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**Condensed Matter: Top Papers 2005 Showcase**

### Ultrahydrophobic surfaces

Towards ultrahydrophobic surfaces: a biomimetic approach

Ulrike Mock, Ralf Förster, Wolfgang Menz and Jürgen Rühe


Many biological surfaces, particularly plant leaves, are hydrophobic. As strongly water-repellent and self-cleaning surfaces are very interesting technologically, many approaches to ultrahydrophobic surfaces have been developed. One such plant is the lady’s mantle, whose leaves are covered with hairs, which apparently help make it ultrahydrophobic. This is surprising as simple theories of wetting on a rough substrate predict that a rough hydrophilic surface should be even more hydrophilic than a smooth one. Herminghaus et al. proposed that the elasticity of the plant hair as well as its area coverage accounts for the water repellence of such hairy leaves.

Jürgen Rühe and colleagues at University of Freiburg, Germany, studied a model surface closely resembling the leaf surface of a lady’s mantle. They used a three-step approach to obtain elastic hydrogel pillars as models for such hairy plant surfaces. They first generated master structures either in steel or through the direct replication of the leaf surface in polymer. This master was moulded against a silicone polymer to yield an elastomer which was a negative of the hairy surface. A subsequent radical polymerization under crosslinking in the negative led to the formation of an elastic hydrogel resembling the natural structure. The hydrogels obtained were hydrophilic, had aspect ratios from four up to 100 as in the natural system and showed elastic properties, so that bundle formation of several pillars could be observed. These models mimic roughly the structure of the leaf of a lady’s mantle.

In further experiments they will concentrate on the choice of appropriate polymers with suitable swelling behaviour and elastic properties. The crosslink density of the polymer networks needs to be controlled and an appropriate choice of the chemical composition of the network-building components will have a great influence on the wetting properties of the resulting hairy surfaces.

### High-energy photoemission in silver

High-energy photoemission in silver: resolving d and sp contributions in valence band spectra

G Panaccione, G Cautero, M Cautero, A Fondacaro, M Gritoni, P Lacovig, G Monaco, F Offi, G Pascaletti, M Sacchi, N Stojic, G Stefani, R Tommasini and P Torelli


Low-energy angle-resolved photoemission spectroscopy (PES), in the UV and soft x-ray range, provides detailed information on electronic states, with a strong sensitivity at higher photon energies, x-ray photoelectron spectroscopy (XPS) increases the probing depth. Hard x-ray PES (HAXPES) offers a more detailed insight, but these experiments are difficult, and very weak signals are expected as the photoionization cross section decreases as E⁻³. High-flux/high-resolution beamlines at third-generation synchrotron radiation sources and recent advances in analyser technology have made HAXPES viable.

G Panaccione (Trieste) and co-workers have obtained high-resolution core level and valence band HAXPES spectra from polycrystalline Ag (left) and Ag(111) (right), compared with the total weighted DOS. The partial s, p, d DOSs are also shown. The vertical lines indicate the Fermi levels of the experimental spectra. Calculated DOSs have been arbitrarily shifted for comparison.

The 3d and valence band HAXPES spectra of polycrystalline Ag display larger bulk sensitivity and improved energy resolution than standard XPS. The surface signal is negligible (less than 3%). HAXPES valence band spectra can be compared with calculated bulk DOS, ignoring the surface contribution. By optimizing the weight of the calculated s, p, and d DOSs to match valence band spectra measured at different photon energies, they found a reduced I(3d)/I(5s + 3p) ratio compared with calculated values, namely ~40 instead of ~70 for XPS and 2.8 instead of 7 at hν = 7912 eV. This enables HAXPES spectra to yield a more accurate picture of the Ag valence band. The 5p-band is responsible for the observed increase of the intensity approaching the Fermi level and has the strongest free-electron-like character, whereas localized s-states are present at the bottom of the d-band.

This technique may be extended to other materials. Comparing DOS calculations with HAXPES data and exploiting the behaviour of photoelectron cross-sections at high kinetic energy will enable the electronic properties of complex systems like transition metal oxides to be studied. Despite the challenging experimental conditions of HAXPES, they anticipate applications to samples of technological interest, thanks to the more relaxed vacuum and surface preparation requirements.

### Opening up photonic bandgaps

Opening up complete photonic bandgaps by tuning the orientation of birefringent dielectric spheres in three-dimensional photonic crystals

Fang Guan, Zhifang Lin and Jian Zi


Photonic crystals are composite structures with a spatially periodic variation of refractive index. Light propagation in them can be strongly modulated not only by the introduced periodicity via multiple Bragg scattering but also by the presence of resonant modes of the building components and is then characterized by complicated photonic band structures. If there exist complete photonic bandgaps between photonic bands, light propagation will be absolutely forbidden and spontaneous emission prohibited within the frequency range of the photonic bandgap, giving rise to unprecedented degrees of freedom in the manipulation and control of spontaneous emission as well as light propagation, leading to many potential applications in photonics, such as frequency selective reflectors, band filters, and low threshold micro-cavity lasers.

