# O 51: Poster Wednesday: Atomic-Scale Studies of Spins on Surfaces with Scanning Tunneling Microscopy

Time: Wednesday 18:00–20:00 Location: P4

O 51.1 Wed 18:00 P4

**Nickelocene molecule as an STM magnetic sensor** — •Andres Pinar Sole, Oleksandr Stetsovych, Pavel Jelinek, Ales Cahlik, Christian Wakerlin, and Jindric Kolorenc — Czech Institute of Physics, Prague, Czech Republic, Email: pinar@fzu.cz

Functionalization of the scanning probe of a scanning tunnelling microscopy (STM) with metallocene molecule allows performing spin-sensitive measurements on magnetic systems. Here, we used a nickelocene molecule (NiCp2), consisting of a Ni atom sandwiched between two cyclopentadienyl rings. As an S=1 system, it presents magnetic-induced spectral features due to the inelastic electron spin-flip.

First, we examined 1D metallorganic coordination polymers (2,5-diamino-1,4-benzoquinonediimines) on Au(111) with Co or Cr atoms as metal sites respectively. Nickelocene IETS conductance spectrum deformation was only sensitive to the out-of-plane magnetic anisotropy of the Cr.

Secondly, the Nc functionalized probe was also used to measure the magnetism emerging from the unpaired electron on the edge of a wave-like graphene nanoribbon (GNR) on Au(111). Here, we observed spectral convolution between a Kondo feature from the edge-state and the nickelocene spectrum.

To understand the IETS from the magnetic sensor, a many-body Hubbard model was proposed, and the system was simplified to a two-site model consisting of the partially filled 3d shell of the nickelocene and a 3d shell in the probed magnetic center.

O 51.2 Wed 18:00 P4

**Yu-Shiba-Rusinov band dispersion of infinite Mn chains on top of a semi-infinite Nb(110) surface** — •Rik Broekhoven, Artem Pulkin, Antonio Manesco, Sander Otte, Anton Akhmerov, and Michael Wimmer — Delft University of Technology, Delft, The Netherlands

Chains of magnetic atoms on s-wave superconductors have been proposed to have a topological non-trivial phase, when the induced in-gap Yu-Shiba-Rusinov (YSR) bands are p-wave gapped by for example spin-orbit coupling. In order to determine the topological phase diagram, experiments were previously limited to probing local quantities of the chain. Recent improvements in STM methodology have made it possible however to now also probe the YSR band dispersion relation. It was found to be highly dependent on the chain spacing and orientation with respect to the superconductor lattice.

Motivated by this discovery, here we present a method to evaluate the in-gap dispersion relation of chains with different orientations and spacing. In contrast to previous works, we work with infinite chains on a semi-infinite surface to make sure the system is larger than the superconductor coherence length. We focus on Mn atoms on top of superconducting Nb(110). First, we derive an effective tight-binding model from ab initio calculation, and subsequently we use the multidimensional Green's function formalism to extend to a semi-infinite system and solve for the corresponding in-gap YSR bands.

O 51.3 Wed 18:00 P4

**Unravelling the Magnetic Ground State of All-Organic Diradicals on Au Substrates** — •Alessio Vegliante[1], Saleta Fernandez[2], Ricardo Ortiz[3], Niklas Friedrich[1], Andrea Aguirre[1], Francisco Romero[1], Diego Peña[2], and Thomas Frederiksen[3] — [1]CIC NanoGUNE, San Sebastian, Spain — [2]CiQUS-USC, Santiago de Compostela, Spain — [3]Donostia International Physics Center, San Sebastian, Spain

Open-shell organic molecules have received considerable interest as potential candidates for molecular spintronics. Magnetism can emerge in all-organic molecules due to the presence of one or more unpaired $\pi$-electrons. Organic diradicals, hosting two spin centers, are particularly interesting as model systems for investigating and manipulating magnetic interactions at the atomic scale.

