

TT 3: Magnetic/Organic Interfaces and Molecular Magnetism (organized by MA; with CPP, DS, HL, O, TT)

Time: Monday 9:30–12:15

Location: HSZ 02

Invited Talk TT 3.1 Mon 9:30 HSZ 02

Molecular quantum spintronics with single-molecule magnets — ●WOLFGANG WERNSDORFER — Institut Néel, CNRS, BP 166, 38042 Grenoble, France

We will address the field called molecular quantum spintronics, combining the concepts of spintronics, molecular electronics and quantum computing. Various research groups are currently developing low-temperature scanning tunnelling microscopes to manipulate spins in single molecules, while others are working on molecular devices (such as molecular spin-transistors, spin valves and filters, and carbon-nanotube-based devices) to read and manipulate the spin state and perform basic quantum operations. For ex., we have built a novel spin-valve device in which a non-magnetic molecular quantum dot, consisting of a Single-Wall Carbon Nanotube, is laterally coupled to a TbPc2 molecular magnet. The localized magnetic moment of the SMM led to a magnetic field-dependent modulation of the conductance in the nanotube with magnetoresistance ratios of up to 300%. Using a molecular spin-transistor, we achieved the electronic read-out of the nuclear spin of an individual metal atom embedded in a single-molecule magnet (SMM). We could show very long spin lifetimes (several tens of seconds). Using the hyperfine Stark effect, which transforms electric fields into local effective magnetic fields, we could not only tune the resonant frequency by several MHz, but we also performed coherent quantum manipulations on a single nuclear qubit by means of electrical fields only.

Invited Talk TT 3.2 Mon 10:00 HSZ 02

EPR Studies of Rare-Earth Molecular Nanomagnets — ●STEPHEN HILL¹, SANHITA GHOSH¹, DORSA KOMIJANI¹, SALVADOR CARDONA-SERRA², JOSE-JAIME BALDOVI², YAN DUAN², ALEJANDRO GAITA-ARINO², and EUGENIO CORONADO² — ¹Department of Physics and NHMFL, Florida State University, Tallahassee, FL 32310, USA — ²ICM, Universidad de Valencia, 46980 Paterna, Spain

I will discuss the application of multi-frequency EPR to study the static and dynamic properties of a family of mononuclear Ln(III) (Ln = Ho or Tb) nanomagnets encapsulated in polyoxometallate (POM) cages. The encapsulation offers the potential for spintronics applications on surfaces or in devices, as it preserves the intrinsic properties of the nanomagnet outside of a crystal. A large magnetic anisotropy arises due to a splitting of the Hund's coupled angular momentum ($J = L+S$) ground state in the POM ligand field. High-frequency EPR studies for the Ho(III) compound ($J = 8$) reveal an anisotropic eight line spectrum corresponding to transitions within the lowest $m_J = \pm 4$ doublet, split by a hyperfine interaction with the $I = 7/2$ Ho nucleus. Meanwhile, X-band studies reveal the presence of a large tunneling gap ($\Delta \sim 9$ GHz) within the $m_J = \pm 4$ doublet. Spin-echo measurements allow studies of the coherent spin dynamics, including Rabi oscillations. Remarkably long T_2 times are found, even for the most concentrated samples. It is postulated that this is due to the large gap, Δ , which provides an optimal operating point for coherent manipulations at X-band such that the quantum dynamics are relatively insensitive to dipolar fields.

15 min. break

Invited Talk TT 3.3 Mon 10:45 HSZ 02

On-surface magnetochemistry of spin-bearing metalorganic molecules — ●PETER M. OPPENEER¹, KARTICK TARAFDER¹, EHE-SAN ALI¹, NIRMALYA BALLAV², CHRISTIAN WÄCKERLIN³, and THOMAS A. JUNG³ — ¹Uppsala University, Uppsala, Sweden — ²IISER, Pune, India — ³PSI, Villigen, Switzerland