Fang Guan, Zhifang Lin and Jian Zi of Fudan University, Shanghai have used a multiple-scattering method to study the photonic band structures of three-dimensional photonic crystals consisting of birefringent dielectric spheres. In the multiple-scattering method the whole system is treated as an assembly of scatterers and its scattering properties are taken as sums over individual scatterers. Once the scattering properties of the individual scatterers are characterized by the scattering matrix (or scattering coefficients for an isotropic sphere), the scattering properties of the entire system can be constructed and the band structure of the photonic crystals can be obtained from the stationary-state solution of the systems.

Their results demonstrate the possibility of opening up complete photonic bandgaps in simple three-dimensional lattice photonic systems by changing the orientation of the extraordinary axis of the birefringent spheres. The creation of the complete photonic bandgaps in the photonic crystals also suggests some degree of tunability of the photonic band structure, provided that the extraordinary axis of all constituent birefringent spheres can be rotated while keeping the whole structure of the photonic system unchanged. The application of a strong external electric field may be a handle to achieve this tunability.
Predictive models of iron-based alloys and steels for fusion and advanced nuclear applications must take into account magnetic effects to obtain accurate models of interatomic interactions. It is known that magnetism makes the BCC α-phase of iron more stable than any of the FCC phases, possibly through the effect of electron correlations on interatomic forces. The density functional and tight-binding approaches cannot model systems containing ~100 000 atoms, necessary to account for the long-range elastic interactions causing swelling, embrittlement and creep of irradiated materials. Phenomenological models suitable for fast evaluation of forces between atoms in a magnetic material are required for molecular dynamics simulations of thermally activated processes in irradiated iron and its alloys.

S L Dudarev (Culham) and P M Derlet (Paul Scherrer Institute) have developed such a model combining the Stoner and Ginzburg-Landau (GL) models. The Stoner model describes correlation effects giving rise to magnetism in an electron gas, while GL is the simplest model of a second-order phase transition. They show that the symmetry-broken solutions of the GL model describing spontaneous magnetization of atoms cause the link between magnetism and interatomic forces. They derive a phenomenological embedding function of the many-body interatomic potential. By adjusting the effective pairwise density functions and pairwise interactions they parameterize the energy of interatomic interactions to describe the equation of state both for the non-magnetic and magnetic configurations, and also the energies of vacancy and self-interstitial point defects in iron.

They extend the existing treatment of interatomic interactions, where the energy is a single-valued function of atomic coordinates, and link it with symmetry breaking, leading to multi-branching of the effective potential. Since in a magnetic system the energy depends on both the position of atoms and the configuration of magnetic moments, the total energy is no longer a unique function of atomic coordinates. Instead, in a magnetic system they find that several energy surfaces correspond to the same geometric configuration of atoms. They treat only the ferromagnetic case where the energy surface consists of two (non-magnetic and ferromagnetic) sheets, but the method can be generalized to arbitrary magnetic configurations.
Dephasing in open quantum-dot arrays

Dephasing due to coupling to the external environment in open quantum-dot arrays
M Elhassan, J P Bird, R Akis, D K Ferry, T Isa and K Ishibashi

Raman study of carbon substituted MgB₂

Raman scattering investigation of electron–phonon coupling in carbon substituted MgB₂
T Sakuntala, A Bharathi, S K Deb, N Gayathri, C S Sundar and Y Harirahan

Dewetting of polymer films

Dynamics and structure formation in thin polymer melt films
Ralf Seemann, Stephan Herminghaus, Chiara Neto, Stefan Schlagowski, Daniel Podzimek, Renate Konrad, Hubert Mantz and Karin Jacobs

The discovery of superconductivity at 39 K in MgB₂ has attracted much attention because of the unusual two-gap nature of superconductivity in this system and also because of the possibility of attaining high critical fields. Carbon substitution reduces $T_c$ but increases the critical field. The $T_c$ of MgB₂ with ~10 at.% of the B substituted with carbon is 22 K. This decrease in $T_c$ is much smaller than that expected from rigid band behaviour. Band structure calculations indicate that for $x = 0.2$ the $\sigma$-band holes are still present and for $x = 0.4$ they completely vanish at $T_c$. It is also suggested that the electron–phonon coupling strength mediated by the $E_{2g}$ bond-stretching mode should increase substantially for small C substitutions. This $E_{2g}$ mode is Raman active and couples strongly with the $\sigma$-band holes leading to the high $T_c$ of MgB₂, so Raman scattering helps in understanding superconductivity in MgB₂. The $E_{2g}$ mode in MgB₂ is at ~600 cm⁻¹, much lower than the 980 cm⁻¹ of the isostructural, non-superconducting AlB₂. This is largely due to electron–phonon coupling.

A Bharathi and colleagues at the Indira Gandhi and Bhabha Atomic Research Centres have studied the evolution of the $E_{2g}$ phonon with C substitution in MgB₂-C, for a wide range of composition. From the observed frequency and the linewidth variations of the Raman shift, and the calculated $\sigma$-hole density of states, they evaluated the $e$–$p$ coupling strength as a function of carbon fraction.

They performed room-temperature Raman scattering measurements in MgB₂-Cₓ samples with $x = 0.0–0.2$. The average phonon frequency increased with C substitution, whereas the linewidth increased to a maximum for $x = 0.1$ and then decreased. They calculated the electron–phonon interaction parameter $\lambda_{phon}$ using Allen’s formula. Its value in pristine MgB₂ was in good agreement with that obtained from x-ray inelastic scattering. By suitably incorporating the $\lambda_{phon}$ variation in $\lambda_{phon}$ appearing in McMillan’s equation, they found that the variation of $T_c(x)$ compared well with the measured value.