Here we study the magnetic state of a Chichibabin*s hydrocarbon diradical deposited on a gold substrate, by using scanning tunneling microscopy (STM) and spectroscopy (STS). We investigate the interaction between the two spin centers of the molecule, focusing on the influence of the molecular geometry. With the support of theoretical simulations, we show that the adsorption on the metal surface changes the ground state of the molecule from a triplet, expected in the gas phase, to a singlet state. Furthermore, we demonstrate that it is possible to modify the magnetic state of the diradical through conformational changes induced by the STM tip. These findings represent an important step towards the control of magnetic interactions within purely organic molecules.

O 51.4 Wed 18:00 P4

**Quantifying the interplay between fine structure and geometry of an individual molecule on a surface** — •Manuel Steinbrecher[1], Werner M.J. v. Weerdenburg[1], Etienne F. Walraven[1], Niels P.E. v. Mullekom[1], Jan W. Gerritsen[1], Fabian D. Natterer[2], Danis I. Badrtdinov[1], Alexander N. Rudenko[4,1], Vladimir V. Mazurenko[3], Mikhail I. Katsnelson[1], Ad v.d. Avoird[1], Gerrit C. Groenenboom[1], and Alexander A. Khajetoorians[1] — [1]Institute for Molecules and Materials, Radboud University, Nijmegen, The Netherlands — [2]Department of Physics, University of Zurich, Switzerland — [3]Ekaterinburg — [4]School of Physics and Technology, Wuhan University, China

With spin-resolved scanning tunneling microscopy (SP-STM) and electron spin resonance (ESR) we have probed single TiH molecules deposited on a thin insulating MgO layer in a vector magnetic field at mK temperatures down to MHz frequencies. We find that the molecule retains a non-trivial orbital angular momentum resulting in a strongly renormalized and anisotropic $g$-tensor. As we prove, the latter does not stem from Kondo or Jahn-Teller effects. From quantum chemistry embedded cluster calculations we find an analytical expression for the $g$-tensor, which solely depends on the splitting of the ground states and the spin-orbit coupling. In a dynamic expansion of the model, the position of the H atom and rotational dynamics of the molecule were investigated. [1] Steinbrecher *et al.*, PRB 103, 155405 (2021) [2] v. Weerdenburg *et al.*, RSI 92, 033906 (2021)

O 51.5 Wed 18:00 P4

**Magnetic molecule as a parity sensor in entangled spin and YSR excitation on a superconductor** — •Jon Ortuzar[1], Stefano Trivini[1], Katerina Vaxevani[1], Jingchen Li[5], Ane Garro[1], Miguel Angel Cazadilla[3], Sebastian Bergeret[2,3], and José Ignacio Pascual[1,4] — [1]CIC nanoGUNE-BRTA, San Sebastián, Spain — [2]Centro de Física de Materiales (CFM-MPC), San Sebastián, Spain — [3]Donostia International Physics Center (DIPC), San Sebastián, Spain — [4]Ikerbasque, Bilbao, Spain — [5]School of Physics, Sun Yat-sen University, Guangzhou, China

A magnetic molecule coupled to a superconductor induces Yu-Shiba-Rusinov (YSR) bound states, detected by tunneling spectroscopy as long-lived quasiparticle excitations inside the superconducting gap [1]. The degeneracy of the system can be lifted by intrinsic magnetic anisotropy so that entangled spin and YSR excitations are possible [2]. We tune the exchange coupling between a FeTPP-Cl molecule and the proximitized Au(100)/V substrate to go through a Quantum Phase Transition from an unscreened half-integer spin (even parity) system to a screened integer spin (odd parity) system [3]. We use a single site superconductor model [4] to prove the capability to detect the parity of the system, getting fundamental insight into the interplay of YSR and spin excitation.

