Psi-K Scientific Report of the "FunMol2012" Workshop: "Functional Molecules on Surfaces: New Building Blocks for Nano-spintronics" held at the Gustav-Stresemann-Institut (GSI), 2th-4th November, Bonn, Germany

SUMMARY

Spin-dependent effects and interactions play a very significant role in current research in nanoscience. The study of the electron spin degrees of freedom at the molecular scale has conveyed an increasing attention both from fundamental and technological points of view. Much effort is devoted nowadays to the integration of novel functional metalorganic molecules with tailored electronic and magnetic properties into traditional solid-state nano-electronic devices. Quantum computing, ultra-high density magnetic storage, and spintronics are some of the most promising research areas that could lead to major technological breakthroughs. Functional magnetic molecules play a key role in these fields since they provide tunable nanometer-size magnetic units, which is an essential requirement for constructing new devices. The occurrence of magnetic hysteresis at the molecular level, due to the quantum phenomenon of slow magnetic relaxation in high-spin single molecule magnets (SMM) has raised a tremendous scientific interest and has suggested some revolutionary applications. Recently, an increasing number of molecules has been successfully sublimated or dry-imprinted in ultra-high vacuum conditions. Among them, a dominant role has been attained by the very robust family of monometallic porphyrins, phthalocyanines, and rareearth double deckers; lately complex poly-metallic molecules as Fe₄ and Cr-base molecular rings have been also deposited by liquid phase or under UHV on Au(111) surfaces.

Density-functional methods have played a crucial role in the characterization of molecules in the gas phase and of molecule-surface systems. The emphasis has been placed on different issues, such as the extraction of the magnetic exchange and spin interaction parameters in polymetallic magnetic molecules by total energy calculations, the influence that structural rearrangement or chemical modification have on electronic, magnetic and transport properties, or the development of advanced theoretical methodologies in order to properly account for the molecule-surface interaction.

The efforts made in the last few years brought to important advances in this field. First of all, van der Waals dispersion interactions, the inclusion of which is indispensable to correctly characterize adsorption energies and geometries of molecules on surface, have been taken into account from first principles or by means of simplified parameterizations. Secondly, in order to assess correctly charge-transfer, work-function modifications, molecular orbitals–surface levels alignment and transport across molecule-surface interfaces, methods to correct the incomplete self-interaction cancellation and, in general, account for the electronic correlations beyond local density exchange-correlation functionals have been considered. The use of optimized effective potentials, Hubbard on-site terms, and hybrid functionals, or of the GW approximation are some of the possible approaches towards solutions to these problems.

Simulations of scanning tunneling microscopy and spectroscopy experiments have demonstrated to be essential for the correct assessment of what is actually measured in experiments on molecules. They provide as well a benchmark validating the computational results and theoretical approximations. Finally, in the transport regime, functional molecules might lead to unique spin filtering capabilities or tunable (with structural, electric, magnetic or radiative stimuli) conducting channels, and are candidates themselves as future building blocks for electronic nano-devices.

The theoretical characterization of the above issues is clearly a fundamental step that the scientific community is challenged with.

DESCRIPTION OF SCIENTIFIC CONTENT AND DISCUSSIONS AT THE EVENT

The oral contributions were organized in five sessions:

- Functional molecules on surfaces and in molecular junctions
- Transport and tunneling through functional molecules
- Dispersion forces
- Carbon based nanostructures and graphene
- Functional molecules and networks

Each session was arranged such to have at the early stage a presentation of a key experimental scientist working in the field, to set the stage and frame of reference.

During the sessions tackling the issue of "Functional molecules on surfaces and in molecular junctions" there have been several contributions that gave relevant cues for discussions. The class of magnetic molecules discussed was broad, ranging for purely organic ones (radicals, graphene sheets), to monometallic, i.e. metal-phthalocyanines (MPcs), metal–porphyrines (MPs), metalloces, rare-earth double deckers (DDs), to polymetallic, e.g. Fe₄ and Cr₇M-family, ones.