Thin liquid films on solid surfaces are important in everyday life as lubricants, as coatings, e.g. to protect hardware from rust, to colour surfaces, or to change the wetting properties of substrates. In all these examples it is essential that the liquid wets the substrate: only then can a homogeneous film be achieved. So it is important to understand the origin of dewetting.

Karin Jacobs at Saarland University and co-workers have studied the stability of thin liquid films on solid surfaces. A detailed analysis of the structures that emerge in dewetting has led to a comprehensive picture of thin film stability. They distinguished experimentally three different pathways of dewetting (spinoidal, homogeneous and heterogeneous) that were expected theoretically. Studies on spinodally dewetting films allowed them to derive the effective interface potential. Adilène van der Waals forces were adequate for correctly describing the potential. Experiments recording the dynamics of dewetting gave insight into the viscosity of a thin film. They demonstrated that thin films of polystyrene below the entanglement length also exhibit a reduction of the glass transition temperature. A new theoretical approach was required to explain this. Mode coupling theory explained their experimental findings very well.

They used the Minkowski measures approach to describe the topographies that emerged in simulations and experiments on dewetting liquid films. The experimental and simulated patterns strongly resembled each other, so numerical simulation can be used to test the behaviour of a liquid on a hypothetical substrate and to predict stability conditions.

Future studies will concentrate on the energy dissipation close to the three-phase contact line of a moving front, addressing questions like: Can the front profile be used to describe a liquid’s properties? Does it reveal whether the liquid is sliding over the surface? Do liquids containing particles or blends of liquids behave similarly? Can we enhance the throughput of lab-on-a-chip devices?
Chirality of nanotubes

Non-dispersive and dispersive collective electronic modes in carbon nanotubes

Ricardo Perez and William Que

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Dispersion curves for the collective electronic modes with angular momentum index \( L = 0 \) for three carbon nanotubes. The solid diamonds are experimental results on the dispersive mode from Pichler et al. The Brillouin zone edges for the \((10, 10)\), \((18, 0)\), and \((16, 3)\) carbon nanotubes are at \( q_{∥} \approx 1.26, 0.73\), and \(0.94\,\AA^{-1}\), respectively.

Metals are carbon nanotubes show Luttinger liquid behaviour, by which single-particle excitations are suppressed and collective electronic modes or plasmons play an important role. Momentum-dependent EELS experiments on single-wall carbon nanotubes carried out by Pichler et al in 1998 showed a dispersive mode attributed to the \( \pi \) plasmon and several non-dispersive modes at lower energies whose origin is controversial: at least three different interpretations have been offered, but none of these was consistent with new results from optical absorption measurements.

Ricardo Perez and William Que of Ryerson University, Canada, present their theoretical results on the loss functions of individual single-wall carbon nanotubes and shed some light on the origin of the non-dispersive modes, which they propose are inter-subband plasmons from chiral nanotubes with small Brillouin zones. They use a tight-binding model for \( \pi \) band electrons to study the collective electronic excitations of single nanotubes using the random phase approximation. The calculated dispersion curves of collective electronic modes for \( L = 0 \) are shown in the figure. The dispersion curves terminate at the Brillouin zone edge of the corresponding nanotube. We see that the \((16, 3)\) tube has only optical modes, while the \((10, 10)\) and \((18, 0)\) tubes each have an acoustic mode. This is because the \((16, 3)\) tube is semiconducting while the other tubes are metallic.

Note that, since the experiment of Pichler et al was performed on bulk samples, the measured spectra contain contributions from many nanotubes of different chirality. The non-dispersive modes could be due to chiral nanotubes, and the dispersive mode should be due to armchair and zigzag nanotubes. Since intertube coupling shifts the energies of the collective electronic modes higher, it is not possible to match the calculated energies in this work for individual nanotubes to experimental results on bulk samples where intertube coupling is present. To allow an exact comparison between theory and experiment, it is desirable to obtain momentum-dependent EELS for individual nanotubes, and such experiments should determine the validity of the interpretation offered here. If Perez and Que’s prediction is confirmed experimentally, eventually EELS could become a potential tool for identifying the chirality of individual carbon nanotubes.

Five-wave mixing at surfaces

Femtosecond time-resolved five-wave mixing at silicon surfaces

T Meier, M Reichelt, S W Koch and U Hofer

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A schematic drawing of wave-mixing processes at surfaces in reflection geometry: (a) for two and (b) for three incident laser beams.

Two-photon photoemission (2PPE) measurements are generally restricted to conducting surfaces. T Meier, M Reichelt, SW Koch and U Hofer describe a surface-sensitive time-resolved technique combining four-wave mixing (4WM) with second-harmonic generation (SHG), resulting in a five-wave-mixing (5WM) process and review recent experimental results on silicon surfaces. The diffracted second harmonic generated by sequences of ultrashort laser pulses is detected as a function of the time delay between the pulses. This 5WM technique can be used to measure the temporal evolution of the optical polarization and the photoexcited populations at the surface. At the Si(111)\( \times 7 \) surface, the self-diffracted signal induced by two ultrashort laser beams shows a rapid decay on a timescale comparable with the duration of the incident pulses of less than 15 fs. Numerical solutions of the optical Bloch equations for model systems show that it cannot be decided from the experimental data alone whether this dynamics is due to the decay of individual uncoupled polarizations or is the result of the destructive interference of a system of coupled polarizations. To distinguish these processes, a microscopic modelling of the SHG including all optical matrix elements and further relevant interaction processes is required.