[1] B. W. Heinrich, et. al., Prog. Surf. Sci.93, 1 (2018) [2] N. Hatter, et. al., Nat. Commun.6, 8988 (2015) [3] S. Kezilebieke, et. al., Nano Lett.19, 4614 (2019) [4] F. von Oppen and K. J. Franke, Phys. Rev. B103, 205424 (2021).

O 51.6 Wed 18:00 P4

**Electronic Properties of Dysprosium-based Fe-Porphyrins Metal-Organic Coordination networks on Au(111) and Ag(100) Substrates** — •Serim Jeon[1,3], Lukas Spree[1,2], Corina Urdaniz[1,2], Caroline Hommel[1,2], Andreas Heinrich[1,2], Christoph Wolf[1,2], and Luciano Colazzo[1,2] — [1]Center for Quantum Nanoscience, Institute for Basic Science, Seoul, Republic of Korea — [2]Ewha Womans University, Seoul, Republic of Korea — [3]Department of Physics, Ewha Womans University

Dy has become the cornerstone for many investigations on lanthanide-directed molecular-magnetism, thanks to its strong mag-

netic anisotropy. Iron Tetrapyrrole complexes, on the other hand, have shown promise as materials for quantum information processing. Creating a platform that incorporates both might have a way for the realization of multiqubit architectures. The presented study describes electronic properties within a metal-organic network MOF consisting of Iron-Tetrakis-(4-Cyanophenyl) Porphyrin Fe-TCPP and Dysprosium. Fe-TCPP was deposited on Au(111), Ag(100), and MgO/Ag(100). The deposition of Dy induces coordination between the cyano groups and the lanthanide atoms and gives rise to ordering and the formation of large islands of 2D MOF. The lanthanide-based organic network was examined by scanning tunneling microscopy STM on the substrates. Significant shifts in the energy of LUMO of the MOFs were observed via scanning tunneling spectroscopy STS after deposition of Dy. The results were combined with ab initio calculation to further elucidate the electronic structure of the deposited materials.

O 51.7 Wed 18:00 P4

**Long-lived spin states of Fe atomic chains on $Cu_2N$ via Hamiltonian engineering** — Robbie J. G. Elbertse[1], •Taehong Ahn[2,3], Jiyoon Hwang[2,3], Jeongmin Oh[2,3], Jorn C. Rietveld[1], Sander Otte[1], Andreas J. Heinrich[2,3], and Yujeong Bae[2,3] — [1]Department of Quantum Nanoscience, Kavli Institute of Nanoscience, Delft University of Technology, Lorentzweg 1, Delft 2628 — [2]Center for Quantum Nanoscience, Institute for Basic Science, Seoul, Korea — [3]Department of Physics, Ewha Womans University, Seoul, Korea

A spin-polarized scanning tunneling microscope (STM) operating at various magnetic fields allows us to characterize the spin relaxation time of atomic structures on a surface, enabling Hamiltonian engineering. Here, we introduce 1D Fe atomic chains built on $Cu_2N/Cu(100)$ using a home-built STM and the evolution of their spin lifetime depending on the length of chains and the direction and magnitude of magnetic fields. To measure the spin lifetime ranging from $10^{-6}$ to 10 seconds, we used two different detection schemes; pump-probe [Science 329, 1628-1630 (2010)] and two state switching [Science 335, 196-199 (2012)]. We observed the spin lifetime of Fe chains changes non-monotonically as passing through a diabolic point with varying magnetic fields changes the degree of superposition of the two Neél states in the lowest energy eigenstates. To control the spin lifetime of Fe chains, we use magnetic fields as a control knob. Our work shows a capability of the spin lifetime in a large time scale and the precise control of spin dynamics in engineered atomic structures.

O 51.8 Wed 18:00 P4

**Local characterization of Yu-Shiba-Rusinov excitations in magnetic field** — •Niels P.E. van Mullekom[1], Benjamin Verlhac[1], Werner M.J. van Weerdenburg[1], Hermann Osterhage[1], Manuel Steinbrecher[1], Katharina J. Franke[2], and Alexander A. Khajetoorians[1] — [1]Institute for Molecules and Materials, Radboud University Nijmegen, the Netherlands — [2]Fachbereich Physik, Freie Universität Berlin, Germany.

