O 68: Poster Session V: Poster to Mini-Symposium: Manipulation and control of spins on functional surfaces I

Time: Wednesday 10:30–12:30 Location: P

O 68.1 Wed 10:30 P

Stability of radical-functionalized gold surfaces by self-assembly and on-surface chemistry — •Tobias Junghöfer, Ewa Malgorzata Nowik-Boltyk, and Maria Benedetta Casu — Eberhard Karls Universität Tübingen, Institut für Physikalische und Theoretische Chemie, 72076 Tübingen, Germany

Organic radical thin films are of great interest for organic electronics such as spin filtering devices, data storage devices, and as quantum bits for quantum computing devices. Here we present the functionalisation of a gold substrate by using a derivative of the perchlorotriphenylmethyl (PTM) radical. PTM is a very chemically and thermally stable radical. We investigate the gold/PTM derivative interface by using soft X-ray techniques, such as X-ray photoelectron spectroscopy (XPS) and near-edge X-ray absorption fine structure (NEXAFS) spectroscopy. Our results show that the functionalisation is successful under specific preparation conditions. The radical is still intact and keeps its magnetic character at the interface. Our findings are a significant step forward on the implementation of organic radicals in molecular-based devices with different properties and applications as energy, sensing, imaging, memories, and spintronics.

O 68.2 Wed 10:30 P

Chemical Doping of Individual Polynuclear Molecular Magnets on Surfaces — •Fabian Paschke[1], Vivien Enenkel[1], Tobias Birk[1], Jan Dreiser[2], and Mikhail Fonin[1] — [1]Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany — [2]Swiss Light Source, 5232 Villigen PSI, Switzerland

The controlled deposition, characterization and manipulation of single molecule magnets (SMMs) on surfaces is one of the crucial topics to investigate with regard to their possible implementation as units in future electronic and spintronic devices. Fe_4 derivatives are among the most investigated SMMs showing a giant spin and a variety of quantum mechanical phenomena. We showed that a flat derivative of this SMM is suitable for defined adsorption on decoupling monatomic layers of *h*-BN and graphene [1,2]. We proved the robust molecular magnetism to be retained on a global and single molecule scale, even on metallic substrates [2-4]. In order to manipulate electronic and magnetic properties of individual SMMs chemical doping with alkali atoms has shown to be a feasible technique [5]. Unfortunately, large polynuclear compounds like Fe_4 can host numerous adsorption sites for dopants. Here we present successful chemical doping with a defined adsorption configuration for the prototypical Fe_4 SMM and study the effect on its electronic and magnetic properties.

[1] P. Erler et al., Nano Lett. 15, 4546 (2015). [2] L. Gragnaniello et al., Nano Lett. 17, 7177 (2017). [3] F. Paschke et al., ACS Nano 13, 780 (2019). [4] F. Paschke et al., Quantum Mater. Res. 1:e200002 (2020). [5] C. Krull et al., Nat. Mat. 12, 337 (2013).

O 68.3 Wed 10:30 P

An atomic Boltzmann machine capable of self-adaption — Brian Kiraly[1], •Elze J Knol[1], Werner MJ van Weerdenburg[1], Hilbert J Kappen[2], and Alexander A Khajetoorians[1] — [1]Institute for Molecules and Materials, Radboud University, Nijmegen, the Netherlands — [2]Donders Institute, Radboud University, Nijmegen, the Netherlands

To move beyond the current hybrid approaches to hardware-based artificial neural networks, new architectures, linking physical phenomena to machine learning models, are needed. Here, we realized an atomic Boltzmann machine capable of self-adaption using atomic manipulation with a scanning tunneling microscope. We utilized the concept of orbital memory, derived from single Co atoms on black phosphorus, as the building blocks of the prerequisite multi-well energy landscape. Namely, when gating two Co atoms simultaneously, there is a finite probability in each of the four possible states. This multi-well behavior persists for larger ensembles. Additionally, we found that the coupling between Co atoms is anisotropic, which we exploited to build synapses capable of tuning the neurons' energy landscape, and to introduce two inherent timescales: a fast neural timescale and a slow synaptic timescale. Finally, we observed self-adaption of the synaptic weights in response to external electrical stimuli, opening a path to on-chip learning in atomic-scale machine learning hardware.

B. Kiraly et al., arXiv:2005.01547v2 (2020)

O 68.4 Wed 10:30 P

Tunneling anisotropic magnetoresistance of Pb and Bi adatoms and dimers on Mn/W(110) — •Soumyajyoti Haldar, Mara Gutzeit, and Stefan Heinze — Institute of Theoretical Physics, University of Kiel, Leibnizstrasse 15, 24098 Kiel, Germany

Noncollinear magnetic structures at transition-metal interfaces are very promising candidates for spintronics applications [1]. A Mn monolayer on W(110) is a prominent example which exhibits a noncollinear cycloidal spin-spiral ground state with an angle of about 173° between neighboring spins. This allows to rotate the spin-quantization axis of an adatom or dimer quasicontinuously and is ideally suited to explore the angular dependence of the tunneling anisotropic magnetoresistance (TAMR) using scanning tunneling microscopy. Here [2], using density functional theory, we explored the TAMR effect of Pb and Bi adatoms and dimers adsorbed on this surface as these elements have a very strong spin-orbit coupling. Pb and Bi adatoms and dimers show a large TAMR up to 60% due to strong spin-orbit coupling (SOC) and the hybridization of 6*p* orbitals with 3*d* states of the magnetic layer. For dimers the TAMR also depends sensitively on the dimer orientation with respect to the crystallographic directions of the surface due to bonds formation with the surface and the symmetry of the SOC induced mixing.