The Si(001)c(4 \times 2) surface has been studied using a 3WM set-up which measures the diffracted second-harmonic intensity induced by three femtosecond laser beams. By varying individual time delays between the pulses, this technique can be used to investigate the dynamics of one-photon transitions, and also allows one to monitor the temporal evolution of populations. Using model calculations based on optical Bloch equations, the observed ultrafast response as a function of a particular delay can be assigned to scattering of the excited electrons within the \( D_{\text{max}} \) surface band on timescales of 50–500 fs.

The authors plan similar 5WM experiments using tunable laser pulses to investigate these processes in more detail, analyse the ultrafast optically induced dynamics at other surfaces, and access the largely unexplored electron dynamics of buried semiconductor interfaces. Theoretically, more microscopic approaches will be developed to gain a better quantitative understanding of the material dynamics responsible for the dynamics of nonlinear optical excitations at surfaces and interfaces.

Molecular motor

Basing the random walk of a molecular motor

R Dean Astumian

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Cartoon illustration of the difference between a mechanical and a chemical approach for storing energy by transferring a particle from a low energy well to a well at a higher energy. Because of the ‘softness’ of the potential, in the ‘mesoscopic approach’ an external source provides a force to push the molecule over the barrier. In the ‘chemical approach’ it is the energy of the external source that is the maximum, \( E_F \), resulting in an inefficient motor. In the chemical approach however the input energy is used to destabilize the system in the left-hand well, but the motion itself is driven by thermal activation over the barrier. In this case, the rate of ‘drift’ does not decrease the efficiency.

Biomolecular motors are molecules that convert chemical free energy into directed motion. Rather than talking about levers, springs and clutches, pulleys, rowing cross-bridges, or power strokes, molecular motors should be discussed in terms of equilibrium processes.

The sequence of conformational changes by which a motor protein moves in a random walk, with transitions occurring by thermal activation over energy barriers. Dean Astumian of University of Maine addresses the question of how this random walk is biased by a non-equilibrium chemical reaction (ATP hydrolysis) so the motor molecule moves preferentially in one direction and discusses how these ‘soft matter’ motors can achieve thermodynamic efficiencies of nearly 100%.

The motions of molecular motors are best described as thermally activated processes with Poisson distributed lifetimes. The Brownian motor mechanism is based on thermally activated transistions between states that are very close to ‘local’ equilibrium with respect to their internal degrees of freedom despite the fact that the chemical reaction that drives motion, ATP hydrolysis, is very far from equilibrium. By operating where all conformational states are near to local equilibrium and by using a chemical (stabilization/denaturation) approach rather than a mechanical approach, a biomolecular motor made of ‘soft’, conformationally flexible, protein can operate at nearly perfect efficiency.

Soon the mechanism of biomolecular motors will be clarified experimentally. By observing at a single-molecule level an individual ATP hydrolysis event followed by the completion of a step of the motor along its track, the distribution of time lapse between these two events can be determined. The random walk (Brownian motor) model presented here predicts that the time between ATP hydrolysis and completion of a step will be randomly (Poisson) distributed rather than deterministic as expected from a mechanical model. Resolution of this question will be important not only for understanding the mechanisms of biomolecular motors, but also in the design of synthetic molecular motors.
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Magneetoelectronics with magnetoelectrics

Ch. Binek and B. Doucini

Characterization of hydrogen-like states in bulk Si, Ge alloys through muonium observations
P. J. C. King, R. L. Lichti, S. P. Cottrell, I. Yonenaga and B. Hitti

Heavy fermions

Dynamics and transport properties of heavy fermions: theory
Optical and transport properties of heavy fermions: theory compared to experiment
David E. Logan and N. S. Vidyadhiraja

Variation with alloy composition of the average value of the isotropic component of the MuT HP, with straight line fit, together with the MuT HP.

Heavy electron materials have been extensively investigated, yet even their ‘normal’ paramagnetic phase, be it metallic or insulating, has eluded a unified microscopic description on all temperature (T) and/or frequency (ω) scales. Within the general framework of dynamical mean-field theory David Logan and N.S. Vidyadhiraja (Oxford) have developed a non-perturbative local moment approach to paramagnetic metallic phases of the periodic Anderson model (PAM), with a focus on dc transport and optics, focusing on the Kondo lattice regime relevant to strong correlated heavy fermion (HF) metals, where the problem is characterized by a single, exponentially small coherence scale s. All relevant energy/temperature scales are handled by the theory, from the low-energy coherent Fermi liquid domain out to large multiples of s, where incoherent many-body scattering dominates; followed by the crossover out of the scaling regime to non-universal, high-energy/temperature scales dictated by ‘bare’ model/material parameters. While the emphasis has been on strong correlations, all interaction strengths are encompassed by the LMA, so intermediate valence behaviour can also be addressed.

