SEAGATE

International Conference/Autumn School,
6^{th}-8^{th} September 2017,
SEAGATE Technology,
Derry/Londonderry,
Northern Ireland

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Functional Magnetic Materials: from fundamentals to applications

The scope of this Autumn School is the identification of new functional magnetic materials. To reach this goal experts from fundamental research as well as from applied technology will team up to present a broad overview of this field. The specific topics range from ultrafast magnetic dynamics, magnetic oxides via functional Heusler systems towards future magnetic recording devices and Heat Assisted Magnetic Recording (HAMR). A broad variety of physical interactions must be considered to analyze the functional behavior of the new magnetic materials ranging from strong correlations and ultrashort charge transfer to plasmonic excitations. The strength of combining experiment and theory to tackle the open questions describing the functionality of the systems, will be demonstrated in joint sessions.

Organizers:
Mark Gubbins (Seagate Technology)
Biplab Sanyal (Uppsala University)
Heiko Wende (University of Duisburg-Essen)

Wednesday 06-09-17	Item	Who	Topic / Notes
14:45	Start / Welcome	Mark Gubbins	
15:00	Talk 1	Robert Bowman	Design and fabrication of synthetic ferrimagnets: bringing atomistic simulation into the lab
15:15			
15:30	Discussion		
15:45	Talk 2	Heike Herper	Finding new permanent magnets by computational materials design
16:00			
16:15	Discussion		
16:30	Coffee break	All	
16:45			
17:00	Talk 3	Michael Farle	Functionalized Nanomagnets: Perspectives in Energy Applications and Medical Theranostics
17:15			
17:30	Discussion		
17:45	Talk 4	Markus Gruner	Electron-phonon coupling in LaFe 13-x Si x H y
18:00			
18:15	Discussion		
18:30	Close		
19:30	Walking tour of city walls		Depart from hotel lobby. www.thederrywalls.com

Functional Magnetic Materials: from fundamentals to applications

Thursday 07-09-17	Item	Who	Notes
09:30	Talk 5	Bert Koopmans	Femtosecond laser-induced spin currents and magnetization dynamics
09:45			
10:00			
10:15	Discussion		
10:30	Talk 6	Stefano Sanvito	First principles multi-scale theory for current-driven magnetization dynamics.
10:45			
11:00	Discussion		
11:15	**Coffee break**	All	
11:30			
11:45	Talk 7	Uwe Bovensiepen	Photo-excited spin current induced magnetization dynamics in epitaxial metallic heterostructures.
12:00			
12:15	Discussion		
12:30	**Lunch**	All	To be served in area behind Causeway room
12:45			
13:00			
13:15	Talk 8	Roy Chantrell	All optical magnetisation switching: Basic physics and potential for new recording technology
13:30			
13:45	Discussion		
14:00	Talk 9	Simon Bance	Seagate
14:15			
14:30	Discussion		
14:45	**Coffee Break**	All	
15:00			
15:15	Group Photo	All	Window tour of Seagate Fab
15:30	Fab tours		
15:45			
16:00			
16:15	Talk 10	Vijay Venugopal	Seagate
16:30			
16:45	Discussion		
17:00	Close		
20:00	Meal in Walled City Brewery		www.walledcitybrewery.com

Friday 08-09-17	Item	Who	Notes
09:30	Talk 11	Barbara Brena	Theoretical description of highly correlated 3d electrons in single molecule magnets: the effect of the Hubbard U term
09:45			
10:00	Discussion	All	
10:15	**Coffee break**	All	
10:30	Talk 12	Diana Iusan	Applications of dynamical mean-field theory to strongly correlated oxides
10:45			
11:00	Discussion		
11:15	Close	All	Closing remarks / discussion
11:30	**Lunch**	All	To be served in area behind Causeway room
11:45			
12:00			
12:15	Close		

Design and fabrication of synthetic ferrimagnets: bringing atomistic simulation into the lab

J.N. Scott, W.R. Hendren & **R.M. Bowman**

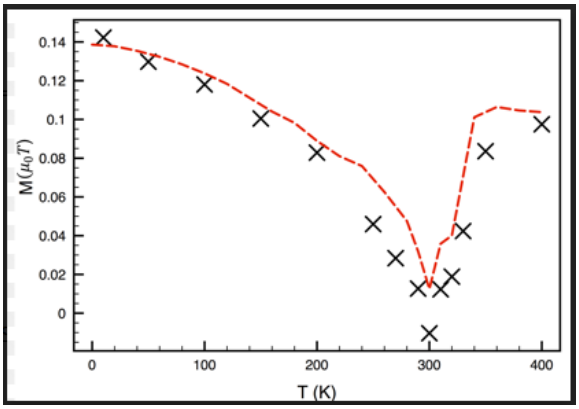
Queen's University Belfast, United Kingdom.