Roberta Sessoli, who started the 1st session of the workshop, reported a systematic investigation on magnetic anisotropies in lanthanides, and unveiled the importance of the whole structure of the molecules, even organic ligands far away from the magnetic ion, revealing non-trivial magnetostructural correlations. She pointed out also the role of molecular packing in thin films, since magnetic exchange between Tb SMM influences the spin-dynamics, even more than the interaction with a magnetic substrate. Such interaction is instead critical in case of Fe₄ molecules deposited on LSMO substrates, where suppression of Quantum Tunneling of the Magnetization at zero field is observed due to some sort of magnetic exchange between molecule and substrate. The choice of LSMO, is driven by the important role that play such substrate in organic spintronic devices, because of its high spin-filter capability being half-metallic. Here the critical point discussed also by Federico Totti, is the knowledge of termination layers of LSMO; DFT calculations predicted very small (ferromagnetic) coupling between Fe₄ and LSMO (1 or 3 µeV depending on the MnO or SrLaO termination). He pointed also out how, exploiting the self-assembly properties of organic radicals on the Au surface, a magnetic network could be achieved. Further work on Fe₄, this time deposited on a non magnetic surface, i.e. Au(111), has been presented by Carlo Canali, that analyzed the stability of the spin ordering and magnetic anisotropy of Fe₄ as a function of several parameters (simulation parameters, and substrate choice). The presence of a surface or lead might alter the charge states of the molecule, and consequently the magnetic properties could be modified. He showed also as an external electric field might further tune the magnetic properties of the molecules, and how such change could be extracted with first-principles studies. He posted an interesting problem that will stimulate further theoretical work, on whether adding self-interaction corrections to the Hamiltonian might lead to a more 'Coulomb Blockade' regime, or if that regime is necessarily obtained only within an out-of-equilibrium transport approach. Further work on electric-field simulation has been presented by Mark Pederson that reviewed the capability of DFT-based method in describing the electric-field effects on the magnetic anisotropy of molecular magnets. This last issue is of critical importance when switching of the spin state of the molecule is required with external stimuli. Graphene nanosheets have been also addressed as possible spin unit to be coupled with standard molecular magnets.

If the above presentations were dedicated to high-spin single-molecule magnets, with possible applications in molecular spintronics and magnetic information storage, **Marco Affronte** has given a comprehensive report on low spin antiferromagnetic molecular wheels, systems of interest to implement quantum bits and quantum computing schemes. The properties of self-assembly of specific derivatives of Cr₇Ni, and of the capability to resolve through XMCD techniques, which selectively probes local magnetic properties such of the metal ions, the magnetic properties, i.e. inter-ring ordering but also the anisotropy of excited magnetic states, of the whole molecules has

been highlighted. Experimental results have been validated by density-functional studies. **Carlo Massobrio** reported on a combined experimental and theoretical study on the stability of ferrocene on Cu(111) susbtrate. By Born-Oppenheimer molecular dynamics (BOMD) calculations and scanning tunneling experiments it was demonstrated how such molecules are stable on Cu, while are known to dismember on Au, and how they assembly in a ML. Calculations suggest also that a Cu atom could stick on top of a ferrocene, and that it acts as a local potential perturbation that pushes the electrons of the interfacial delocalized states, parent to the surface Schottky 2-DEG Cu(111) surface state, into a resonant localized state, opening new perspective in tuning surface states.

Other seminars were devoted to the study of MPcs and MPs, both on non-magnetic and magnetic substrates. **Peter Oppeneer** has reviewed a whole series of experimental and theoretical calculations on on-surface magneto-chemistry events, showing how the magnetic coupling between porphyrins PPs and phthalocyanines PCs on magnetic substrates (Ni, Co) could be tuned by proper axial-ligand absorption (NO or NH₃). Molecule-substrate magnetic interaction could be modified, e.g. from FM to AFM, or spin states of the metal ions in the PP or PC could be modified or turned off. Moreover it has been pointed out that such magnetic interaction arise also if a graphene layer is placed on the magnetic Ni surface, and opening interesting fields in carbon-based spintronics. Further experimental evidence on how the molecule-substrate magnetic coupling could be tailored has been give by **Heiko Wende**, that highlighted in this respect the capabilities of the XMCD technique in extracting magnetic information with sub-monolayer sensitivity. The magnetic coupling could be tuned by acting on the chemical functionalization either of the molecule or the magnetic surface. Structural modification of the molecules could also lead to a switch of the magnetic state of the molecule, for instance by exploiting the tensile stress felt by on a di-vacancy in a graphene sheet.