In the second paper they make a direct comparison with dc transport and optical conductivities of CeB6, YbAl3, CeAl3 and CeCoIn5. YbAl3 is an intermediate valence material, and the others typify heavy fermion behaviour, from the strongly correlated Kondo lattice regime of CeAl3 and CeB6, to the somewhat weaker coupling case of CeCoIn5. Most features of the optics and transport of these materials are captured, the natural exception, omitted from the model itself, being crystal field effects which may (or may not) show up in the experimental resistivity as a reduction below one-channel behaviour at suitably high temperatures. The theory performs well quantitatively, and also captures notable features specific to individual systems, e.g. the existence of a low-frequency shoulder in the optical spectra of YbAl3, or the absence of any significant direct gap/mR absorption in CeAl3. The model thus appears to provide quite a comprehensive and successful description of experiment. This also authorises both to the dominance of the local electron scattering inherent to the model itself and the need to provide an adequate theoretical description of such on all experimentally relevant frequency and temperature scales.
**Novel superconductivity in CePt$_3$Si**

Novel superconductivity coexisting with incoherent electric-multipolar order in CePt$_3$Si.

M Ishikawa, S Yamashita, Y Nakazawa, N Wada and N Takeda


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**Short-range attractions in proteins**

Tuning short-range attractions in protein solutions: from attractive glasses to equilibrium clusters.

Anna Stradner, George M Thurston and Peter Schurtenberger


**s–p- and d-ferromagnetism**

Are s–p- and d-ferromagnetisms of the same origin?

Antonis N Andreiotis, R Michael Sheetz and Madhu Menon


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C$_p$/T versus ln T as a function of several magnetic fields for an annealed sample of CePt$_3$Si. $T_{Q1}$, $T_{Q2}$ and $T_c$ are respectively two quadrupolar-like transitions and superconducting transition temperature.

There is much interest in strongly correlated electron systems, e.g., the unconventional superconductivity in f-electron heavy-fermion compounds including Ce$_2$Pt$_7$S$_{12}$, CeRh$_2$Si$_2$, CeCu$_2$Si$_2$, UPt$_3$ and CePt$_3$Si. Paradoxes mediated by fluctuations of spin, valence, density have been proposed. CePt$_3$Si is claimed as a new superconductor without inversion symmetry, and its pairing mechanism is actively sought.

M Ishikawa and co-workers in Japan recently reported that an annealed sample of CePt$_3$Si exhibits non-magnetic heavy-fermion behavior. To reveal the precise nature of the 2.2 K transition, they measured $C_p$ above 0.6 K in fields up to 10 T. The plot of $C_p$/T versus ln T shows a small but distinct anomaly at 2.2 K and a shoulder around 2.6 K at zero field, denoted $T_{Q1}$ and $T_{Q2}$, respectively. The former is rapidly depressed and absorbed by the latter below about 4 T, and the latter becomes sharper and grows into a distinct peak as the field increases. This resembles the quadrupolar transitions in CeB$_6$ and Ce$_2$Pd$_7$S$_{12}$. The transition at $T_{Q1}$ may be an incipient quadrupolar transition. However, in CeB$_6$, an AF transition occurs at 2.5 K in the quadrupolar-ordered phase, while the present transition at $T_{Q1}$ is not AF but something related to the transition at $T_{Q2}$. Superconductivity emerges below these temperature transitions, and it is destroyed by a field around 4 T as the $T_{Q2}$ peak is smeared out. The new phase at $T_{Q2}$ may assist the appearance of superconductivity.

Why is such coexistence possible in CePt$_3$Si? The heavy-fermion state with relatively large exchange interaction parameter $J$ is formed closer to an intermediate-valence region rather than a quantum critical point on the verge of an AF phase. A large $J$ and high Kondo temperature are inferred from the exceedingly low magnetic entropy at these low temperatures, i.e., it is in a state where strong fluctuations of any kind are conceivable near the presumed multipolar transition, and the superconductivity could be mediated via such fluctuations of spin, valence or charge, as proposed for superconductivity in other heavy-fermion compounds like CePd$_2$Si$_2$ and CeCu$_2$Si$_2$. It is important to decide which type of fluctuation is most effective for the superconductivity in CePt$_3$Si.

Effective structure factors $S(q)$ for γ-B-crystallin solutions plotted vertically as a function of $q$ and protein concentration $c$, compared with the Baxter sticky sphere structure factor model with use of sphere diameter 3.6 nm and thickness parameter $1/\sigma = 8.62$

Anna Stradner and Peter Schurtenberger of Fribourg University, Switzerland, and George Thurston of Rochester Institute of Technology, USA, have carried out small-angle scattering experiments with two different types of model proteins, γ-B-crystallin and lysozyme. They discuss the results in the context of recent suggestions that globular proteins possess a short-ranged attractive potential, and that simple models from colloidal science could help to rationalize the best route for obtaining protein crystals and to interpret their complex phase diagrams. The short-range attraction leads to an extremely interesting phase behavior with a liquid–gas coexistence curve that is metastable with respect to the liquid–solid (crystal) boundary and the occurrence of an attractive glass. They demonstrate that for γ-B-crystallin, the scattering data are indeed in good agreement with predictions for an interaction potential consisting of short-ranged attraction and hard sphere repulsion, and they also provide evidence of a dynamically arrested glasslike state at high concentrations. They also report on a systematic study of the effect of a weak screened Coulomb repulsion in highly concentrated lysozyme solutions.

