MA 42: Molecular Magnetism and Magnetic Particles / Clusters II

Time: Thursday 9:30–12:30 Location: HSZ/0004

MA 42.1 Thu 9:30 HSZ/0004

Towards a Physics-Informed Deep Learning Model for Parameterizing the Magnetism in 4f based Single-Molecule Magnets — •Zayan Ahsan Ali and Oliver Waldmann — Physikalisches Institut, Universität Freiburg, Germany

Single-molecule magnets (SMMs) have attracted interest in recent decades for their intriguing magnetic behavior and potential applications in quantum computing and spintronics. 4f based SMMs stand out because lanthanide ions can provide large magnetic anisotropies. However, the ligand environments that govern their magnetic properties involve up to 27 ligand-field parameters, while common experimental data such as temperature dependent magnetic susceptibility measured on powdered samples are comparatively featureless. Inferring ligand field parameters from such data is therefore a highly overparameterized inverse problem. Machine learning approaches have shown promise in addressing this challenge [1]. Two central difficulties are identification of physically relevant regions of the ligand field parameter space and learning of a highly complex one-to-many mapping. This work presents a machine learning framework tailored to overcome both obstacles. It is shown that an informative training data set can be constructed via active learning with uncertainty sampling, and that incorporating the energy spectrum as an intermediate representation significantly improves the learnability of the high dimensional inverse mapping. The resulting architecture is found to be capable of predicting multiple possible ligand field parameter sets.

[1] Z. A. Ali *et al.*, PRB 112, 064403 (2025).

MA 42.2 Thu 9:45 HSZ/0004

Graphene-based quantum heterospin graphs — Gabriel Martínez-Carracedo[1], Amador García-Fuente[1], László Oroszlány[2], •László Szunyogh[3], and Jaime Ferrer[1] — [1]Universidad Oviedo, Spain — [2]Eötvös Loránd University, Budapest, Hungary — [3]Budapest University of Technology and Economics, Hungary

Harnessing quantum-regime functionalities without relying on rare-earth elements represents an important step toward developing globally accessible quantum technologies. In this contribution, we investigate a range of low-dimensional open quantum spin systems constructed from magnetic nanographene structures containing spin-1/2 and spin-1 triangulenes and/or olympicenes. These graphene nanostructures act as localized spins and can be effectively modeled using a quantum bilinear*biquadratic Heisenberg Hamiltonian. We compute the energy spectrum and the quantum numbers associated with the low-energy eigenstates. We identify a double degeneracy in the total spin quantum number S of the first excited state in three-leg spin graphs (3-LSGs) and in other heterospin nanostructures. This degeneracy depends on both the number of sites and the spin species, and arises from a swapping-transformation symmetry of the Hamiltonian. Numerical simulations further show that this degeneracy remains largely robust in $N = 7$ spin-1 3-LSGs under realistic perturbations relevant to experimental conditions. [1]

[1] G. Martínez-Carracedo *et al.*, DOI: 10.1103/v3fm-lvsh (2025)

MA 42.3 Thu 10:00 HSZ/0004

Femtosecond spin-state switching dynamics of Fe(II) complexes condensed in thin films — •Manuel Gruber[1], Lea Kämmerer[1], Gérald Kämmerer[1], Laurent Mercadier[2], Andreas Scherz[2], Felix Tuczek[3], Peter Kratzer[1], Uwe Bovensiepen[1], and Heiko Wende[1] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen, Germany — [2]European XFEL, Schenefeld, Germany — [3]Institute for Inorganic Chemistry, Kiel University, Germany

Significant progress has been made in tailoring spin-crossover films, driven by their potential for technological applications. However, studies of ultrafast switching in such films remain limited compared to their solution-phase counterparts. Here, we investigated photoinduced spin-state switching in a molecular film at room temperature, using the new capabilities offered by X-ray free-electron lasers. The sub-picosecond transition from the $S = 0$ low-spin state to the $S = 2$ high-spin state is tracked via transient changes in the Fe L_3 X-ray absorption edge. Our results reveal the involvement of an intermediate state in the switching dynamics [Kämmerer et al., ACS Nano 18, 34596 (2024)].

