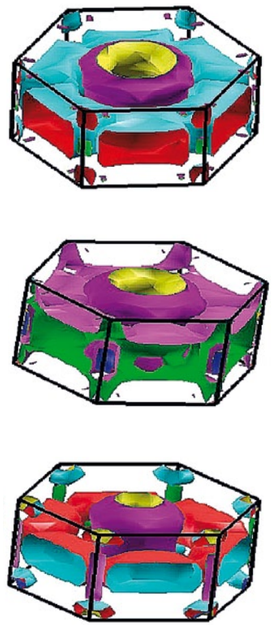
• *Ab initio Calculated Electronic Structure and X-ray Magnetic Circular Dichroism of Gadolinium*

Materials based on rare-earth metals offer interesting magnetic properties for the field of spintronics in general and dilute magnetic semiconductors in particular, due to the unfilled and highly localized $4f$ orbitals. Through various calculations, including the spin-orbit coupling (SOC), within the local-spin-density approximation (LSDA), the generalized-gradient approximation (GGA), the LSDA+U (where U is the onsite Hubbard interaction) and the GGA+U, it is clearly shown that the latter two methods are the most adequate for describing the electronic and magnetic structures as well as the x-ray absorption spectra and x-ray magnetic circular dichroism of the strongly correlated $4f$ electrons of gadolinium metal.

It is interesting to notice that the SOC reduces slightly all Fermi surface areas (FSA), whereas the U has a much important effect. First, it reduces also the FSA of both spin up and spin down bands crossing the Fermi level. Secondly, because of the shifting of the energy bands towards low energies a new electron pocket with a sizeable FSA appears. We can therefore conclude that both the SOC and the U parameter have an effect on physical properties involving the Fermi surface, like the thermal properties, the quantum transport or the magneto-crystalline anisotropy.
This research will be extended to novel materials for spintronics and is supported by the ANR P-nano and a new Berkeley-France research grant with Prof. W. Pickett. ■



Three dimensional total Fermi surface per spin of gadolinium calculated, respectively, in GGA+SOC, GGA, and GGA+U methods.

Samir Abdelouahed, N. Baadji, M. Alouani
Phys. Rev. **B 75**, 094428 (2007).

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➜ *International Relationships*

The 7th France-Japan Workshop on Nanomaterials has been organized by the French C'Nano network together with IPCMS and took place in "Le Bischenberg, France" from 23rd to 26th October 2007. It gathered about 70 invited scientists from both countries and was the occasion to discuss the very recent breakthroughs in nanomaterials and nanosciences. It was also the opportunity to develop and strengthen collaborations in materials science between the two countries.

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Editorial

This issue of ***IPCMS News*** is centered on recent results obtained in our laboratory in the fields of nanomagnetism and spintronics. Symmetry-conserved tunneling results show how a chromium ultrathin layer acts as a tunnel barrier in a Fe/MgO(001) system. Then, a new process of recording and reading information in magnetic media, by using a confocal magneto-optical Kerr microscope working in a pump-probe configuration is demonstrated. As a third contribution, transport measurements on a hybrid ferromagnetic/organic semiconductor junction are presented; they reveal the overarching role of defects and/or trap levels present in the structurally ordered organic spacer on the spin-transport response. Finally, the first "Mn_{12}" based fluid mesophases with 3D and 1D positional order are reported. This was obtained through a functionnalization of Mn_{12} by mesogenic ligands to favor self-organization.

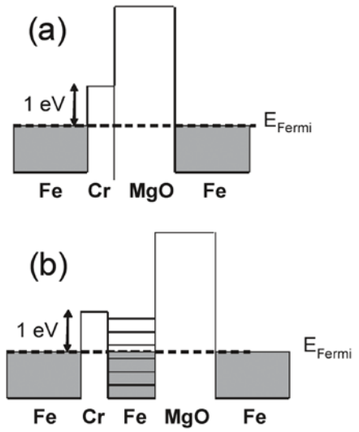
Further, this issue is also the opportunity to emphasize the involvement of the laboratory into a new partnership with the students of art, jewelry and communication from the "Ecole Superieure des Arts Decoratifs de Strasbourg". (**www.esad-stg.org**)
Researchers and engineers from the laboratory have helped these art students to produce nanoimprints thanks to the nanofabrication platform of the institute. These objects have been imprinted on the nanoscale, so that the size of the patterns on these works of art can vary from a few nanometers to a few micrometers. These nanoimprint techniques deploy the "direct writing" of patterns thanks to an electron beam that is focused onto a wide ranging number of substrates –glass, silicon, metals, polymers... The art work that has resulted from these experiments is made accessible to a broader public through projections onto a wide screen, and in addition could be used against illegal trading. The corresponding exhibition took place at IPCMS from 23rd October to 2nd November 2007.