They have previously shown that a combination of short-range attraction and long-range repulsion results in the formation of small equilibrium clusters, which is clearly relevant for e.g., nucleation processes during protein crystallization, protein or DNA self-assembly, and the formation of cluster and gel phases in colloidal suspensions. In the current study they investigate the effect of variations in temperature, which allows them to carefully tune the balance between soft repulsion and short-range attraction and investigate its influence on the cluster formation.

Any attempt to use the theoretical framework for strongly interacting colloidal particles, e.g., to use mode-coupling theory to evaluate particle dynamics close to dynamical arrest near a glass or gel line, requires precise knowledge of the static structure factor $S(q)$, so they used a combination of small-angle x-ray and neutron scattering to determine $S(q)$ as a function of concentration, ionic strength and temperature for both lysozyme and γ-B-crystallin. This provides structural information on the spatial correlations between individual proteins in concentrated solutions.

There is much current interest in the exotic s–p magnetism in organic materials such as C$_60$-based polymers and some non-traditional inorganic materials such as hexaborides. These materials show several common features, such as the presence of structural and/or topological defects, significant charge transfer, a degerenate ground state, and in some cases, a resonant ground state.

Antonis N Andreiotis of FORTH and R Michael Sheetz and Madhu Menon of University of Kentucky have examined the results in more detail, emphasizing the defect-related magnetism in the C$_60$-based polymers and elucidated the underlying mechanism of their magnetism. They draw analogies with the well known McConnell model for ferromagnetic charge-transfer salts.

The existence of the 2 + 2 cycloaddition bonds (which provide sp$_2$-bonded carbon atoms) in coexistence with vacancies can explain the magnetism in polymerized-C$_60$ materials. The vacancies and the 2 + 2 cycloaddition bonds provide the necessary unpaired spins, while also initiating the charge-transfer processes which create and sustain large electric dipole moments. The latter develop the necessary ferromagnetic coupling mechanism among the unpaired spins, leading to a ferromagnetic state.

These observations show the common origin and common features of s–p magnetism and the usual d-magnetism. Charge-transfer processes and orbital degeneracy seem to be key factors. However, the charge-transfer processes have to be large enough to develop and sustain strong fields to provide the necessary kinetic exchange interaction for promoting the high spin states as ground states, and this is more apparent in s–p magnetism. The differentiation between the two types of magnetism in the literature through various models reflects the leading terms that are kept in the implementation of the e–e correlations and the underlying physical picture of such an approximation.
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Shape-memory effect
Fermi-surface orbits responsible for each frequency (see (B)).
R D McDonald, J Singleton, P A Goddard,
F Drymiotis, N Harrison, H Harima,
M-T Suzuki, A Saxena, T Darling, A Migliori,
J L Smith and J C Lashley

Chirality and protein folding
Fermi-surface orbits responsible for each frequency (see (B)).
R D McDonald, J Singleton, P A Goddard,
F Drymiotis, N Harrison, H Harima,
M-T Suzuki, A Saxena, T Darling, A Migliori,
J L Smith and J C Lashley

Magnetotransport in epitaxial films of the degenerate semiconductor Zn$_x$Co$_{1-x}$O films
R C Budhani, Priya Panti, R K Rakshit,
K Senapati, S Mandal, N K Pandey and
Jitendra Kumar

The calculated Fermi surfaces for (A) the austenite phase and (B) martensite phase of AuZn, the small letters label the orbit giving rise to various dHvA oscillations. (C) (from left to right) dHvA frequencies from the band-structure calculations for the martensite domain with the [1 1 1] zone-axis rotated along the austenite (111) direction, the (110) and (111) directions and the (110) direction and the sum of all domain orientations, with the observed dHvA frequencies on the right. The coloured bands are a guide to the eye, a-f indicate the Fermi-surface orbits responsible for each frequency (see (B)).

Martensites are widely found materials that undergo diffusionless, solid-state transitions. Some of them exhibit the shape-memory effect (SME) - after deformation of the low-temperature martensitic phase, they recover their high-temperature shape on warming.

A group led by John Singleton (Los Alamos) has identified the primary electronic mechanism responsible for the martensitic transition (MT) in the shape-memory alloy AuZn through detailed measurements of its Fermi surface and comparing the data with band-structure calculations.

As the temperature is lowered through the MT, the unit cell is distorted in the [1 1 0] shear direction. A strain and commensurate shuffle of every third unit cell results in a hexagonal primitive unit cell formed from nine primitive cubic cells of the parent phase.

The figure shows the calculated Fermi-surface sections of the martensite phase (B) along with their cell results in a hexagonal primitive unit cell formed from nine primitive cubic cells of the parent phase.

A problem in modelling the kinetics of protein folding is to know when the system has reached the native conformation. Simple and widely used criteria of folding are based on a variable crossing a predefined threshold value, e.g. the root mean square deviation (RMSD) distance away from the native state, or the fraction, Q$_n$ of the established native contacts. A third criterion, based on the angular properties of the protein backbone, involves checking whether the bond and dihedral angles are within a chosen range of their native values.