Jens Kortus has, in addition to further combined calculation-experiments of CoPc on magnetic and non magnetic substrate, discussed the case of a bilayer of a heterojunction created by the interface of two films of fluorinated CoPc and of MnPc, grown on Au(111). Charge and spin transfer happens at the interface, and this might modify sensibly transport properties across such junctions, issue of clear interest when designing organic electronic devices. Comparison of XAS and EELS calculated spectra with experimental ones could help in sorting the correct stacking of an assembly of molecules. Another important feature that metal phthalocyanines exhibits on metal substrates is the Kondo regime. **Nicolas Lorente** presented a nice overview on Kondo effects on MPc on Ag(100) as a function of the metal ion, showing how the presence or not of Kondo peaks has to be traced back on the type of charge transfer acting at the molecule-metal interface. Moreover, in case of TbPc₂ on Au(111), it has been discussed how Kondo features could be switched on/off, by modifying the registration angle between the two PCs composing the double decker. These results are of relevance when the understanding of transport properties across such molecules is sought.

Further cues on the transport issue has been given by **Jeffrey Neaton** that pointed out how the correct description of molecule-metal level alignment is a fundamental issue in electronic and transport calculations in these systems, showing how several approaches have been attempted, from the construction of refined density-functionals, containing short range exchange and correlation effects, e.g. HSE functional, to more computational demanding GW methods. Band-gap closing due to polarization of the substrate is completely missing within DFT, and still lacking in large part in short-range hybrid functionals, while captured with GW. Along this line, **Kristian Sommer Thygesen** described the issue that a charged molecule on a metal surface gives rise to image charge effects, which modify the molecular orbitals and in turn the transport properties. Standard DFT overestimates the conductance of molecular junction as compared to experiments. An improvement comes again from the GW approximation, as a consequence of an improved alignment of the molecular levels with respect to the metal Fermi level.

Several other seminars, that focused on issues related to transport simulations and experiments through scanning-tunneling microscopies, were collected in the session "Transport and tunneling

through functional molecules". Here, leading experimentalists coming from the surface science and chemical synthesis gave an important contribution in highlighting the capability of scanning tunneling microscopies and manipulation techniques.

Richard Berndt showed how conductance experiments at the single molecule level could be performed by utilizing a STM tip. This approach allows to perform single molecule contacts with precise control of the junction geometry. Experiments revealed how the geometry of the contact crucially affects the conductance of the device. Moreover, manipulations techniques allow to modify the molecules by switching their configuration, removing, adding, substituting atoms. Analyzing the emitted photons and the shot noise allows for a deeper insight into the molecular junction properties. **Mario Ruben** concentrated on TbPc₂ double decker molecules and on the interaction with different substrates. Depending on the substrate, i.e. Cu(111), Au(111) or Co/Ir (111), he showed how different type of coupling are achieved. On Cu, the organic radical on the lower Pc is quenched by the interaction with the substrate, while on Au the molecule behaves as a S=1/2 Kondo system. On Co, instead, clear evidence of a spin-splitted molecular orbital is reported, sign of a some kind of exchange coupling between the molecule and the magnetic substrate atoms.

Another presentation, given by **Saw Wai Hla**, was devoted to the capability of STM in resolving electronic properties of adsorbed molecular structures. When two types of molecules having tendencies to accept and donate the electronic charge are put together, charge transfer can lead to engineer materials with intriguing properties. For example, clusters composed of BETS and GaCl₄ molecules on Ag(111) exhibit superconductivity, while McnE combined with TCNQ on Au(111) behaves as a molecular motor for which a controlled directional rotation can be achieved with electron injection from a STM tip. The manipulation capabilities of STM has been ultimately demonstrated by **Germar Hoffmann** that showed how the chirality in TbPc₂ could be tuned, rotating the upper Pc with respect to the lower one, opening potential nanotechnological applications. Molecular spin chains could also be assembled by atomic manipulation, and STM could reveal intra-chain difference in the Kondo effects shown when adsorbing such nanostructures on Au(111).