Nothing is forever - *Hector Lasso*


Le regard mâle - *Selma Lepart*

Marc Drillon
Director

• Spintronics and quantum wells in metals



Potential landscape for Δ_1 electrons in epitaxial Fe/Cr/MgO/Fe (a) and Fe/Cr/Fe/MgO/Fe (b) stacking. Chromium plays the role of an additional tunnel barrier and can confine Δ_1 electrons in a quantum well as in (b). This confinement effect is observed in transport measurement leading to an oscillation of the differential conductance (shown for 7, 14 and 21 Fe atomic layers in the quantum well).

In collaboration with LPM in Nancy, we have observed that Chromium behaves as an insulator for electron of a given symmetry in monocrystalline systems. We inserted a few Cr atomic layers in a magnetic tunnel junction to observe the transport properties in a Fe/Cr/MgO/Fe stacking. In the absence of Cr, the magneto-resistance is higher than 100%. Upon inserting Cr, we strongly decrease the conductance when both magnetisations are parallel, whereas the anti-parallel conductance is not modified by Cr insertion.
This proves that the symmetry of tunnelling electrons is different in both magnetic configurations. Indeed, in the parallel one, the transport properties are dominated by Δ_1 electrons, for which Cr is an insulator. In the anti-parallel one, the main role is played by Δ_5 electrons for which Cr is conducting. By changing the magnetic configuration we thus change the actual tunnel barrier thickness for electrons, thus explaining the decrease of the magneto-resistance to a few percents.

This effect enabled us to observe a quantum well that is selective in electronic symmetry. Indeed by growing an epitaxial Fe/Cr/Fe/MgO/Fe stacking we could confine Δ_1 electrons and only Δ_1 electrons in the Fe layer between MgO and Cr. By applying a voltage bias we observed oscillations of the differential conductance when injecting electrons from the right electrode into the left. This is due to the modulation of the electronic state density in the well as in semi-conductors quantum wells. This effect was only observed in the parallel magnetic configuration thus confirming that only Δ_1 electrons are involved. ■

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Phys. Rev. Lett. **99**, 187202 (2007)

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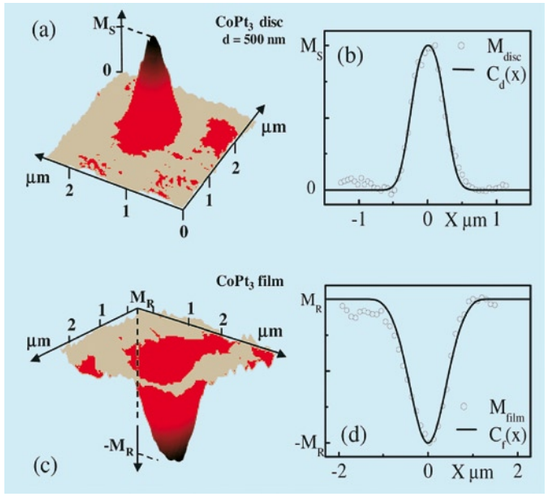
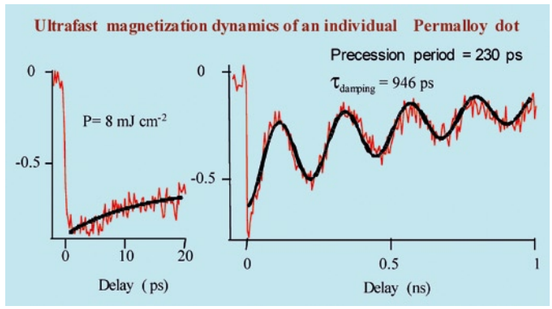
• Ultrafast spin-photonics microscopy

The processes of recording and reading information in magnetic media, like those used in computer hard drives, is performed via a sequence of magnetic field pulses. This process is limited not only by the capacity of the ferromagnetic medium (density in bits/inch²) but also by the speed to address each magnetic bit (typically 1 ns). During the past years we have developed at IPCMS a new approach allowing us to explore the ultimate limits for the recording and reading processes. It is based on the use of femtosecond optical pulses which can demagnetize and switch magnetic dots. Our preceding studies have shown that laser pulses with a duration of ~100 fs are ideal for obtaining information on a variety of mechanisms occurring in the ferromagnetic magnetic materials.



Magnetization imaging of an individual 500 nm $CoPt_3$ disc (a) and of a switched dot on a $CoPt_3$ film.

