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Chemical Tailoring of Double Exchange in Mixed Valence Diiron Molecules

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Molecules are promising building blocks for future generations of functional materials. A particularly interesting niche are molecules that contain metal-ions in different oxidation states, since double exchange can contribute to the molecular magnetic properties in addition to conventional Heisenberg exchange. The most promising prospect coming from competition between these exchange mechanisms are molecules that switch from a low-spin to a high-spin ground state when an electric field is applied [1]. However, the mechanisms that govern double exchange in molecules are poorly understood and the full potential of mixed valence molecules is not realised.

We have studied a series diiron Fe^{II}/Fe^{III} molecules with S = 9/2 ground states using inelastic neutron scattering (INS) and high-field electron paramagnetic resonance (HF-EPR). These techniques probe the energies of spin excited states and the crystal field-induced splitting within the ground state manifold, respectively, giving complete information about the spin dynamics. Comparison of experiments with simulated INS and HF-EPR spectra, calculated from parametrised Hamiltonian models, allowed us to quantify the influence of bridge functionalisation and capping ligand chirality on the exchange and crystal field parameters. Thereby, we have shown the potential for INS and HF-EPR to collaboratively unveil the mechanisms governing double exchange in molecules.

[1] C. S. Bosch-Serrano *et al.*, *ChemPhysChem.*, 13, 2662 (2012)

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