Department of Physics, University of York, United Kingdom.

We have identified a transition metal based synthetic ferrimagnet (SFi) as a technologically feasible media for All Optical Magnetic Switching (AOMS). These SFi are constructed from two magnetic transition metal films, exchanged coupled via a non-magnetic spacer layer through the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction. Exploitation of the ab-initio code, VAMPIRE [1], is aiding understanding of the magnetization dynamics of the SFi, with experimental parameters supplied directly into the simulations and the output compared straight to the experimental result. It is hoped that in this way, simulations can be used not only to explain the magnetic behaviour of the structures, but to guide the creation of tailored synthetic ferrimagnet samples.

In this presentation we describe the integration of atomistic simulation using VAMPIRE code to design and identify a synthestic ferrimagnet Ni3Pt/Ir/Co and the validation against samples fabricated by UHV sputtering. The Ni3Pt/Ir/Co structure was chosen to achieve room temperature compensation and for future work to afford two distinct ferromagnetic layers that would subsequently allow optical or X-ray probe measurements to investigate dynamic switching of the stack and the individual ferromagnetic layers.

In the figure we show VAMPIRE simulation of a 10 x 10 x 13.5nm stack of antiferromagnetically exchange coupled Co and Ni3Pt layers compared to a Ni3Pt(10nm)/Ir(0.5nm)/Co(1nm) SFi remnanent magnetization values taken from SQUID derived hysteresis loops. A good agreement is obtained and subsequent refinements will be presented and discussed.



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Finding new permanent magnets by computational materials design

Heike C. Herper

Department of Physics and Astronomy, Uppsala University, Uppsala, Sweden

Magnetic materials are an inherent part of our everyday life and key materials in many technological fields. They are used in data storage devices, cars and wind power plants as well as in sensors and actuators. The demand of magnetic materials will further increase in view of increasing environmental friendly energy production and solutions based on abundant materials and avoiding critical elements such as rare earth are needed. A cheap and recourse saving way to predict new or novel phases with desired properties is by computational materials design. This talk focusses on new phases for permanent magnets which were obtained by systematically modifying and optimizing known systems or novel phases derived from high throughput studies.

The systems are characterized using a combination of different state of the art first principles methods (VASP [1], RSPt [2]). Finite temperature properties are obtained from mapping the system on a spin model using UppASD [3]. Examples for rare earth free magnets from known phases (Heusler-type), rare earth lean magnets with ThMn 12 structure, and Fe-rich novel phases will be discussed.

In the first case a series of tetragonal Ni-based Heusler alloys Ni 2 YZ with (Y = Mn, Fe, Co) and Z varying from B to Sn has been investigated showing that systems with Y=Fe tend to have a uniaxial magnetocrystalline anisotropy (MAE). We show that the MAE can be systematically tuned by changing the geometry and by varying the occupation of the Z sublattice. Even though the MAE of this systems is quite large, the Curie temperatures and the magnetic moments might be too small for high performance applications. These problems can be avoided by using RE-lean magnets with ThMn 12 structure. However, for light RE such as Nd ferromagnetism is achieved only if Mn is replaced by Fe, which destabilizes the phase. To overcome this partial replacement of Fe by nonmagnetic atoms is necessary but degrades the magnetic properties. Though REFe 12 compounds have been studied for years, the interplay between Fe reduction, interstitial elements and the concentrations needed to stabilize the phase and substantially increase the MAE are not completely understood. Here, a series of Nd 1-x Y x Fe 12−y Ti y phases has been systematically investigated. To avoid RE completely high throughput calculations have been performed for Fe-rich ternary compounds searching for new uniaxial phases. In case of Fe x CoTa (x= 6,8,10) uniaxial phases with MAE values larger than 1MJ/m 3 could be identified. This work is supported by the European Research Project NOVAMAG (EU686056) and STandUP for energy (Sweden).