For example, one can observe in real time the thermalization of the spins as well as their equilibrium dynamics with the lattice. It is also a powerful approach for studying the precession and damping of the magnetic vector around the effective magnetic field.
The next important step, which we have achieved in the present work, was to combine the ultrashort femtosecond temporal resolution with the spatial resolution in order to study the dynamics of magnetic nanostructures. We can now perform such femtosecond magneto-optical experiments at the scale of optical diffraction (a few hundreds of nanometers). We name this new approach Ultrafast Spin-Photonics Microscopy. The apparatus which we have developed consists in a confocal magneto-optical Kerr microscope working in a pump-probe configuration. Two collinear frequency non-degenerated femtosecond pulses are focused on the sample mounted on a XY-piezo. The magnetization state of the studied material is monitored in the confocal plane of the microscope by an appropriate polarization analysis. The overall spatial and temporal resolutions are respectively : 300 nm and 150 fs as can be seen in the figure showing the magnetization of a single $CoPt_3$ dot (a) and of a single dot switched on a film with the femtosecond pulses (b).



Ultrafast demagnetization and optically induced ferromagnetic resonance on an individual permalloy dot.

The method can be used for example to study the demagnetization and precession dynamics of single magnetic dots as seen in the figure beside for a permalloy disc. Note that the non-invasive character of optics opens the way to investigate a large variety of magnetic nanostructures at the femtosecond time scale. An even better spatial resolution could be achieved beyond the diffraction limit either by hyper-focusing (~80 nm) or through near-field optical probing (~50 nm). ■

A. Laraoui, M. Albrecht, J.-Y. Bigot, Optics Letters **32**, 936-938 (2007)

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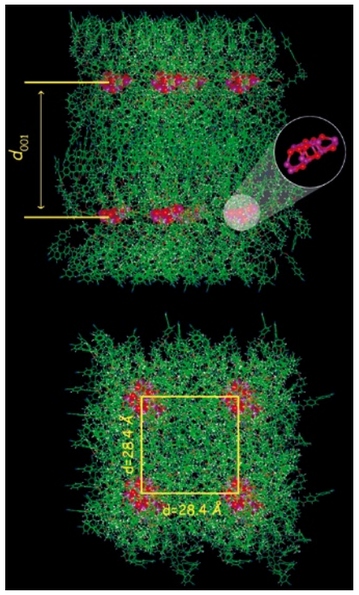
• Liquid-crystalline Single Molecule Magnets

Chemists from IPCMS have recently reported for the first time the endowment of the famous Single Molecule Magnet "Mn_{12}" with liquid-crystalline phases.

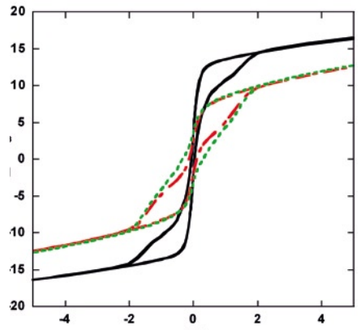


Simulated views (in accordance with the XRD data) of the lamellar organisation of the molecules and their substituants in the smectic phase.

Single Molecule Magnets (the archetype of which is the so-called "Mn_{12}", a polymetallic Mn complex, of formula $[Mn_{12}O_{12}(OAc)_{16}(H_2O)_4]$) have the remarkable property of showing an extremely slow relaxation of their magnetization below a blocking temperature (D. Gatteschi, R. Sessoli, *Angew. Chem. Int. Ed.* 2003, **42**, 268-297 and references therein). This hysteresis of purely molecular origin allows foreseeing the ultimate scale of information storage in a single molecule. Moreover, the quantum tunnelling of the magnetization, observed on these molecules, may open huge opportunities on the way to quantum computing. Nevertheless, the most important challenges before the eventual use of this type of molecules in a quantum computer remain their self-organization and their addressing.

Our approach consists in functionalizing the Mn_{12} by mesogenic ligands in order to favour the self-organisation into liquid-crystalline phases. Depending on the characteristics of the mesogenic ligands (size and position of the substituting groups), clusters possessing fluid mesophases with 3D (cubic) or 1D (smectic) positional order have been obtained. Even though short ranged, the intra-layer ordering of the molecular cores in the smectic phase is square-like. The magnetic properties are preserved upon functionalization and the molecules are thermally stable up to 150°C. Another very interesting result is the fact that the main molecular axes of the magnetic cores share a common alignment direction, in a nematic sense.
It seems reasonable to expect that these remarkable features may facilitate the 2D ordering of these clusters on surfaces, which is the ultimate goal. In order to tailor more precisely the mesomorphic behaviour of these SMMs, the modification of the ligand structure as well as the regioselective substitution of two different ligands (at the axial and equatorial positions) are in progress in our laboratory. ■

Hysteresis curves for different liquid-crystalline "Mn_{12}" molecules.



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Angew. Chem. Int. Ed., **47**, **3**, 490-495 (2008)

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