Research Projects in the Boskovic "Inorganic Molecular Materials" Group - 2019

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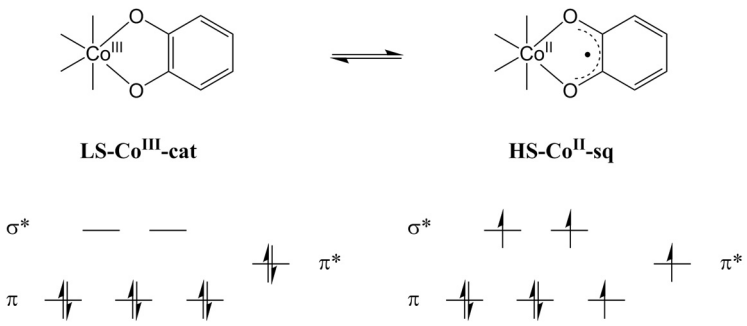
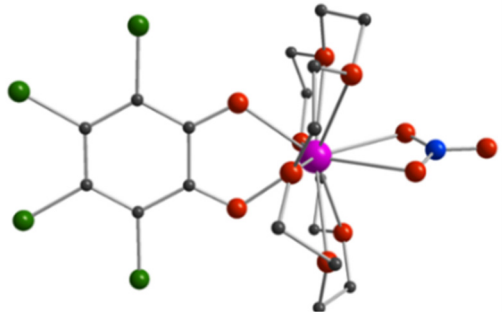
Molecular materials with physical properties that can be controlled by external parameters, such as temperature, light or magnetic field are important synthetic targets because they form the basis of molecular devices. The miniaturisation required by technological advances in electronics makes the demand for such nanoscale devices inevitable. Research in our group is focused on the exploration of different families of inorganic molecules that can display functionality arising from their electronic structure: single-molecule magnets (SMMs), valence tautomeric (VT), spin crossover (SCO) and redox-switchable complexes. We are particularly interested in complexes of *3d* and *4f* metals

Research in our group involves organic and inorganic synthesis, crystallisation and crystallography, electrochemistry, magnetic and photomagnetic studies, NMR and EPR spectroscopy and inelastic neutron scattering. We collaborate widely with numerous local and international collaborators, including for density functional theory and ab initio calculations on our compounds.

(1) Valence tautomerism.[1,2] Valence tautomerism involves stimulated intramolecular electron transfer between redox-active ligands and metals. The most common example is the thermally stimulated transition between low spin Co(III)-catecholate complexes and high spin Co(II)-semiquinonate complexes. Projects will involve investigation of discrete mono- and polynuclear Co complexes, as well as coordination polymers.



(2) Redox-activity/switchability in lanthanoid complexes.[3] We are investigating complexes of redox-active lanthanoid metals (Ce(III/IV), Eu(II/III), Yb(II/III) with redox-active ligands towards new redox switchable and valence tautomeric systems.



(3) Lanthanoid single-molecule magnets.[4] Single-molecule magnets are molecules that can retain magnetization at low temperature, as well as display magnetization quantum tunneling. Projects will focus on the investigation of how the lanthanoid(III) coordination environment correlates with the mechanisms of magnetisation relaxation.

(4) Inelastic neutron scattering of metal complexes.[5] We use INS at ANSTO to explore exchange interactions and lanthanoid crystal field splitting or transition metal zero-field splitting.

References

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(3) Fedushkin, I. L.; Maslova, O. V.; Morozov, A. G.; Dechert, S.; Demeshko, S.; Meyer, F. *Angew. Chem. Int. Ed. Engl.* **2012**, *51*, 10584.
(4) Rousset, E.; Piccardo, M.; Boulon, M.-E.; Gable, R.; Soncini, A.; Sorace, L.; Boskovic, C. *Chem. - A Eur. J.* **2018**, *24*, 14768.
(5) Vonci, M.; Giansiracusa, M. J.; Gable, R. W.; Van den Heuvel, W.; Moubaraki, B.; Murray, K. S.; Yu, D.; Mole, R. A.; Soncini, A.; Boskovic, C. *Inorg. Chem.* **2017**, *56*, 378.