



Contribution ID : 98

Type : Oral

## Elucidation of the electronic structure in lanthanoid-radical systems by inelastic neutron scattering

Wednesday, 24 November 2021 16:35 (15)

Single-molecule magnets (SMMs) are metal organic compounds which exhibit magnetic hysteresis and slow magnetic relaxation at low temperature. They have potential applications in high density data storage, quantum computing, and molecular spintronics. Coordination complexes of the trivalent lanthanoid (Ln(III)) ions are the current best performing SMMs, with examples showing hysteresis above liquid nitrogen temperature.[1]

The magnetic properties of Ln(III) ions stems from the crystal field (CF) splitting of the ground Russel-Saunders state. These CF states give rise to the energy barrier to reversal of magnetisation, and can be tuned by modification of the ligand environment around the Ln(III) centre. Slow magnetic relaxation in Ln-SMMs can also be modulated by the introduction of magnetic exchange coupling with another magnetic moment, such as that of an organic radical ligand.[2] Quantifying the magnitude of magnetic exchange coupling in many Ln(III) systems is, however, difficult using conventional magnetometric techniques, due to the often large spin-orbit coupling.

Inelastic neutron scattering (INS) is an ideal spectroscopic tool to measure both CF splitting and magnetic exchange coupling in Ln(III) systems.[3] We have used INS measurements to elucidate the magnetic exchange coupling and CF splitting in Ln(III)-semiquinonate complexes. Using this information we have rationalised the magnetic properties of these compounds, with the hope that a better understanding of the magnetic exchange in these systems can be used to design SMMs with improved performance.

[1] Guo et al. Science 2018, 362 (6421), 1400–1403

[2] Demir et al. Coord. Chem. Rev. 2015, 289–290, 149–176

[3] Dunstan et al. Eur. J. Inorg. Chem. 2019, 8, 1090–1105

### Level of Expertise

Student

### Presenter Gender

Woman

### Pronouns

She/Her

### Which facility did you use for your research

Australian Centre for Neutron Scattering

### Students Only - Are you interested in AINSE student funding

Yes

**Do you wish to take part in the Student Poster Slam**

No

**Condition of submission**

Yes

**Primary author(s) :** DUNSTAN, Maja (University of Melbourne); CALVELLO, Simone (The University of Melbourne); Prof. SONCINI, Alessandro (University of Melbourne); Dr KRAUSE-HEUER, Anwen (ANSTO); MOLE, Richard (ANSTO); BOSKOVIC, Colette (University of Melbourne)

**Presenter(s) :** DUNSTAN, Maja (University of Melbourne)

**Session Classification :** Chemistry, Soft Matter & Crystallography

**Track Classification :** Chemistry, Soft Matter & Crystallography