Contribution ID: **312** Type: **Poster Presentation**

4fN energy level schemes for the di-, tri-, and tetravalent lanthanides

Thursday, 28 June 2018 15:00 (2 hours)

Since the refinement of the famous Dieke diagram (DD) [1] to include all higher energy levels, not much progress has been made in this field. It is now clear, though, that the purely theoretical methods have still a long way to go to yield the 4fN (or 5fN) energy levels in any accuracy. This is because the new applications, e.g. up- and down-conversion, require energy levels that are ever more accurate. In fact, these processes are the most efficient when quasi-resonant condition is reached. The proven phenomenological methods to calculate the energy level schemes (and wave functions required by many applications) are still the most reliable, accurate and fastest way. Unfortunately, some of the published data [2] are so inaccurate that they are of little or no use. In this work, the energy level schemes for the di-, tri-, and tetravalent lanthanides were calculated taking into account the crystal field effects as well. The effect of the host was synchronised for both the R2+ and R3+ series by the use of isomorphic crystal structures (BaFCl and ROCl, respectively) facilitating the comparison between them. Utmost care was taken to compare the calculated data with the experimental one which was easy for the R3+ but much more scarce for the R2+ series. For the RIV series, experimental data is virtually inexistent. The energy level schemes for the R3+ are the most useful ones whilst the 4fN levels of the R2+ series are often masked in practice by the low-energy 4fN-15d1 configuration. The 4fN levels of the RIV series are practically inaccessible because of the low-energy charge transfer transitions and the initial low-energy positions of the 4fN levels of RIV species.

References
[1] R.H.T. Wegh, A. Meijerink, R.-J. Lamminmäki, J. Hölsä, J. Lumin. 87-89 (2000) 1002.
[2] C.-G. Ma, M.G. Brik, D.-X. Liu, B. Feng, Ya Tian, A. Suchocki, J. Lumin. 170 (2016) 369.

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Session Classification: Poster Session 2

Track Classification: Track A - Physics of Condensed Matter and Materials