Scientific Program - *Spin+X* Summer School Molecular Spintronics 2018

	October 08th Monday	October 09th Tuesday	October 10th Wednesday
09:00 - 10:30		**Alberto Riminucci** "Interplay between charge and spin conductance in molecular semiconductors and its applications to neuromorphic computing"	**Benjamin Stadtmüller** "Spin-dependent phenomena at metal-organic interfaces – Functionalization of spin-interfaces"
		coffee break	
11:00 - 12:30	welcome coffee	**Roberta Sessoli** "Spin dynamics of magnetic molecules"	**Matteo Mannini** "Organization and characterization of magnetic molecules assembled on surfaces and interfaces"
13:30	Welcome Eva Rentschler	lunch break	
14:00 - 15:30	**Andrea Droghetti** "A (biased) overview about molecular spintronics"	Poster Flash-Presentations	**Erik R. McNellis** "First-Principles and Multi-Scale Modeling in Molecular Spintronics Development"
		break	
16:00 - 17:30	**Andrea Cornia** "Designing magnetic molecules and their spin Hamiltonian"	Poster Session	**Marco Affronte** "Towards devices at single molecule scale"
			Farewell
		Dinner	

www.ak-rentschler.chemie.uni-mainz.de/MolSpin-School-2018

The school aims to provide a deep and comprehensive understanding of the state of the art of scientific activities in the field of Molecular Spintronics. Molecular spintronics combines the ideas of spintronics and molecular electronics striving for manipulating spins and charges in electronic devices containing only one or few molecules.
The weak spin-orbit interaction in organic molecules is likely to preserve spin-coherence over time and distance much longer than in conventional metals or semiconductors. Moreover, the interaction of molecules with electrodes surface can be used to tune the energy level alignment at hybrid interfaces and thus facilitate an efficient spin injection. Currently, there is an increased activity on embedding in spintronics devices functional molecules. Among them, magnetic molecules, either showing magnetic bistability at low temperature or long quantum spin coherence, are particularly attractive also in connection with quantum information technology.

CONFIRMED SPEAKERS

Marco Affronte (Universitá di Modena, Italy)
Andrea Cornia (Universitá di Modena, Italy)
Valentin Alek Dediu (Institute of Nanostructured Materials ISMN-CNR, Bologna, Italy)
Andrea Droghetti (ETSF Sab Sebastian, Spain)
Matteo Mannini (Universitá di Firenze, Italy)
Erik R. McNellis (JGU Mainz, Germany)
Alberto Riminucci (Institute of Nanostructured Materials ISMN-CNR, Bologna, Italy)
Roberta Sessoli (Universitá di Firenze, Italy)
Benjamin Stadtmüller (TU Kaiserslautern, Germany)

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Financially supported by the

SPIN+X SFB/TRR 173 Kaiserslautern • Mainz

MATERIALS IN MAINZ SCIENCE

A (biased) overview about molecular spintronics

Andrea Droghetti

University of the Basque Country and European Theoretical Spectroscopy Facility

Spintronics is the study of spin-related phenomena in materials at the most fundamental level towards applications for data storage and processing technologies.

In the first part of this lecture, I will introduce the most important spintronic devices realized with solid state materials and explain the key effects underlying their functionalities. These include spin-filtering, the giant-magnetoresistance effect, spin-transfer torque and spin-to-charge conversion driven by spin-orbit coupling. I will then explain how spintronic devices can be shrunk to the single-molecule scale and present a comprehensive overview of new emerging quantum behaviors. These can potentially allow for either electrical- or current-induced control over molecular and atomic spins. Along with my treatment, I will provide a basic introduction to quantum transport from a theoretical perspective.

Finally, I will introduce a new class of interfaces, called spinterfaces, obtained by adsorbing molecules on either ferromagnetic surfaces or materials with large spin-orbit coupling. Spinterfaces have mostly been studied because of their spin-filter properties. Yet, spinterfaces can also host new quantum phenomena, which may be exploited to translate externally controllable input signals, such as charge currents, electric and magnetic fields, into a number of chemical and physical functionalities.

Designing magnetic molecules and their spin Hamiltonian

Andrea Cornia

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In his seminal book “The Theory of Transition-Metal Ions” J. S. Griffith described the spin Hamiltonian as “a convenient resting place during the long trek from fundamental theory to the squiggles of an oscilloscope which are the primary result of electron resonance experiments”. Spin Hamiltonians are still of unrivaled usefulness to model the electronic structure and physical properties of magnetic systems.

The lecture will give an introduction to the spin-Hamiltonian formalism for molecules containing one, two or more than two magnetic centers. It will then focus on the relationship between molecular structure and spin-Hamiltonian parameters and on simple design principles that have recently led to molecules of top interest in spintronics.

Suggested readings:

J. S. Griffith, The Theory of Transition-Metal Ions, Cambridge University Press, Cambridge, 1961.
J.-P. Launay, M. Verdaguer, Electrons in Molecules: from Basic Principles to Molecular Electronics, Oxford University Press, Oxford, 2014.