From the theoretical point of view, Michael Rohlfing showed how the electronic structure of molecules can be strongly modified by the interaction with a surface. He pointed out that, in order to correctly describe the spectrum, a combination of DFT, many-body perturbation theory and renormalization group theory might be necessary, and this methodology was successfully applied to the case of PTCDA on Ag(111). Stefano Sanvito dedicated the seminar to the physics of spincrossover compounds that exhibit transition between two spin states. The switch between the two can be achieved with an external electric field that modifies the exchange interaction between the two magnetic units of the molecule; in describing the transition between high and low-spin states, the choice of the exchange correlation functional is crucial. Transport across such molecules has been discussed, in terms of possible application in spintronics devices. Giovanni Cuniberti has introduced the interesting case of how helical molecular systems, even if non-magnetic such as DNA, can act as spin filters. The charge flowing along the molecule axis experiences a helical electrostatic potential that is at the origin of an unconventional Rashba-like spin-orbit interaction. This, in combination with a small dispersion, leads to a low mobility of the charges and allows even weak spin-orbit interactions to be effective. The electronic and magnetic properties of Mn12 adsorbed on Bi have been investigated by Kyungwha Park, employing DFT+U+spin-orbit methods. It is outlined the effect that a strongly spin-orbit coupled substrate has on the singlemolecule magnet, and that the inclusion of the on-site Coulomb interaction (U) considerably affects the HOMO-LUMO gap. Dipole corrections were found to be important for this system. Andrea Floris discussed supramolecular networks of Mn- and Cs-TCNQ4, where the nature of the metal-TCNQ bond determines the geometry and the chirality. The size of the total and induced dipole moments affects the electrostatic energy.

A whole session has been dedicated to a critical issue in theoretical methodologies tackling molecule-substrate systems, namely the correct description of van der Waals forces.

Stefan Grimme described how to include the dispersion corrections within density functional theory (DFT) by using a semiempirical approach for which the molecular dispersion coefficients are deduced from ab intio calculations based on high accurate wave-function type methods. He presented several approaches that account for the van der Waals interactions and discussed them in relation to density functional methods which use non-local correlation functionals to account for the van der Waals interactions. Ikutaro Hamada presented a thoroughly analysis of the van der Waals nonlocal density functional (vdW-DF) applied to several adsorption systems. A very important part of his presentation was also focused on how to improve the accuracy of the vdW-DF functional by using several approximations for the exchange functional. Wei Liu presented the results for several molecules and substrates, spanning the whole range from physisorption to chemisorption employing two different dispersion-inclusive density-functional methods. Most interestingly, he demonstrated that van der Waals interactions play an important role also in those cases where covalent binding is active between the molecule and the substrate. Yoshitada Morikawa discussed about firstprinciples investigations of dipole layer formation at the hybrid organic/metal interfaces. His results showed how the interfaced dipole layer modifies the alignment of the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular level (LUMO) of a molecule with respect to the Fermi level of the metal. Interestingly, the substrate dependence of interface dipole for physisorbed systems mainly comes from the difference in the interface geometry, especially the organic-metal distance that requires the inclusion of van der Waals dispersion forces in the theoretical simulations. Predrag Lazic spoke about the role of the nonlocal correlation (NL) effects in the surface adsorption of several pi-conjugated organic systems adsorbed on metal surfaces. Even more interestingly, he demonstrated how the correct treatment of the NL effects within DFT improves also the description of the chemisorbed systems and solves the well-known "CO puzzle".

Another session was dedicated to functional carbon-based nanostructures. Lapo Bogani reviewed how to exploit the outstanding transport characteristic of graphene and carbon nanotubes, and how chemically-tailored nanomagnets can be selectively grafted onto them, creating hybrid materials. The aim is to develop novel spintronic devices, and sensors able for single molecule detection. Bart **Partoens** showed systematic studies how to modify and manipulate the electronic structure of graphene by using the processes of (i) physisorption of small organic molecules which leads to a charge transfer and (ii) chemisorption of hydrogen and fluorine atoms which induce distortions into the pi-aromatic system. Claudia Draxl presented a very exiting talk on the adsorption of piconjugated organic molecules inside Carbon nanotubes. Her convincing theoretical studies demonstrated how these organic hybrids could be used as nano-sized light emitting nano-peapods. Finally a session was devoted to the search of functional molecules and networks.