Financial support from CRC 1242 is gratefully acknowledged.

MA 42.4 Thu 10:15 HSZ/0004

Chirality-induced spin selectivity without intrinsic spin-orbit coupling: Role of non-equilibrium molecular orbital moment — •Sumit Ghosh[1] and Daniel E. Bürgler[2] — [1]The Institute of Physics of the Czech Academy of Sciences, 16200 Prague, Czech Republic — [2]Peter Grünberg Institut (PGI-6), Forschungszentrum Jülich GmbH, 52428 Jülich, Germany

We present an alternative theory of chirality induced spin selectivity (CISS) that does not require any intrinsic spin orbit coupling (SOC). The proposed mechanism is based on the formation of circulating currents in the molecular rings. In each ring, this current generates a non-equilibrium molecular orbital moment (MOM) which interacts with the spin of an injected electron, giving rise to CISS. The direction of the MOM is governed by the gauge field that arises from the chirality-induced structural distortion of the molecule. Being non-relativistic in nature, the gauge field induced MOM can be stronger than the effect generated by SOC. The presence of such a gauge field also overcomes the hurdle posed by Onsager's reciprocity. Finally we demonstrate that a non-equilibrium MOM can also form in the absence of the gauge field. However only the presence of the gauge field can produce the experimentally observed crossing I-V curve which is a characteristics of the CISS effect.

MA 42.5 Thu 10:30 HSZ/0004

Magnetocaloric effect of the centered-square, centered-hexagon, and double-pyramidal spin models — •Hamza Meel and Jürgen Schnack — Bielefeld University, Faculty of Physics, Bielefeld, Germany

Molecular magnetocalorics have been proposed as a replacement to ^{3}He for cryogenic applications, however the search for the best compound for such an application is still ongoing. Specifically, magnetic molecules exhibiting a high adiabatic entropy change in the kelvin and sub-kelvin range are sought after. Such an entropy change could for instance be achieved by a molecule whose ground state is highly degenerate. We investigate three frustrated systems, the centered square, the centered-hexagon, and the double-pyramidal spin models. Their figures of merits and their magnetocaloric effect are discussed.

MA 42.6 Thu 10:45 HSZ/0004

Exchange-biased toroidal moments in a family of homochiral Cu_6Ln_3 complexes studied by high-field EPR — •Jan Arneth[1], Deepanshu Chauhan[2], Sagar Paul[3], Bapan Jana[2], Wolfgang Wernsdorfer[3], Maheswaran Shanmugam[2], Gopalan Rajaraman[2], and Rüdiger Klingeler[1] — [1]Kirchhoff Institute for Physics, Heidelberg University, Germany — [2]Department of Chemistry, Indian Institute of Technology Bombay, India — [3]Physikalisches Institut, Karlsruhe Institute of Technology, Germany

The vortex-like arrangement of the individual magnetic moments renders single-molecule toroics (SMT) promising candidates for application in quantum computing, molecular spintronics and the development of magneto-electric coupling in multiferroic devices. Here, we report the magnetic investigation of a family of heterobimetallic nonanuclear Cu_6Ln_3 (Ln = Y,Gd,Dy) clusters, featuring a homochiral Cu_3-Ln_3-Cu_3 triangular core, using combined theoretical *ab-initio*, ac and dc susceptibility, μ-SQUID and high-field EPR studies. Numerical analysis of our experimental data allow for the determination of the microscopic spin Hamiltonian parameters, which reveal an antiferromagnetic inter-triangular coupling between the two spin-frustrated Cu_3 units. In particular, Cu_6Dy_3 exhibits both single-molecule magnet (SMM) and SMT behaviour with a non-magnetic ground state persisting up to magnetic fields as high as $B \simeq 1.3$ T. The large excitation gap is found to result from the ferromagnetic Cu-Dy exchange interaction coupling the toroidal Dy_3 unit with the adjacent Cu_3 triangles.

