MS22-02 | Elucidating the Mechanisms of Single Molecule Magnets using Diffraction Methods

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Single-molecule magnets (SMM) are special molecules, which are able to preserve an induced magnetization after the removal of an external magnetizing field. Such tiny magnets have potential technological applications in e.g. spin-based electronics. The functionality of these materials relies on strong magnetic anisotropy caused by orbital angular momentum. Both lanthanide-based [1] as well as more abundant transition-metal based SMMs exist, and the origin of the magnetic properties in the two types are slightly different. In this talk, I will show how X-ray and neutron diffraction studies of SMMs add valuable insight into the properties of SMMs.

Firstly, I will show selected results of experimental charge density (CD) studies of transition-metal based SMMs, from which we are able to extract quantitative magnetic properties such as that described using the zero-field splitting parameter. Secondly, I use CD studies of two dysprosium SMMs to experimentally confirm the predicted oblate shape of the valence density while also indicating the mixed nature of the ground state [2]. Finally, I will show how polarized neutron single crystal data can lead to quantitative knowledge of the local susceptibility tensor in related dysprosium-compounds [3].

[1] K. R. Meihaus, J. R. Long, *J. Am. Chem. Soc.* **2013**, *135*, 17952-17957.
[2] C. Gao, A. Genoni, S. Gao, A. Soncini, S.-D. Jiang, J. Overgaard, *submitted*.
[3] E. A. Klahn, C. Gao, B. Gillon, A. Gukasov, X. Fabreges, R. O. Piltz, S. D. Jiang, J. Overgaard, *Chemistry* **2018**, *24*, 16576-16581.