[1] A. Fert et al. Nat. Nanotechnol. **8**, 152 (2013). [2] S. Haldar et al. Phys. Rev. B **100**, 094412 (2019)

O 68.5 Wed 10:30 P

Local electronic structure of lanthanide metallofullerene single-molecule magnets — •Tobias Birk[1], Fabian Paschke[1], Alexey Popov[2], and Mikhail Fonin[1] — [1]Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany — [2]Leibniz Institute for Solid State and Materials Research, Helmholtzstr. 20, 01069 Dresden, Germany

Dimetallofullerenes with single-electron lanthanide-lanthanide (Ln-Ln) bonds are new promising single-molecule magnets with exceptional robustness and high blocking temperatures up to 25 K [1]. These molecules are well suited for STM based magnetization relaxation and spin excitation measurements due to their high blocking temperature and exceptional stability.

Here we present the first successful deposition of the lanthanide metallofullerene single-molecule magnet $Dy_2@C_{80}(CH_2Ph)$ on graphene/Ir(111) using electrospray deposition (ESD). Scanning tunneling microscopy (STM) and spectroscopy (STS) measurements are performed in order to study ordering behavior and electronic properties on this weak coupling substrate. The observation of LUMO resonances in combination with varying topographic appearances reveal different adsorption configurations of the molecules on the surface. Additional comparison between molecules with Dy and Er atoms as magnetic centers show a shift in LUMO energies proving that electron tunneling mediated by the single-electron Ln-Ln bond is possible.

[1] F. Liu et al. Nat Commun 10, 571 (2019).

O 68.6 Wed 10:30 P

Complete reversal of the atomic unquenched orbital moment by a single electron — •Rasa Rejali[1], David Coffey[1], Jeremie Gobeil[1], Jhon W. González[2], Fernando Delgado[3], and Alexander F. Otte[1] — [1]Delft University of Technology, Delft, The Netherlands — [2]Universidad Técnica Federico Santa María, Valparaíso, Chile — [3]Universidad de La Laguna, Santa Cruz de Tenerife, Spain

Efforts to downscale information storage to the single-atom limit have largely focused on readily probing and manipulating the spin of single magnetic atoms adsorbed on surfaces. This emphasis on the spin is primarily due to orbital quenching combined with spin-orbit coupling: the orbital angular momentum of these systems is often diminished due to the local symmetry of the surface, and what remains of it typically delineates the direction of the electron spin. This limits the scope of information processing based on these atoms to essentially one magnetic degree of freedom: the spin. By coordinating a Fe atom atop the fourfold symmetric nitrogen binding site of the $Cu_2N/Cu_3Au(100)$ surface, we gain independent access to both the spin and orbital degrees

of freedom. We demonstrate a full rotation of the orbital moment, without altering the spin state of the atom; and a distinct spin excitation, which does not affect the orbital moment. The full inversion of the unquenched moment is a seemingly forbidden transition ($\Delta m = 4$) that defies the selection rules that apply to the spin ($\Delta m = 1$); we justify this apparent violation of momentum conversation in terms of the Einstein-de Haas effect.

O 68.7 Wed 10:30 P

Hyperfine fields of magnetic adatoms on ultrathin insulating films — •SUFYAN SHEHADA[1,2], Manuel dos Santos Dias[1], Filipe Souza Mendes Guimarães[1], Muayad Abusaa[3], and Samir Lounis[1,4] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, 52425 Jülich, Germany — [2]Department of Physics, RWTH Aachen University, 52056 Aachen, Germany — [3]Department of Physics, Arab American University, Jenin, Palestine — [4]Faculty of Physics, University of Duisburg-Essen, 47053 Duisburg, Germany

Individual nuclear spin states can have very long lifetimes and could be useful as qubits. Promising steps in this direction were realized on MgO/Ag(001) via STM detection of the hyperfine interaction (HFI) of Fe and Ti adatoms [1] and the electrical control of the nuclear polarization of Cu adatoms [2]. Here, we report on systematic first-principles calculations of the HFI for $3d$ adatoms (Sc–Cu) atop ultra-thin insulators (MgO, NaF, NaCl, h–BN and Cu_2N) [3]. We analyze the trends and the dependence of the computed HFI on the filling of the magnetic s and d-orbitals of the adatoms and on bonding type and strength with the substrate. Finally, we identify promising candidates for future experimental investigations with scanning probe techniques.
–Work funded by the Palestinian-German Science Bridge (BMBF–01DH16027) and Horizon 2020–ERC (CoG 681405–DYNASORE).
[1] Willke *et al.*, Science **362**, 336 (2018); [2] Yang *et al.*, Nat. Nanotechnol. **13**, 1120 (2018); [3] Shehada et al. ArXiv:2012.11639.