f^{N-1}5d¹ transitions as well as charge transfer transitions [2].

In this talk, the empirical energy level models for lanthanides will be introduced and applied to the luminescent material SrAl₂O₄:Eu²⁺. Co-doped with Dy³⁺, this material features a strong green afterglow, well-known from emergency signalization and a lot of different gadgets [3].

Although this phenomenon was discovered in the 1990's, the exact mechanism of the energy storage is not yet completely resolved. The delayed light emission of the persistent luminescence is thought to be the consequence of the temporary trapping of charge carriers after photoionization of the Eu²⁺ ion. The exact nature of the trapping centers as well as the role of the Dy³⁺ ion is not clear [3].

To resolve these issues, energy level modeling of the lanthanide defects can be an interesting tool to get a deeper understanding on the incorporation of the lanthanide ions as well as their possibilities to capture charge carriers.

On the other hand, the SrAl₂O₄ host poses a specific challenge for the empirical energy level modeling as two nonequivalent defects are expected due to incorporation on two different Sr sites in the crystal structure [4]. To enable the construction of a realistic energy level scheme for this material, the conventional energy level model is extended to accommodate materials in which two – or more – nonequivalent lanthanide defects exist. This obviously requires site-selective spectroscopy. In the case of SrAl₂O₄:Eu²⁺, we show that a blue emission band which only appears at sufficiently low temperature can be related to the second type of europium defect [4].

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