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Functionalized Nanomagnets: Perspectives in Energy Applications and Medical Theranostics

Michael Farle *(IEEE Magnetics Society Distinguished Lecturer for 2017)*
University of Duisburg-Essen, Germany, and Immanuel Kant Baltic Federal University, Russia

Let's dream of materials that store and release energy reversibly by temperature changes between day and night or provide a non-invasive treatment of cancer. These visions may be realized by using magnetic nanoparticles that are functionalized to be biocompatible, environmentally stable and recyclable, self-healing, and low-cost.
In this presentation I will discuss the basic concepts of magnetic nanomaterials and their magnetic properties with a focus on how to tune parameters in a controlled fashion. I will highlight state-of-the-art experimental approaches [1,2,3] that allow us to synthesize multifunctional particles and to understand microscopic properties and interactions in relation to electronic structure changes caused by changes in size, shape, and composition of nanomaterials. The apparently complex behavior of hybrid metal/metal, metal/oxide, or oxide/oxide interface materials –core-shell materials - can be understood from the three fundamental interactions in magnetism: magnetic exchange interaction due to orbital overlap, spin-orbit interaction due to inner- and intra-atomic relativistic corrections (e.g., crystal field effects) and the long-range magnetic dipolar interaction. Several examples will be presented, including the formation of above-room-temperature ferromagnetic interface layers between low-temperature antiferromagnetic layers and the evolution of lattices of magnetic textures (skyrmions) in confined dimensions.
Work supported by European Union and Deutsche Forschungsgemeinschaft. The fruitful collaboration with many colleagues and students is thankfully acknowledged.

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Michael Farle received his Diploma in experimental physics, Doctorate, and Habilitation degrees from Freie Universität Berlin in 1984, 1989, and 1998, respectively. During this time he spent three and a half years as a senior researcher at Stanford University, California, and Université de Strasbourg, France. In 1999, he moved to Technische Universität Braunschweig, Germany, where he became a full professor. Since 2002, he has been working as a professor at the Universität Duisburg-Essen, Germany, where he has served as Vice-Rector for Research and Junior Scientific Staff. In 2016 he became, in addition, an adjunct professor at Immanuel Kant Baltic Federal University, Kaliningrad, Russia. Prof. Farle has published over 230 technical articles in peer-reviewed journals, including Book chapters and review articles, and has given more than 60 invited presentations. He coordinated two European Research Networks and served as the vice-spokesman of Collaborative Research Center: Magnetic Heterostructures (SFB 491). Since 2014 he is chairman of the Magnetism Section of the German Physical Society. For many years he has been active on the program committees of several international conferences on magnetism. He is a member of the IEEE Magnetics.

Electron-phonon coupling in LaFe 13-x Si x H y

PD Dr. Markus E. Gruner

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Fully hydrogenated La-Fe-Si is one of the most interesting candidates for room temperature magnetic refrigeration. The first order nature of the magnetic transition is connected to its itinerant electron metamagnetism, which relates to a particular coupling between the microscopic degrees of freedom. By combining first principles calculations in the framework of density functional theory (DFT) and nuclear resonant inelastic X-ray scattering (NRIXS) we investigate the interplay of electronic structure, magnetism and vibrational degrees of freedom in fully hydrogenated La-Fe-Si.

We demonstrate that the adiabatic electron-phonon coupling which leads to a cooperative contribution of magnetic, electronic and vibrational degrees of freedom to the entropy change in the non-hydrogenated La-Fe-Si and is thus responsible for the superior magnetocaloric properties, is again important for the hydrogenated compound. Since full loading with hydrogen involves the occupation of only a part of the available sites 24d, we also discuss the site-occupation of hydrogen based on total energy calculations and by comparing vibrational density of states from DFT Involving different distributions of hydrogen with the NRIXS measurements.

Femtosecond laser-induced spin currents and magnetization dynamics

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Novel schemes for controlling the ferromagnetic state at the femtosecond time scale by pulsed laser excitation have received great current interest recently. Driving systems into the strongly non-equilibrium regime, it has been shown possible not only to quench magnetic order by femtoseond laser pulses, but also to drive systems through a ferromagnetic phase transition, and even switch the magnetic moment by single pulses of circularly polarized light. More recently, it has been proposed that pulsed laser excitation can also induce spin currents over several to tens of nanometers, which can act as an additional source of sub-picosecond magnetization dynamics. Thereby, an interesting link between the fields of ultrafast magnetization dynamics and spintronic transport physics has emerged. In all these processes transfer of angular momentum between different sub-systems plays and essential role.