Joanna Kwiecińska and Marek Gieplak of Polish Academy of Sciences, Warsaw show that such simple criteria may prompt one to declare folding even though fragments of the resulting conformations have the wrong chirality. The figure shows an example of this with the Q criterion. The folding process may generate a left-handed α-helix instead of the true right-handed one, even though all native contacts are within their respective values of Q$_n$ and the RMSD distance from the native state is only around 2.5 Å.

They propose combining the simple criteria with the requirement that all local values of the chirality should be nearly native. They show that setting the local chiralities to native-like values may or may not precede the ‘call’ resulting from the simple criteria, but the compound requirement allows for more accurate studies of folding and typically generates structures that appear to be of correct topology.

Dihedral angles are the backbone dihedral angles that determine the chirality of a protein. The chirality-based criterion relates to the criterion involving the bond and dihedral angles and whether it is better to use potentials that favour the native sense of chirality or those which favour the native values of the bond and dihedral angles. They find the chirality potential to act in a comparable way to the angular potential, but its usage is much more economical in simulations. They also find that simple modelling of the side groups by the β carbon atoms does not automatically make the chirality in the folded state correct.

Conformations of crambin in the backbone representation. Left: the native structure (1crn in the Protein Data Bank). Right: the conformation in which all native contacts are established through a folding process accomplished through a molecular dynamics evolution in the Go-like model. Some local chiralities are opposite to what they should be.

The zero-field longitudinal resistivity of the films with x = 0.0, 0.10, 0.20 and 0.30 plotted as a function of temperature. The inset shows the variation of the room temperature resistivity as a function of the cobalt concentration.

ZnO doped with transition metal (TM) is a strong candidate for a dilute magnetic semiconductor (DMS). The origin of the long-range ferromagnetic order observed well above 300 K is controversial. In some cases the magnetism was related to isolated clusters of the TM or its oxides, whereas in others a seemingly homogeneous solid solution orders via alignment of 3d spins at the TM ion sites.

The solubility of Co is larger in thin films than in bulk samples, but there are conflicting reports on the magnetic character of these films. R C Budhani and co-workers at Indian Institute of Technology, Kanpur have performed magnetotransport measurements over a broad range of temperatures and magnetic fields on heavily degenerate n-type Zn$_x$Co$_{1-x}$O epitaxial films. The cobalt-free samples are characterized by a metallic resistivity ρ(T) down to 2 K, a negative and predominantly isotropic magnetoresistance and optical transmission above 85% in the visible range. X-ray diffraction measurements showed that, while for x < 0.20 all cobalt atoms occupy the tetrahedral sites of the wurtzite structure of ZnO, a phase separation into CoO is seen for x > 0.2. In the solution phase, they did not observe any signatures of a spontaneous ordering of the cobalt spins despite a large concentration of mobile electrons (>10$^{20}$ cm$^{-3}$).

The absence of anomalous Hall resistance is consistent with this observation. Over the entire range of x, the carrier concentration remains above the Mott limit for the insulator-to-metal transition in a doped semiconductor. However, while the Co-free samples are metallic (T $>$ 2 K), there is a resistivity minimum followed by ln T divergence of ρ(T) at low temperatures with increasing x. The magnetoresistance of these samples is negative and predominantly isotropic and tends to follow a log H behaviour at high fields. These observations, including the Kondo-like minimum in the low resistivity, suggest transport in these dilute magnetic semiconductors is dominated by s$^-$ exchange.
Hydrogen production from ethanol on Pt(111)

Modelling of ethanol decomposition on Pt(111): a comparison with experiment and density functional theory

E. Vesselli, G. Codovich, G. Comelli and R. Rosci

Dynamics of active filaments

Some aspects of the dynamics of active filament solutions

Tanniemola B Liverpool

Liquid–liquid phase transitions

On the abundance and general nature of the liquid–liquid phase transition in molecular systems

Rei Kurita and Hajime Tanaka

Surface concentration of the stable species during a simulated ethanol decomposition experiment on Pt(111), as a function of temperature, on the basis of the results obtained with the simple UBI-QEP model. Arrows indicate the temperature range in which the species are found to be stable on the basis of real time temperature dependent EPS data.

The ethanol reforming reaction catalysed by Pt or Rh is a candidate for hydrogen production. E. Vesselli and co-workers in Trieste have studied ethanol decomposition on clean Pt(111) in the zero-coverage limit in the unity bond index quadratic-exponent potential (UBI-QEP) model.

DFT identifies ethanol, CH₃CHOH, CH₃COH, CH₃CO, CH₂CO, CH₂CO, CH₃CHO and CCO as the most stable intermediates for each dehydrogenation step from ethanol to CCO CH₂CHO has the lowest transition state energy for C-O cleavage, while CHCO shows the lowest decarbonylation barrier.

It is proposed that CH₃CO dehydrogenates to CHCO (unstable), yielding CO and CH or CH₃ groups via C–C bond cleavage. It is proposed that CH₂CO dehydrogenates to CH₂CO (unstable), yielding CO and CH₂, which rehydrogenate to methane. Vesselli et al. used the UBI-QEP model to simulate the most probable decomposition pathway. They found good estimates for adsorption energies and dehydrogenation barriers but their C–C and C–O bond cleavage barriers (though in line with experiment) disagreed with DFT estimates. Their kinetic picture can explain these discrepancies. The proposed reaction mechanism predicts the formation of CH₂ and CH groups on the surface by distinct parallel reaction paths. Then, the methyl groups can rehydrogenate to methane or dissociate to surface carbon and hydrogen. The proposed stable intermediate is CH₂CO, which is not incompatible with the spectroscopic data. This work is a further step in predicting catalytic behaviour.