Interplay between charge and spin conductance in molecular semiconductors and its applications to neuromorphic computing

Alberto Riminucci

Magnetic Nanostructures for Spintronics and Nanomedicine
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Building on the spectacular success of solid state spintronics, Molecular Spintronics aims at harnessing the power of spin phenomena in molecular semiconductors. After giving the background on spin injection from ferromagnetic electrodes into molecular semiconductors and transport therein, the lecture will cover the experimental techniques available to study these processes. It will then focus on magnetoresistance and on its interplay with multilevel resistive switching, with a discussion of the fundamental implications of such interplay. Finally, the lecture will provide an introduction on how these phenomena can be used effectively in neuromorphic computing and in sensing.

Spin dynamics in magnetic molecules

Roberta Sessoli

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Though magnetic molecules can share with traditional magnetic materials a classical property like occurrence of hysteresis in the magnetization cycle, the origin of the latter is intrinsically molecular in nature rather than cooperative.

This lecture will review the basic mechanisms of magnetic relaxation in paramagnetic materials, focalizing on two aspects that can be relevant for application in molecular spintronics and in quantum information technology with spins. The two key topics will be magnetic bistability of magnetically anisotropic molecules and the coherent spin dynamics that characterizes principally isotropic spin systems, in particular S=1/2 molecules. Quantum effects in magnetization dynamics, as well as they key role played by low energy optical phonons that characterize molecular materials will be also introduced. Most common technique to characterize the magnetization dynamics at different time-scales will be discussed.

Suggested readings:

1. Gatteschi, D.; Sessoli, R.; Villain, J., Molecular nanomagnets. Oxford University Press: Oxford, UK, 2006.

Spin-dependent phenomena at metal-organic interfaces – From a basic understanding towards the functionalization of spin-interfaces

Benjamin Stadtmüller

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The future success of molecular complexes in next-generation spintronic applications crucially depends on our ability to tune and control the spin-dependent properties of metal-organic interfaces according to device-relevant functionalities. In this context, organic complexes are particularly intriguing material systems since their intrinsic properties can be designed by chemical functionalization on a single molecular level. On surfaces, however, the spin-dependent properties of molecular complexes are determined by a delicate balance between the different interaction mechanisms occurring at the interface. These partly chemical interactions can result in a strong modification of the intrinsic molecular functionalities as well as in a modification of the spin-dependent properties of the underlying surface.

In this lecture, I will provide an overview of the basic spin-phenomena of metal-organic hybrid interfaces and how they can be studied experimentally by various spectroscopic techniques. I will start with an introduction into the interactions at metal-organic interfaces and their influence on the spin-dependent electronic band structure of the interface. Subsequently, I will turn to well-chosen examples which will demonstrate the capability of different experimental techniques to image the spin-dependent properties of metal-organic interfaces and to study the spin injection from the magnetic surface into the molecular film. Finally, I will highlight the latest efforts in molecular interface science to actively functionalize magnetic and spin-textured surfaces by the adsorption of organic molecules.

Organization and characterization of magnetic molecules assembled on surfaces and interfaces

Matteo Mannini

LAboratory for Molecular Magnetism (LA.M.M.)
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Embedding magnetic molecules in hybrid devices with the aim of influencing spin-injection and transport processes is far from trivial. Before studying the role of these molecular object in spintronic devices, the stability of molecules in the device environment has to be validated. The organization of molecules in the desired architectures has to be mastered in order to carefully control the interactions between the substrates and molecular layers. Single Molecule Magnets has been used to establish the playground for these concepts. This lecture will be focused on the nanostructuration protocols adopted to assemble SMMs on surfaces and an overview of the multi-technique characterization approach we established to study these hybrids.

First-Principles and Multi-Scale Modeling in Molecular Spintronics Development

Erik McNellis

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Electronic structure simulations from first-principles theory have revolutionized several areas of nano-science. Multi-scale modeling is a solution to the computational effort of such simulations for large-scale material models, in which energy-, time- and length-scales are bridged by several levels of interlinked approximations retaining relevant information while minimizing the cost of evaluation. Ideally, multi-scale first-principles modeling offers a toolbox optimally balanced between predictive accuracy and efficiency of evaluation for phenomena at any scale.

Spin dynamics in semiconductors are often sensitively dependent on e.g. material and charge dynamics properties, especially so in molecular semiconductors. This sensitivity stresses the need for non-empirical, high quality modeling. We have developed an accurate and transferable multi-scale modeling toolbox for spintronic materials and components from single molecules to bulk material scales.

I will begin by briefly covering the basics and history of first-principles modeling, continuing with the goals and general framework of our work. Our techniques modeling all spin relaxation mechanisms in organic semiconductors from first-principles theory will be presented. The value of these techniques both as standalone tools providing fast, high-throughput evaluations of specific properties of interest, and combined in large, semi-classical stochastic models will be discussed from the perspective of utility to a non-theorist developer of molecular spintronics. Finally, current challenges and cutting-edge development will be discussed.

Towards devices at single molecule scale

Marco Affronte

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When spintronic devices are scaled down to single molecule level, novel approaches for realizing electronic circuits need to be used. We shall first focus on the use of graphene and carbon nanotubes as platform for molecular architectures and devices, while gold junctions are successfully employed to trap single molecules. Functioning of archetypical molecular devices will be described. Surprisingly, their behaviour goes beyond simple mimicking that of current spintronic devices, revealing the intrinsic quantum nature of magnetic molecules.