In this lecture I will start with a brief review of the field of fs control of the magnetic state by pulsed laser excitation. Proposed mechanisms for ultrafast loss of magnetic order upon fs laser heating as well as all-optical switching will be discussed. Next, different processes that give rise to laser-induced spin currents will be distinguished. In particular I will address recent experiments that have demonstrated laser-induced *spin transfer torque* on a free magnetic layer, using a collinear multilayer configuration consisting of a free in-plane layer on top of a PMA injection layer and separated by a nonmagnetic spacer. As it will be shown, these non-collinear fs spin currents are absorbed within a few nanometers, and thereby provide ideal conditions for exciting GHz spin waves, their quantum mechanical manifestation called magnons. This allowed us in recent experiments to map out the dispersion of the frequency, $\omega(\vec{q})$, and the Gilbert damping, $\alpha(\vec{q})$, of thin Co and CoB layers. Finally, attempts to treat both the local dissipation of angular momentum and the induced spin currents on equal footing will be discussed. If time permits, the role of spin currents on all-optical switching will be briefly addressed as well.

First principles multi-scale theory for current-driven magnetization dynamics.

Stefano Sanvito

School of Physics, AMBER and CRANN, Trinity College, Dublin 2, Ireland

Many devices and device concepts are based on driving the dynamics of the magnetic order parameter, either the magnetization of the N_eel vector, with a spin-polarized current. This, in general, produces a torque, which enables switching and dynamics. The modelling of such dynamics is a complex task because the Physics involved spans over different time and space scales, and it is strictly materials and devices speci_c. On the one hand, one can model the current-induced torques by using _rst principles methods, which can be applied very generally to any materials class without the need of external parameters, but can deal with static or at best steady-state quantities. On the other hand, spin-dynamics can be very efficiently computed by using a vast range of micromagnetic techniques. These can tackle the time-dependent problem, but unfortunately depends on parameters, usually extracted from experiments or some other level of theory.

Here we present a computational scheme, which combines such two worlds and aims at providing a general tool for materials-specific current-induced spin dynamics. Our method computes the spin-transfer torques by using a combination of density functional theory (DFT) and steady-state transport theory, implemented within the non-equilibrium Green's function formalism. The torques are derived from time-dependent DFT and can be extracted from the transport calculations [1]. Then such torques are used as an input for atom-istic spin-dynamics calculations [2], with a net result that a fully ab initio theory for spin dynamics can be implemented. Together with the theory backbone I will show a few examples of such computational scheme. In particular I will look at dynamics in Fe/Co-based magnetic tunnel junctions and look at the possibility of constructing and all-antiferromagnetic current-driven device [3].

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Photo-excited spin current induced magnetization dynamics in epitaxial metallic heterostructures analyzed in all optical pump-probe experiments

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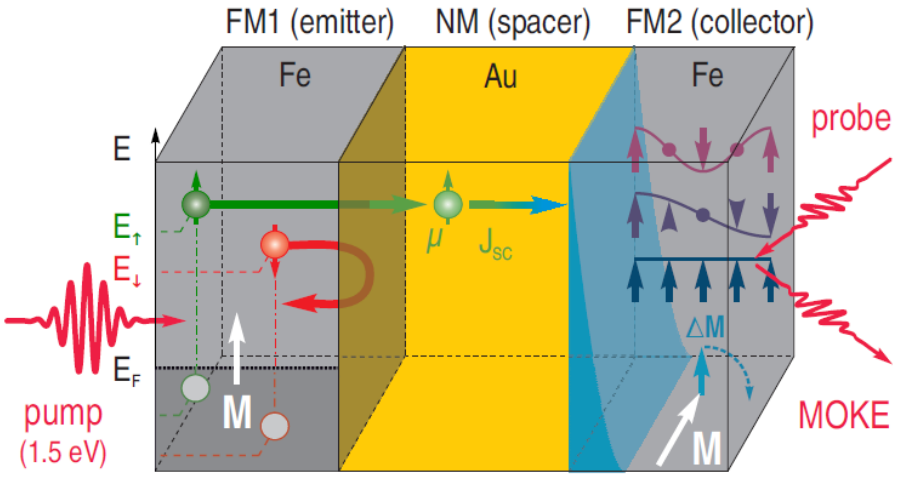
Optical excitation of ferromagnets results in spin-polarized hot electrons, which relax locally on femtosecond time scales within the ferromagnet and are transferred into adjacent constituents leading to transient spin currents. We analyze such spin currents and the photo-excited magnetization dynamics in epitaxial heterostructures combined of transition metal ferromagnets and noble metals by time-resolved magneto-optical techniques. Pump-probe experiments on Co/Cu(001) detecting the complex, linear magneto-optical Kerr effect (MOKE) [1] and the second harmonic optical response allow to disentangle the magnetization dynamics near the surface and the inner interface. The dynamics of local demagnetization due to spin flip scattering and spin transfer into Cu is distinguished. Back pump – front probe experiments in epitaxial heterostructures Fe/Au/Fe/MgO(001) facilitate the analysis of the currents directly [2]. Employing detection of the second harmonic generation we have identified a non-linear magneto-optical response which represents the symmetry breaking generated by the spin currents [3]. Furthermore, we report up 0.5 THz standing spin waves driven by the spin current induced spin transfer torque in the collector Fe layer, see figure. A spectral analysis of the spin wave frequencies allows to estimate the depth in which the spin transfer torque acts to a few nanometer [4].