Eliseo Ruiz elected mononuclear transition metal complexes, exhibiting single-ion magnet behavior, as possible spin units, and presented systematic CASSCF-RASCI calculations. By analyzing the mathematical expression of the anisotropy parameters, he suggested how to predict, by tuning the electronic configuration and coordination, which 3d metal ions can present large axial magnetic anisotropy. **Mihail Atanasov** discussed first-principles insights of the magnetic anisotropy in linear high-spin complex molecular networks based on iron. His studies indicated that these types of materials have a large spin-orbit coupling that leads to large orbital moments, which contribute to the total magnetic moment. These molecular networks are suitable candidates to be drafted on surfaces and possible building blocks for larger magnetic clusters with increased the total spin and therefore the relaxation time. **Alessandro Stroppa**, who concluded the Workshop, focused on metal-organic frameworks (MOFs). Employing ab-initio methods, he described how orbital order induced ferroelectricity could be found. Most interestingly, the switching of the polarization direction implies the reversal of the ferromagnetic component, electing this emerging class of functional materials as breakthrough candidates for various technological applications.

ASSESSMENT OF THE RESULTS AND IMPACT OF THE EVENT ON THE FUTURE DIRECTIONS OF THE FIELD

The objective of the Workshop was to bring together an international forum of computational scientists from different areas: molecules with spin, molecular magnets, magnetism, surface science, molecular electronics and spintronics complemented by expert experimentalists and chemists to create a interdisciplinary environment to explore the challenges and opportunities of this novel field of molecular spintronics. The goal was to induce stimulating discussions on effective strategies for controlling and tuning the spin degrees of freedom in molecule-surface systems by means of interaction with the environment. This is possible, on one side, by chemical modification or structural reorganization due to molecule-surface interactions, on the other side, by tuning the magnetic properties with external stimuli, e.g. electric field, addition or removal of electrons, electromagnetic radiation or mechanical switching.

The Workshop was mainly devoted to the theoretical characterization of functional magnetic molecules on surfaces by means of density-functional based theoretical methodologies. A limited (\approx 15-20%), but scientifically representative, embassy of leading experimental scientists was necessarily considered, and has contributed to the success of the Workshop. In order to support idea exchange and in-depth discussions, the sessions where mainly composed by invited seminars (30+5 minutes) plus a few contributed talks (15+5); a poster session was also scheduled for contributing authors / participants. There were 54 participants.

The success of the Workshop was intimately related to the high-level of all the speakers and on the presence of world-leading experimentalists. Not only several issues on the theoretical methodology were discussed (inclusion of vdW, role of electronic correlation and surfaces dipole formation in the energy level alignment between the molecules and the substrate) but a more broad view on the problem was offered discussing the role of carbon-based materials, the ultimate capabilities of the XMCD and STM techniques, and possible switching mechanisms of the magnetic properties by exploiting structural or electromagnetic (electric fields, charging effects during tunneling, magnetic fields) stimuli. This Workshop followed another meeting organized in Uppsala in 2011 by B. Brena, B. Sanyal, P. Oppeneer and T. Saha-Dagupta, where similar thematics were addressed and several speakers were in common. The importance of arranging similar meetings with continuity was evident in the audience and it was proposed to organize them possibly with a cadence of two year.

ANNEX I: PROGRAM OF THE FUNMOL2012 WORKSHOP

Tuesday 2nd October

8.50 - 9.00	Welcome			
	Session: "Functional molecules on surfaces and in molecular junctions I"			
9.00 - 9.35	Roberta Sessoli: "Single molecule magnets on surfaces: achievements and challenges"			
9.35 - 10.10	Federico Totti: "Molecular magnets on surfaces: from tailoring to the catwalk"			
10.10 - 10.45	Carlo Maria Canali: "Magnetic properties of the charged states of Fe ₄ SMM on surfaces and in			
	molecular junctions"			
10.45 - 11.15	Coffee break			
	Session: "Transport and tunneling through functional molecules I"			
11.15 - 11.50	Richard Berndt: "A surface science approach to molecular conductance"			
11.50 - 12.25	Kristian Sommer Thygesen: "Quasiparticle calculations for metal / molecule interfaces"			
12.25 - 14.00	Lunch break			
14.00 - 14.35	Mario Ruben: "Supramolecular quantum spintronics"			
	Session: "Dispersion forces"			
14.35 - 15.10	Stefan Grimme: "Dispersion corrections for density functional theory"			
15.10 - 15.45	Ikutaro Hamada: "Van der Waals density functional applied to adsorption systems"			
15.45 - 16.05	Wei Liu: "Benzene adsorbed on metals: concerted effect of covalency and van der Waals bonding"			