An isolated spin, typically derived from an atomic or molecular adsorbate, can interact with a BCS superconductor leading to so-called Yu-Shiba-Rusinov (YSR) excitations. These excitations can be probed with scanning tunneling microscopy/spectroscopy (STM/STS), which are often characterized by resonances that reside in the superconducting gap and are linked to the excitation energies. These spin-based excitations to date have been poorly studied in magnetic fields, due to influence of magnetic fields on typical BCS superconductors. Here, utilizing STM/STS at milliKelvin temperatures, we report on a study of the YSR excitations of individual adsorbates in variable magnetic field.

O 51.9 Wed 18:00 P4

**Extending the spin excitation lifetime of a magnetic molecule on a proximitized superconductor** — •Katerina Vaxevani[1], Stefano Trivini[1], Jingcheng Li[1], Jon Ortuzar[1], Dongfei Wang[1], Danilo Longo[1], and Jose Ignacio Pascual[1,2] — [1]CIC nanoGUNE-BRTA, 20018 Donostia-San Sebastian, Spain — [2]Ikerbasque, Basque Foundation for Science, 48013 Bilbao, Spain

Magnetic molecules adsorbed on surfaces have been used as a platform to individually address and manipulate spins. Long spin-relaxation times are required in order to be able to use atomic spins in quantum information processing and data storage. Normally, coupling of the spin with the conduction electrons of metallic substrates can quench the excited state lifetime and lead to short relaxation times, but the presence of superconducting paring effects in the metal substrate can protect the excited spin from relaxation[1]. Here, we use a substrate of a few monolayers of gold epitaxially grown ontop of an oxygen reconstructed 1x5-V(100) surface to decouple the molecular spin of an iron-porphyrin-chloride from itinerant electrons. The gold film exhibits a proximitized superconducting gap with in-gap de Gennes-Saint James resonances, which protects molecular spin excited states and results into a lifetime of $\tau$=80ns. The spin lifetime decreases with increasing the film thickness due to the gradual gap-closing by the in-gap states. Our results elucidate the use of proximitized gold electrodes for addressing quantum spins on surfaces, envisioning new routes for tuning the value of their spin lifetime.

[1] B. W. Heinrich et al., Nature Physics 9, 765 (2013).

O 51.10 Wed 18:00 P4

**The Emergence of Magnetism in [5]-Aza-Triangulene** — •Lorenz Meyer[1], Francisco Romero Lara[1], Niklas Friedrich[1], Alessio Vegliante[1], Manuel Vilas Varela[2], Unai Uriarte Amiano[1], Natalia Koval[1], Emilio Artacho Cortés[1], Diego Peña Gil[2], and Jose Ignacio Pascual[1] — [1]1 CIC nanoGUNE, San Sebastian (Spain) — [2]Centro Singular de Investigación en Química Biológica y Materiales Moleculares (CIQUS), Santiago de Compostela (Spain)

Zigzag-edged Graphene triagulenes are known to host a magnetic ground state due to sublattice imbalance. The magnetic properties of these structures can be tuned by the size of the triangulene or via heteroatom substitution. This makes them intriguing for future spintronic applications paving the way towards organic logical devices. So far, the influence of heteroatoms in larger triangulenes seems to be unknown. In our work, we report the bottom-up synthesis of [5] aza-Triangulene by means of surface-assisted cyclodehydrogenation on a Au(111) surface. Electronic transport measurements carried out with a scanning tunneling microscope reveal the high-spin ground state of this molecule via low energy phenomena. Additionally, we shine light on not only the influence of heteroatoms but also of additional Hydrogen atoms and defects which are able to tune the magnetic ground state. Density functional theory and Mean-Field-Hubbard calculations confirm the spin texture and the electronic structure of the observed molecules.