15 min break

MA 42.7 Thu 11:15 HSZ/0004

Fully Quantum-Mechanical Simulations of Spin Crossover Behaviour in an Iron(II) Complex — •Ethan Crawford, Solveig Felton, and David Wilkins — Queen's University Belfast,

Belfast, Northern Ireland

Spin-crossover (SCO) complexes change spin state when exposed to external stimuli such as light, temperature or pressure, allowing them to be used as sensors or magnetic memory devices. Predicting with precision when a crossover occurs would bring the technology closer to fruition, but it remains a significant challenge. Single-point energy calculations using Density Functional Theory (DFT) have been employed with limited accuracy, because they neglect the vibrational and other entropic contributions present at finite temperatures. Furthermore, a given calculation setup is not necessarily transferable to another complex. We trained a committee neural network potential (c-NNP) using data generated via Ab Initio Molecular Dynamics for an Iron (II) SCO complex. Two c-NNPs were trained, to model both the highest and lowest spin states respectively, encompassing all intramolecular interactions. The models were systematically improved using the query by committee approach. These systems were extended from a single complex to a bulk system combining the c-NNPs with a classical forcefield to account for the intermolecular interactions. The spin state for each complex is individually assigned to simulate experimental transitions. During the transition window, neither model can accurately predict the behaviour of the complex, but combining the three forcefields should replicate experimental behaviour.

MA 42.8 Thu 11:30 HSZ/0004

Symmetric finite-temperature Lanczos method for anisotropic magnetic molecules — •Jürgen Schnack — Bielefeld University, Faculty of Physics, Bielefeld, Germany

The finite-temperature Lanczos method (FTLM) constitutes a valuable approximation scheme for Hilbert space problems that exceed the dimension tractable by complete numerical diagonalization [1,2]. Several large magnetic molecules have been successfully modeled using FTLM [3]. It has been noted earlier that the method converges best for problems where the z-component of total spin commutes with the Hamiltonian. For anisotropic Hamiltonians the convergence is much poorer [4]. Here, we discuss conceptional improvements [5] as well as realizations on nowadays supercomputing architectures that employ CPUs as well as GPUs.

[1] J. Jaklic, P. Prelovsek, Phys. Rev. B 49, 5065 (1994). [2] J. Schnack, J. Richter, R. Steinigeweg, Phys. Rev. Research 2, 013186 (2020). [3] T. Tziotzi, D. Gracia, S. Dalgarno, J. Schnack, M. Evangelisti, E. Brechin, C.J. Milios, JACS 145, 7743 (2023). [4] O. Hanebaum, J. Schnack, Eur. Phys. J. B 87, 194 (2014). [5] M. Aichhorn, M. Daghofer, H. G. Evertz, W. von der Linden, Phys. Rev. B 67, 161103(R) (2003).

MA 42.9 Thu 11:45 HSZ/0004

Investigation of Magnetic Properties of Ce-Doped Ni-Based Composites as Near Infrared Absorbers Based on Soft-XAS and XMCD Measurements — •Timuçin Emre Tabaru[1], Ali Karatutlu[2], Iremnur Duru[1], and M. Fatih Kilicaslan[3] — [1]Department of Electrical Electronics Engineering, Sivas University of Science and Technology, 58000 Sivas, Turkey — [2]National Nanotechnology Research Center (UNAM), Bilkent University, Ankara 06800, Türkiye — [3]Department of Engineering Fundamental Sciences, Sivas University of Science and Technology, 58000 Sivas, Turkey