16.05 - 16.35	Coffee break
16.35 - 17.10	Yoshitada Morikawa: "First-principles investigation of dipole layer formation at organic/metal
	interfaces"
17.10 - 17.45	Predrag Lazic: "The role of the nonlocal correlation in surface adsorption"
17.45 - 19.00	Poster session
19.00	Dinner

Tuesday 3rd October

 9.00 - 9.35 Marco Affronte: "Control in the deposition of functional molecular nanomagnets on surfaces" 9.35 - 10.10 Carlo Massobrio: "Structural, electronic and magnetic properties at the ferrocene/Cu(111) interface" Jeff Neaton: "Electronic structure and energy conversion at organic-inorganic interfaces, from junctions to assemblies" 10.45 - 11.15 Coffee break Session: "Functional molecules on surfaces and in molecular junctions III" 11.15 - 11.50 Peter Oppeneer: "Magnetic interactions at the metal-organic molecule / substrate interface: Insight from first-principles calculations" 11.50 - 12.25 Heiko Wende: "Utilizing molecule/substrate interactions to create new spin-hybrid systems" 12.25 - 14.00 Lunch break Session: "Transport and tunneling through functional molecules II" 14.35 - 14.55 Michael Rohlfing: "Molecular electronic spectrum on a metal substrate: quasiparticle energies and Kondo resonance" 14.55 - 15.30 Stefano Sanvito: "Molecular spintronics with spin crossover compounds" 16.35 - 17.10 Lapo Bogani: "Carbon nanostructures and graphene" 16.35 - 17.10 Lapo Bogani: "Carbon nanostructures and molecular magnets: from ultra-high sensitivity to molecular spintronics" 17.45 - 18.20 Claudia Draxl: "Organic pi-conjugated molecules inside carbon nanotubes: nano-sized light-emitting hybrids" 		Session: "Functional molecules on surfaces and in molecular junctions II"				
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hybrids"	17.10 - 17.45	Bart Partoens: "Hydrogenation and fluorination of single and bilayer graphene"				
19.00 Conference dinner	17.45 - 18.20					
	19.00	Conference dinner				

Thursday 4th October

	Session: "Functional molecules on surfaces and in molecular junctions IV"				
9.00 - 9.35	Germar Hoffmann: "Interviewing a molecular spin state"				
9.35 - 10.10	Kyungwha Park : "Effect of a strongly spin-orbit coupled substrate on a single-molecule magnet Mn_{12} "				
10.10 - 10.30	Andrea Floris: "Stereoselectivity and electrostatics in charge-transfer Mn- and Cs-TCNQ ₄ networks on Ag(100)"				
10.30 - 11.00	Coffee break				
	Session: "Transport and tunneling through functional molecules III"				
11.00 - 11.35	Jens Kortus: "Metal-phthalocyanines: materials for molecular spintronics"				
11.35 - 12.10	Nicolas Lorente: "Magnetic properties of phthalocyanine derivates on metal surfaces: from magnetic IETS to the Kondo effect"				
12.10 - 12.30	Mark Pederson: "DFT-based Modeling of field-dependent control and response of nanomagnetic molecules"				
12.30 - 13.30	Lunch break				
	Session: "Functional molecules and networks"				
13.30 - 14.05	Eliseo Ruiz: "Mononuclear transition metal complexes: a simple alternative"				
14.05 - 14.40	Mihail Atanasov: "Chemical bonding, vibronic coupling and magnetic anisotropy in linear iron(II) complexes"				
14.40 - 15.00	Alessandro Stroppa: "Polar and magneto-electric properties of anti-ferrodistortive ordered Jahn- Teller distortions in a metal-organic multiferroic"				
15.00	Conclusions				

ANNEX II: FULL LIST OF SPEAKERS AND PARTICIPANTS (organizers, invited speakers, contributed speakers)

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