Funding through the DFG, the BMBF, the EU, and MERCUR is gratefully acknowledged.



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All optical magnetisation switching: Basic physics and potential for new recording technology

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Since the pioneering demonstration of ultrafast demagnetization in Ni [1], the field has produced a series of remarkable discoveries, including that of magnetization reversal driven by circularly polarized light [2] giving rise to the intriguing concept of all-optical magnetic recording on the picosecond timescale. Previous experimental studies [3] using large magnetic fields showed that conventional reversal on this timescale was not possible due to a 'fracturing' of the magnetization structure. It was shown [4] that all-optical reversal was achieved due to the elevated temperatures achieved in the pulsed laser process, which accessed the so-called 'linear' reversal mechanism capable of switching on the sub-picosecond timescale. The talk will firstly outline the physics of these processes, leading to the discovery of Thermally Induced Magnetisation Switching (TIMS) in ferrimagnets, in which magnetization switching occurs in the absence of an externally applied field. This effect is discussed in terms of a 2-magnon bound state, which is responsible for the transfer of angular momentum between sublattices, which drives magnetization reversal. This can be interpreted as arising from a large effective field due to the strong inter-sublattice exchange. In terms of recording technology this field has considerable significance since it has been shown [5] that basic thermodynamic considerations lead to the requirement of fields larger than accessible to conventional inductive switching. The implications of TIMS for future magnetic storage devices is considerable, in terms of the reduction in complexity of write transducers, increased data rate and power reduction. Arguably, a recent paper [6] has brought the technology closer by demonstrating TIMS using ultrafast current pulses, potentially accessible to CMOS technology. We will finally consider potential recording densities and the materials required for their achievement.

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Theoretical description of highly correlated 3d electrons in single molecule magnets: the effect of the Hubbard U term

Dr. Barbara Brena

We have considered a series of 3d transition metal Phthalocyanines (Pcs), like Mn, Fe, Co, Ni and CuPc [1,2]. Pcs are organic macrocycles with a metal atom in the centre, widely used as dyes, and highly appealing for applications in photovoltaics and in spintronics as single molecule magnets.

Density functional theory (DFT) in the generalized gradient approximation (GGA), as well as in the local density approximation (LDA), cannot properly describe highly correlated and localized d-electrons. To overcome this limitation, the GGA+U method, where U is the Hubbard U term [3,4,5], is commonly employed. The U term, accounting for the intra-atomic Coulomb interactions, is selectively added to to the d orbitals of the transition metal.

In DFT studies of such molecules, effective U values of 3 or 4 eV are usually chosen for the 3d electrons, but the choice of U is often solely based on previous literature reports.

We have therefore performed a systematic characterization in the Dudarev implementation [4] of how different U values affect the structure, density of states and magnetic properties of such molecules. We have compared GGA+U calculations for various values of U with results obtained from hybrid functionals (B3LYP[6], HSE06[7]) and with valence band photoelectron measurements. We discuss which U values can be appropriate for each molecule and highlight the importance of estimating the value of U for each system studied.

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Applications of dynamical mean-field theory to strongly correlated oxides

Diana Iusan

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In this talk I will present the applications of the local density approximation (LDA) plus dynamical mean-field theory (DMFT) to two strongly correlated oxides: $BiFeO_3$ and NiO. The local impurity problem within DMFT was solved using the exact diagonalization solver. The calculated valence band spectra of $BiFeO_3$ shows a good agreement with the measured hard X-ray photoelectron spectroscopy (HAXPES) and resonant photoelectron spectroscopy (RPES) for the Fe *3d* states. The inclusion of static corrections only via LDA+*U* fails to reproduce the experimental results, confirming thus the importance of dynamical electron-electron correlations. As for NiO, we show that the incorporation of non-local correlations via the GW method in addition to DMFT is necessary in order to accurately describe the electronic structure of this compound.