O 70: Gerhard Ertl Young Investigator Award

Time: Thursday 11:15–13:45 Location: WIL C307

O 70.1 Thu 11:15 WIL C307

A chemical switch for molecular spins undergoing exchange coupling with magnetic substrate — Chriatian Wäckerlin[1], Dorota Chylarecka[1], Armin Kleibert[2], Kathrin Müller[1], Cristian Iacovita[3], Frithjof Nolting[2], Thomas A. Jung[1], and •Nirmalya Ballav[1] — [1]Laboratory for Micro and Nanotechnology, Paul Scherrer Institut, 5232 Villigen, Switzerland — [2]Swiss Light Source, Paul Scherrer Institut, 5232 Villigen, Switzerland — [3]Department of Physics, University of Basel, 4056 Basel, Switzerland

The regulation of oxygen affinity in hemoglobin by the iron-porphyrin moiety as shown in nature has been used as a designed concept to perform the switching event of single molecular spins on the surface. This degree of control is achieved upon modifying the coordination sphere of the metal ion of a cobalt(II)tetraphenylporphyrin (CoTPP) molecule ferromagnetically coupled to a nickel (Ni) thin film substrate by the nitric oxide (NO) functioning as an axial ligand. On NO addition, coordination sphere of the Co-ion is modified and a NO-CoTPP nitrosyl complex is formed, which corresponds to an off-state of the Co spin. Thermal dissociation of NO from the nitrosyl complex restores the on-state of the Co spin. The NO-induced reversible off-on switching of surface adsorbed molecular spins observed here is attributed to a spin-trans effect. Use of external stimuli to control single molecular spins at magnetic-interfaces is of potential interest for spintronics and quantum information.

O 70.2 Thu 11:45 WIL C307

Manipulation of the spin structure of metallic QWS and topological insulators. — •Hugo Dil[1,2], Fabian Meier[1,2], Bartosz Slomski[1,2], and Juerg Osterwalder[1] — [1]Physik-Institut, Universitat Zurich, Winterthurerstrasse 190, 8057 Zurich, Switzerland — [2]Swiss Light Source, Paul Scherrer Institute, 5232 Villigen PSI, Switzerland

The electronic structure of non-magnetic low-dimensional materials can acquire a spin structure due to the breaking of the inversion symmetry at the surface or interface. This so-called Rashba effect is a prime candidate for the manipulation of the electron spin without using any magnetic fields. This is crucial for the emerging field of spintronics, where the spin of the electron instead of its charge is used to transport or store information. Spin and angle resolved photoemission is currently one of the main experimental methods to measure the spin resolved electronic structure, which contains all the relevant information for spintronics [1]. Here it will be shown how the knowledge obtained from model Rashba systems can be applied to increasingly complex systems and result in the possibility to manipulate the spin structure of ultrathin Pb films [1] and topological insulators [3].

[1] For a review see: J. Hugo Dil, J. Phys.: Condens. Matter 21 403001 (2009). [2] H. Dil et al. Phys. Rev. Lett. 101, 266802 (2008). [3] D. Hsieh et al. Nature 460, 1101 (2009).

O 70.3 Thu 12:15 WIL C307

Substrate-Induced Mechanical Transformations in Graphene Films: A Basic Surface Science Approach Towards Controlled Nanoscale Engineering — •Nicola Ferralis — University of California, Berkeley, CA 94720, USA

Compared to research into graphene's remarkable electronic properties, much less is known about how its mechanical and elastic properties are affected by the presence of a supporting substrate. Yet, the response of graphene films to mechanical stimuli is an important fundamental surface science and nanotechnology topic, with potentially far reaching applications in high performance linear and nonlinear electronic, photonic, electrochemical and electromechanical elements. Here, the results of direct investigations of graphene's elastic and mechanical properties at the graphene-substrate interface are presented. Substrate-induced strain in epitaxial graphene grown on SiC surfaces is found to be related to the large difference in the linear expansion coefficient of graphene and the substrate. Furthermore, the amount of strain induced by the substrate is found to be tunable, through optimized graphene growth conditions, from strain-free to up to 0.1%. A comprehensive description of the temperature dependent evolution of the graphene Raman spectra is used to determine and quantify the strength of the graphene-substrate pinning. Through a comprehensive modeling of the interaction of interatomic potentials, it is found that the degree of pinning is substrate-dependent. While graphene on SiC shows a high degree of pinning, graphene grown on metal surfaces behaves as freestanding graphene.

O 70.4 Thu 12:45 WIL C307

Measuring Nanosecond Spin Dynamics at the Atomic Scale — •Sebastian Loth — IBM Research - Almaden, San Jose, CA, USA

Transition metal atoms that were placed on a monolayer-thin film of copper nitride (Cu$_2$N) on Cu (100) exhibit unusually large magnetic anisotropy that enables long electron spin lifetimes. The magnetic atoms exhibit discrete spin states that can be probed by inelastic electron tunneling spectroscopy (IETS). We make use of a quantized analogue of spin-momentum transfer to interact with the local spin. A large spin-polarized tunnel current pumps the spin of the magnetic atoms into highly excited states allowing us to quantify the lifetimes of different spin excitations.

Direct access to the dynamical evolution of magnetic atoms in the time domain can be obtained by combining spin-polarized scanning tunneling microscopy (SP-STM) with an all-electronic pump-probe measurement scheme: a continuous train of fast voltage pulses is applied to the tunnel junction where a pump pulse excites the magnetic atom and a time-delayed weaker probe pulse monitors the post-excitation dynamics with nanosecond precision. We find that the spin relaxation time of a Fe atom on Cu$_2$N can be increased beyond 200 ns by placing a Cu atom adjacent to it. This enables studies of quantum tunneling of magnetization that occurs in these dimers.

The ability to probe individual nanostructures with atomic spatial and nanosecond temporal resolution opens a new avenue to explore spin dynamics and other dynamical phenomena on the intrinsic length scale of the underlying interactions.

O 70.5 Thu 13:15 WIL C307

Towards accurate modeling of van der Waals interactions for surfaces and interfaces — •Alexandre Tkatchenko — Fritz-Haber-Institut der MPG, Berlin, Germany

Density-functional theory (DFT) is the method of choice for the modeling of properties and functions of surfaces and interfaces, typically yielding reasonable trends for strong chemical bonding. In the quest for a predictive method for interface modeling, the most pressing issue is thus an accurate description of the long-range van der Waals (vdW) interactions [1,2]. We have recently developed a set of efficient methods for an accurate description of intermolecular vdW interactions in DFT and MP2 theories [2,3]. When applied to the adsorption of nitrogen on graphite, our methods yield quantitative agreement with all experimentally measured data. Our PBE+vdW method also leads to accurate adsorption geometries for complex switches on metallic surfaces [4], as well as for the isophorone/Pd(111) system, where a balanced description of both the chemisorbed and the physisorbed state is essential. Despite these successes, the adsorption energies for molecules on metallic surfaces are systematically too large. The inclusion of screening effects inside the bulk by approximate methods leads to an improved agreement with experimental desorption enthalpies. The comparison of our theory with the non-local vdW-DF functional [1] and the many-body EX+cRPA method will be discussed. [1] M. Dion *et al.*, PRL 92, 246401 (2004); [2] A. Tkatchenko and M. Scheffler, PRL 102, 073005 (2009); [3] A. Tkatchenko *et al.*, JCP 131, 094106 (2009); [4] G. Mercurio *et al.*, PRL 104, 036102 (2010).