Contribution ID : **7** Type : **Poster**

Theoretical Study of a Family of Lanthanoid-Dioxolene Single-Molecule Magnets

Monday, 19 November 2018 11:30 (20)

Lanthanoid Single-Molecule Magnets (SMMs) are molecular materials that exhibit slow relaxation of the magnetization of molecular origin, thus making them promising targets for the development of spintronic devices and molecular memories. Since the electronic and magnetic properties of lanthanoid-based SMMs are strongly dependent on the characteristics of the electrostatic crystal field induced by the ligands on the lanthanoid ion, a thorough understanding of such magneto-structural correlations is crucial to develop molecules displaying SMM behavior at sufficiently high temperatures to warrant commercial applications. For this reason, ab initio calculations have proven to be valuable tools to elucidate the details of the electronic structure of SMMs and improve the understanding of their effect on magnetic properties and relaxation mechanisms.

In this work, we have performed a set of ab initio calculations on the family of molecules [Ln(bpy)2(Cl4Cat)(Cl4CatH)(MeOH)] (Ln = Tb, Dy, Ho), employing the CASSCF/RASSI-SO method, and we have compared the predicted electronic and magnetic properties with the experimental data. These molecules, recently synthesized, are expected to display SMM behavior due of their structural similarity to other SMMs previously described in literature, with their low-lying energy spectrum determined with Inelastic Neutron Scattering (INS) for Ln = Tb, Ho. We show that there is a good agreement between computational and experimental results, thus confirming the validity of theoretical predictions of electronic and magnetic properties of lanthanoid-based SMMs.

Topic

Physics

Primary author(s) : Dr CALVELLO, Simone (The University of Melbourne, ANSTO); Dr SONCINI, Alessandro (The University of Melbourne)

Co-author(s) : Mr ATKIN, Aiden (The University of Melbourne); Dr MOLE, Richard (ANSTO); Dr BOSKOVIC, Colette (University of Melbourne)

Presenter(s) : Dr CALVELLO, Simone (The University of Melbourne, ANSTO)

Session Classification : Topical Session 1: Advanced Materials

Track Classification : Physics