Title	**Computational Design of Single-Molecule Magnetic Skyrmions**
PI	**SONCINI Alessandro**
Research Group	**Molecular Materials & Modeling (M3)**
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Project description:

Single Molecule Toroics (SMTs) are polynuclear complexes in which 3d/4f unpaired electrons can couple to form vortex magnetic configurations with a vanishingly small magnetic moment and a large *toroidal moment.* They are molecular versions of *magnetic skyrmions* found in ordered magnetic materials, topologically stable spin structures in which, by virtue of spin-chirality, spins can be flipped via electric fields, and the spin-polarization of spin currents can be rotated, opening new avenues to develop logic devices for a future generation of reduced power consumption molecualr computers. SMTs are also investigated as spin-qubits for quantum computation, where an open problem consists of devising a suitable experimental protocol to control the quantum dynamics of the toroidal moment.

The PhD project consists of the extension and application of computational modelling strategies impemented in a software (CERES) developed in our group, to achieve the following objectives:

- Identify magneto-structural correlations underlying stable toroidal states in polynuclear clusters, also via the development of Neural Networks trained via ab initio calculations and experimental data.
- Identify the signatures of molecular toroidal and skyrmionic states in magnetic resonance spectroscopies, and scattering (neutron and X-ray) experiments.
- Simulate the quantum dynamics of toroidal moments induced by microwave radiation pulses to identify a suitable protocol to (i) initialise toroidal states (ii) implement one and two-qubit gates on a toroidal computational basis.

The research will be carried out in collaboration with experimental groups in Europe and Australia.

Publications

1. A. Soncini, M. Piccardo (2022). Ab initio non-covalent crystal field theory for lanthanide complexes: a multiconfigurational non-orthogonal group function approach. PHYS CHEM CHEM PHYS, 24, 18915.
2. Gao C., Genoni A., Gao S., Jiang S., Soncini A., Overgaard J. (2020). Observation of the asphericity of 4f-electron density and its relation to the magnetic anisotropy axis in single-molecule magnets. NATURE CHEMISTRY, vol. 12, p. 213-219.
3. Calvello S., Piccardo M., Rao S. V., Soncini A. (2018). CERES: An ab initio code dedicated to the calculation of the electronic structure and magnetic properties of lanthanide complexes. JOURNAL OF COMPUTATIONAL CHEMISTRY, vol. 39, p. 328-337.
4. Crabtree J. M., Soncini A. (2018). Toroidal quantum states in molecular spin-frustrated triangular nanomagnets with weak spin-orbit coupling: Applications to molecular spintronics. PHYS. REV. B, 98,094417.
5. Vignesh K. R., Soncini A., Langley S. K., Wernsdorfer W., Murray K. S., Rajaraman G. (2017). Ferrotoroidic ground state in a heterometallic {$CrDy_6$} complex displaying slow magnetic relaxation. NATURE COMMUNICATIONS, vol. 8, 1023.

Hosting group(s) for the period abroad (tentative list, may change):

- Prof. Nick Chilton, School of Chemistry, University of Manchester (UK).
- Dr. Stu Langley, Adv. Mat. & Surface Eng. Research Centre, Manchester Metropolitan Univ. (UK).
- Dr. Elizaveta Suturina, Department of Chemistry, University of Bath (UK).