

Dr. Irina Kühne

Department of Functional Materials, Division of Condensed Matter Physics

Applications of Mn(III) Spin Crossover Complexes

A Short Overview of my Research

The phenomenon of spin crossover in metal complexes is known since the early 1930s, and has since then attracted a lot of interest. Through their possible hysteretic effects, potential applications of these molecules include their use as molecular switches in data storage and in displays. At low temperatures, it is energetically favorable for spin crossover compounds to be in a low spin state, and by application of an external stimulus, such as heat, light, pressure or applied magnetic field, it is possible for the spins to occupy the energetically higher orbitals, resulting in a high-spin state of the molecule. While the SCO phenomenon is rather common in Fe(II), it is still quite rare in Mn(III). We have developed a ligand system that promotes SCO in Mn(III) and we have synthesized various Mn(III) complexes based salicylaldehyde Schiff base ligands using different substituents on the salicylaldehyde: (i) nitro groups in para- and ortho- position,[1] (ii) methoxy groups in the meta-position,[2] (iii) methyl groups in the ortho-position[3] and (iv) bulky naphthaldehyde groups [4]. We have investigated their different magnetic behavior and their structural features using also different counterions to understand this additional influence. Density Functional Theory calculations were able to correctly describe the energetics of intermediate spin/high spin transitions in the complexes.

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