Planar spin-bearing metalorganic molecules such as metal-porphyrins and -phthalocyanines are paramagnetic in the gas phase, however an interface exchange coupling develops when these molecules are assembled on magnetic surfaces, which induces spontaneous molec-

ular magnetic order at room temperature. To unveil fundamental origins of the exchange interaction leading to the metalorganic molecule/substrate spin-interface we use ab-initio DFT+U calculations with dispersion corrections added. Our calculations provide detailed, orbitally-resolved insight in the molecule-surface exchange interactions as well as the spin-switching induced by additional ligation in the free ligand position of the metal ion by small molecules such as NO and NH₃. We find that on-surface coordination chemistry of planar metalorganic complexes gives rise to novel magnetochemical effects, which challenge the notions of classical coordination chemistry. A key to these magnetochemical effects is the weak bonding to the surface, i.e. a "surface" trans effect. Our calculations further reveal that certain systems, as e.g. Cu-phthalocyanine on Co, are liable to formation of novel spin-polarized interface states that are expected to be particularly suited for spin-polarized electron injection in metalorganic layers.

Invited Talk TT 3.4 Mon 11:15 HSZ 02

Interfacing single-molecule magnets with metals — ●ANDREA CORNIA¹, VALERIA LANZILOTTO², LUIGI MALAVOLTI², MATTEO MANNINI², MAURO PERFETTI², LUCA RIGAMONTI¹, and ROBERTA SESSOLI² — ¹Dip. di Scienze Chimiche e Geologiche, Univ. di Modena e Reggio Emilia & INSTM, Modena, Italy — ²Dip. di Chimica U. Schiff, Univ. di Firenze & INSTM, Sesto Fiorentino (FI), Italy

Encoding and manipulating information through the spin degrees of freedom of individual molecules are central challenges in molecular scale electronics. With their large magnetic moment and long spin relaxation time, single molecule magnets (SMMs) are of special importance in this field. The electrical addressing of individual SMMs is now well within reach using scanning probe methods, which require organizing molecules on electrically conductive surfaces [1,2]. Herein we present the latest achievements in the deposition of SMMs on metal substrates, like ultraflat surfaces [3] and nanoparticles [4]. Special emphasis is placed on the design of molecular structures that withstand processing by solution [3,4] or vapour-phase [5,6] methods as well as on chemical strategies for controlling molecular orientation. Rewardingly, these efforts have shown that the distinctive property of SMMs, i.e. slow spin relaxation, can persist in metal-wired molecules [3,4].

[1] S. Loth, et al. *Science* 2012, 335, 196. [2] A. A. Khajetoorians, et al. *Science* 2013, 339, 55. [3] M. Mannini, et al. *Nature* 2010, 468, 417. [4] M. Perfetti, et al. *Small* 2013, DOI: 10.1002/smll.201301617. [5] L. Rigamonti, et al. *Inorg. Chem.* 2013, 52, 5897. [6] L. Malavolti, et al. *Chem. Commun.* 2013, 49, 11506.

Invited Talk TT 3.5 Mon 11:45 HSZ 02

Linking magnetic molecules to themselves, to others and to surfaces — ●RICHARD WINPENNY — University of Manchester, United Kingdom

We are learning how to link together polymetallic compounds to give complex structures [1]. During this presentation recent work will be discussed in two distinct approaches. Firstly, we will describe recent work creating new hybrid inorganic-organic rotaxanes [2] and in the second approach we will discuss functionalising polymetallic rings so that they can act as ligands for other metal complexes and surfaces [3,4]. We will also describe the use of pulsed EPR spectroscopy to measure weak interactions between these molecular magnets.

1.G. A. Timco, T. B. Faust, F. Tuna and R. E. P. Winpenny, *Chem. Soc. Rev.*, 2011, 40, 3067-3075. 2.C.- F. Lee, D. A. Leigh, R. G. Pritchard, D. Schultz, S. J. Teat, G. A. Timco and R. E. P. Winpenny, *Nature*, 2009, 458, 314-318. 3.G. A. Timco, S. Carretta, F. Troiani, F. Tuna, R. G. Pritchard, E. J. L. McInnes, A. Ghirri, A. Candini, P. Santini, G. Amoretti, M. Affronte and R. E. P. Winpenny, *Nature Nanotechnology*, 2009, 4, 173-178. 4 G. F. S. Whitehead, F. Moro, G. A. Timco, W. Wernsdorfer, S. J. Teat and R. E. P. Winpenny, *Angew. Chem. Int. Ed.*, 2013, 52, 9932-9935.