In this study, the X-ray Magnetism Circular Dichroism (XMCD) spectra of Ni-based composites produced by melt spinning and rapid solidification with ~75% Ni, ~10% Cr, ~8% Si, ~5% Fe, ~2% B, and 1% Ce doping were determined according to different Fe and Cerium (Ce) contents using soft X-ray absorption spectroscopy (XAS) at the HESEB beamline at the Synchrotron-Light For Experimental Science And Applications In The Middle East (SESAME). The L2 and L3 edges of Ni, Fe, and Ce were investigated for both Ce-doped and undoped samples. The areas under the XAS and XMCD spectra obtained from these measurements were determined, and the spin and orbital magnetic momenta of each sample were calculated. The results confirmed that the materials mentioned exhibit paramagnetic properties, in agreement with the literature. Ni-based composite doped with Ce demonstrated enhanced broadband infrared (IR) absorption, reaching a maximum efficiency of 93% in the 3-5 μm mid-IR window and maintaining over 80% absorption across the entire 3-15 μm spectral range.

MA 42.10 Thu 12:00 HSZ/0004

Magnetic Hexagonal Nanoferrite-Based Electrode: Structural Characterization and Electrochemical Detection of Caffeine in Drinks — •Sajjad Hussain — The Begum Nusrat Bhutto Women University, Sukkur, Sindh, Pakistan

Caffeine is a pharmacologically active alkaloid that is frequently incorporated into a wide range of food and beverage formulations. V-type hexagonal ferrite nanoparticles (SrSnFe*O**-NPs) were prepared through a sol*gel-based green auto-combustion route and analyzed using a range of advanced characterization techniques, including X-ray diffraction (XRD), X-ray absorption fine structure (XAFS), scanning electron microscopy (SEM), atomic force microscopy (AFM), Brunauer*Emmett*Teller (BET) surface area analysis, and vibrating sample magnetometry (VSM). The V-type hexaferrite exhibits a single-phase crystalline structure with an average crystallite size exceeding 30 nm. The local atomic structure was confirmed using XAFS analysis, while the surface morphology and particle size were examined through SEM and AFM. BET was used to confirm the surface area 209.6 m*/g. The magnetic studies revealed soft magnetic behavior. Furthermore, the synthesized V-type hexagonal ferrites were employed to modify a glassy carbon electrode (GCE), developing SrSnFe*O**-NPs/GCE for the electrochemical sensing of caffeine. Cyclic voltammetry studies revealed conductive and diffusion-controlled behavior, with the SrSnFe*O**-NPs/GCE demonstrating high sensitivity and selectivity for caffeine detection (linear ranges: 0.5 to 80 *M; detection limits: 0.025 *M, while the LOQ was 0.078 *M.

MA 42.11 Thu 12:15 HSZ/0004

Strain control of three-dimensional magnetic nanostructures — •José Claudio Corsaletti Filho, Mohammad Sedghi, Elina Zhakina, Markus König, Elena Gati, and Claire Donnelly — Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

The study of nanoscale objects in three-dimensions has led to new discoveries and opportunities for technological development. Recent studies have shown that the magnetic landscape of 3D nanostructures can be controlled by geometrical effects, enabling innovations in design and magneto-mechanical devices. Consequently, a method to reversibly tune the properties of a three-dimensional nanostructure is highly desirable. Strain represents a particularly promising approach, as it directly influences the geometry. Indeed, while strain has been extensively applied to magnetic thin films for the tuning of global material properties, there the substrate restricts global strains to 0.7-1%. In this work, we describe how we strained 3D magnetic nanostructures and map out their geometrical changes through in situ electron microscopy. We are able to achieve ultimate strains of up to 20%, but we also identify regimes associated with the elastic and plastic deformations of 3D nanostructures with different geometries. By determining the mechanical properties of the nanowires, we obtain the fundamental insight to achieving reversible tuning of the geometry - and therefore the magnetic properties - of 3D nanostructures. Such reversible tuning will be of key interest for future technological applications.