

**ELECTRONIC STRUCTURE AND MAGNETIC ANISOTROPY
IN F-BLOCK MOLECULAR NANOMAGNETS**J. J. Baldoví^a, E. Lucaccini,^b A. Gaita-Ariño,^c L. Sorace^b and E. Coronado^c^a Nano-Bio Spectroscopy Group, Universidad del País Vasco CFM CSIC-UPV/EHU-MPC & DIPC, Av. Tolosa 72, 20018 San Sebastián, Spain^b Department of Chemistry "U.Schiff" and UdR INSTM, Università degli Studi di Firenze, Via della Lastruccia 3-13, 50019 Sesto Fiorentino (FI), Italy^c Instituto de Ciencia Molecular, Universidad de Valencia, C/Catedrático José Beltrán 2, Paterna E-46980, Spain

Owing to their attractive physical properties and novel quantum phenomena arising from their chemical nature, lanthanide single-ion magnets (SIMs) have excited a large number of researchers working in molecular magnetism. [1] These systems have been proposed as encouraging candidates for the development of high-density magnetic memories, magnetic refrigeration, quantum computing devices and several applications in molecular spintronics [2]. Nevertheless, any future technological realization is subordinate to a profound understanding of their static and dynamic behaviour, which still remains an open problem. From an experimental point of view, the combination of spectroscopic and magnetic data is the only way to obtain a detailed description of their electronic structure and magnetic anisotropy, via the phenomenological determination of the symmetry-allowed crystal-field parameters (CFPs). From a theoretical point of view, the CFPs can be estimated using the real structure of the compounds and then benchmarked against the experiment. These predictive methods include Complete Active Space *ab initio* calculations [3] and effective electrostatic models, such as the semi-empirical Radial Effective Charge (REC) model [4].

In this contribution, we deal with both perspectives presented above. On the one hand, we simulate the electronic structure and magnetic properties of the Ln(trensal) family, (where H₃trensal is = 2,2',2''-Tris-(salicylideneimino)triethylamine) by combining spectroscopic and thermodynamic magnetic data, i.e. following a purely phenomenological approach. Subsequently, the determined CFPs are used as starting point to reproduce the magnetic data of a new family of lanthanide complexes, Ln(trenovan) (where H₃trenovan = tris(((3-methoxysalicylidene)amino)ethyl)amine), which only differs in a methoxy-substituted position on the ligand, from the Ln(trensal) family. [5] On the other hand, we concern the possible synergies between the different theoretical models, discussing how we can exploit their complementarity in order to help as starting point in the rationalization of the electronic structure and magnetic anisotropy of f-block molecular nanomagnets. [6]

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