

## MA 26: Molecular Magnetism

Time: Wednesday 15:00–16:00

Location: H48

MA 26.1 Wed 15:00 H48

**Density functional theory studies of a Fe(II) spin-crossover complex** — ●GERALD KÄMMERER and PETER KRATZER — University Duisburg-Essen, Duisburg, Germany

We investigate the spin-state switching of a Fe(II) spin-crossover complex ( $[\text{Fe}(1\text{-bpp} - \text{COOC}_2\text{H}_5)_2](\text{BF}_4)_2\text{CH}_3\text{CN}$ ) from a diamagnetic low-spin ( $S=0$ ) to a paramagnetic high-spin ( $S=2$ ) state in the framework of density functional theory (DFT). The calculations were carried out with FHI-Aims code using PBE and B3LYP functionals. Due to the switching, the bond length Fe-N increases by up to 20%. In addition, calculations for Raman spectra were done for both spin-states and compared to temperature-dependent Raman measurements. This allows us the analysis of a unique fingerprint of the molecular bondings as well as the assignment of specific Raman modes. The financial support by DFG within CRC 1242 (*Project B 02*) and computation time on the MagniUDE supercomputer system are gratefully acknowledged.

MA 26.2 Wed 15:15 H48

**Inelastic Neutron Scattering and Magnetic Studies on Families of 3d-4f Heterometallic  $\text{M}_2\text{Ln}_2$  Single-Molecule Magnets** — ●JULIUS MUTSCHLER<sup>1</sup>, THOMAS RUPPERT<sup>2</sup>, YAN PENG<sup>2</sup>, JACQUES OLLIVIER<sup>3</sup>, QUENTIN BERROD<sup>3</sup>, JEAN-MARC ZANOTTI<sup>3</sup>, CHRISTOPHER E. ANSON<sup>2</sup>, ANNIE K. POWELL<sup>2</sup>, and OLIVER WALDMANN<sup>1</sup> — <sup>1</sup>Physikalisches Institut, Universität Freiburg, D-79104 Freiburg, Germany — <sup>2</sup>Institut of Inorganic Chemistry, Karlsruhe Institute of Technology (KIT), D-76131 Karlsruhe, Germany — <sup>3</sup>Institut Laue-Langevin, F-38042 Grenoble Cedex 9, France

The discovery of slow relaxation and quantum tunnelling of the magnetization in the single molecule magnets (SMMs) two decades ago has led to a flurry of research towards improving their magnetic properties. This class of molecules has been expanded to heterometallic clusters incorporating transition metal and rare earth ions. The 4f ions are of interest because of their large angular momenta and magnetic anisotropies, but exactly the latter feature leads to unexpected challenges in the numerical analysis of experimental susceptibility and magnetization curves. Inelastic neutron scattering (INS) experiments were performed on the time-of-flight disk-chopper spectrometers IN5 and IN6 at ILL on the SMMs  $\text{Mn}_2\text{Ln}_2$ -squares with  $\text{Ln} = \text{Y}, \text{Tb}, \text{Ho}, \text{Dy}$ , and the  $\text{M}_2\text{Ln}_2$ -butterflies with  $\text{M} = \text{Fe}, \text{Al}$  and  $\text{Ln} = \text{Dy}, \text{Er}$ . High quality INS data were recorded, even for the Dy containing species besides the strong neutron absorption of this ions. The analysis and interpretation of the INS data, and of magnetic data, by means of a linked fit approach and using effective models is presented.

MA 26.3 Wed 15:30 H48

**Study of VOPc/TiOPc layers on Ag(100) using X-ray absorption spectroscopy** — ●JAEHYUN LEE<sup>1,2</sup>, STEFANO REALE<sup>1,2</sup>,

KYUNGJU NOH<sup>1,2</sup>, LUCIANO COLAZZO<sup>1</sup>, DENIS KRYLOV<sup>1</sup>, CHRISTOPH WOLF<sup>1</sup>, ANDRIN DOLL<sup>3</sup>, ANDREAS HEINRICH<sup>1,2</sup>, YUJEONG BAE<sup>1,2</sup>, and FABIO DONATI<sup>1,2</sup> — <sup>1</sup>Center for Quantum Nanoscience — <sup>2</sup>Ewha Womans University, Seoul, Republic of Korea — <sup>3</sup>Swiss Light Source, Paul Scherrer Institut (PSI), Villigen Switzerland

Vanadyl Phthalocyanine (VOPc) shows spin 1/2 and long coherence time of almost 1 microseconds up to room temperature [M. Atzori et al., J. Am. Chem. Soc. 138, 2154 (2016)]. Investigating the orbital splitting when absorbed on a surface and the interactions between the molecular spin and the supporting substrate is crucial to optimize their quantum coherence properties. Here, we use x-ray absorption spectroscopy to investigate the spin properties of VOPc on Ag(100) and on TiOPc/Ag(100). To interpret our data, we simulate x-ray spectra combining machine learning with multiplet calculations. We find that the interaction with the metal surface changes the orbital structure of VOPc when directly on the Ag(100). Decoupling from the metal using a TiOPc layer is sufficient to restore the spin and orbital structure of the free standing VOPc, which shows no changes upon annealing up to 450K. This robust molecular spin architecture shows the potential in quantum computing technology.

MA 26.4 Wed 15:45 H48

**High-frequency EPR studies on monomeric 4f complexes** — LENA SPILLECKE, CHANGHYUN KOO, and ●RÜDIGER KLINGELER — Kirchhoff Institute for Physics, Heidelberg University, Germany

Tuning of magnetic anisotropy by appropriate design of crystal fields in 4f monomeric complexes is guided by experimental determination of relevant parameters – here by high-frequency electron paramagnetic resonance (HF-EPR) studies – and by numerical results. Our recent study on pentagonal-bipyramidal Er(III) [1] complexes is motivated by a reported difference in relaxation behavior [2]. Evaluating the data in a  $S = 1/2$  pseudo spin approximation for each Kramers doublet (KD) results in the precise determination of the crystal field splitting energies and effective g-values of the three lowest KDs. Relaxation behaviour is directly traced back to changes in electronic structure, induced by the crystal field and are attributed to a pronounced non-axiality of the ground-state g-tensor promoting a fast QTM magnetic relaxation. Another confirmation of a guided approach is provided by recent data on a set of [Ln(III)L12]-complexes ( $\text{Ln} = \text{Dy}, \text{Tb}$ ) involving tetradentate ligands [3] as well as by studies of a novel nonadentate bispidine-based ligand where the experimentally determined relaxation barrier of  $46 \text{ cm}^{-1}$  is rather modest but in excellent agreement with that predicted by ab-initio calculations [4].

[1]L. Spillecke et al., Dalton Transactions 50, 18143 (2021) [2]T.A. Bazhenova et al., Molecules 26, 6908 (2021) [3]P. Comba et al., Chemistry-Eur. J. 24, 5319 (2018) [4]P. Cieslik et al., J of Inorg. Gen. Chem. (Z. Anorg. Allg. Chem.) 647, 843 (2021)