Soft active systems are a new and exciting class of complex fluids to which energy is continuously supplied by internal or external sources. Examples from biology include cell membranes and biopolymer solutions driven by chemical reactions, living cells moving on a substrate, and the cytoskeleton of eukarotic cells. The cytoskeleton is a complex network of long filamentary proteins cross-linked by smaller proteins. Among the latter are clusters of motor proteins, such as myosin and kinesin, that use chemical energy from the hydrolysis of ATP to ‘walk’ along the filaments. This out-of-equilibrium chemical activity in motor–filament solutions leads to complex cooperative behaviour including pattern formation and creation of dissipative structures.

The transition state energy for C–O cleavage, while CHCO shows the lowest decarbonylation barrier.

The rich behaviour of mixtures of filaments and motors is far from being completely understood. The simple picture considered needs to be tested by experiment. Even in the isotropic regime, an active solution could be pre-stressed, and it is possible that imposing a shear flow could decrease the stress. It is assumed that the tube has the same properties as the structure, being neither perfectly homogeneous nor universal. For TPP and n-butanol, for example, hydrogen bonding may be crucial in the formation of such structures. The identification of the locally favoured structures of these liquids remains a future problem.

Even a single-component liquid may have more than two kinds of isotropic liquid state. Although there are clear examples of liquid–liquid transitions (LLT) for atomic liquids, there was until recently no direct evidence for molecular liquids. LLT in water has been suggested by experimental evidence of LLT in a molecular liquid, triphenyl phosphate (TPP). Both nucleation-growth-type and spinodal-decomposition-type phase transformations were directly observed with optical microscopy. The glass transition of a normal liquid and a distinct thermal signature of the glass transition of a second liquid were both detected. They also observed a critical-like anomaly associated with the mean-field spinodal behaviour of LLT.

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Pattern observed with phase contrast microscopy at T_g = 120 K for various annealing times t_a: (a) 30 min, (b) 45 min, (c) 50 min, (d) 50 min, (e) 60 min, (f) 80 min, (g) 90 min, (h) 120 min, and (i) 180 min. The scale bar corresponds to 20 µm. Initially there is only liquid I (or (i)), and then droplets of liquid II with dark contrast appear and grow with time.

This study may shed new light on the basic nature of a liquid: even an ordinary molecular liquid such as n-butanol or TPP may have a hierarchical energetic structure, being neither perfectly homogeneous nor random, but possessing long-lived short-range order with cooperativity. So, the liquid may not be a unique state of matter, but there can often be more than two liquid states even for single-component matter. LLT may be hidden by either crystallization or glass transition. The former may be the case of liquid water.
Theoretical phase diagram for hard spheres of radius $R$ with a square well attractive interaction of width $\lambda$ and depth $u_0$. Curves are labelled by the relative well width, $\lambda/R(2\pi)$. Note the $\omega$-exponent shape of the lines separating the fluid region in the glassy regions for $\lambda < 5\%$. For $\lambda > 3\%$, a line separating the attractive and the repulsive glass phases ends in the $A_5$ singular point. The $A_5$ singular point (critical curve) is estimated to be located on the $\lambda = 4.11\%$ line (not shown for clarity).

Luca Cipelletti and Laurence Ramos from Montpellier review recent experimental work on the slow dynamics in soft matter, focusing on four closely related areas: the existence of two different glass states (attractive and repulsive), the dynamics and the ageing of systems far from equilibrium, the effect of an external perturbation on glassy materials, and dynamical heterogeneity. Many unified approaches have been sought to account for the similarities in the slow dynamics of many soft materials and analogies with hard condensed matter glasses and granular media, notably mode coupling theory (MCT). Recent theoretical evidence that MCT can make quantitative predictions on dynamical heterogeneity: they need to be tested experimentally.

The jamming scenario can rationalize fluid-to-solids transitions in systems ranging from colloidal suspensions to molecular glasses and granular materials. It is supported by analogies in the local dynamics between glass formers and granular media (cage effect, dynamical heterogeneity). While MCT and jamming describe systems approaching the non-ergodicity transition from the fluid phase, materials deeply quenched in an out-of-equilibrium phase are less well understood. The effective temperature concept may prove useful to describe out-of-equilibrium soft materials and analogies with hard condensed matter glasses and granular media.

Slow dynamics in glassy soft matter has been investigated by a combination of theory, simulation, and experiments. New experimental techniques have extended measurements to out-of-equilibrium and very slowly relaxing systems, aiming to obtain spatially and time-resolved information on the dynamics, and to identify the most insightful quantities to characterize heterogeneous behaviour. Future advances will probably include the combined use of these methods, to achieve a more complete understanding of the various physical mechanisms driving the relaxation of glassy soft matter, and of their interplay. The focus will be in identifying and explaining the ‘universal’ features of the slow dynamics in vastly different systems.

Flow-induced structures in colloids

Flow-induced structure in colloidal suspensions

J. Vermaart and M.J. Solomon


Schematic of the changes in the suspension microstructure as characterized by an FFT of an initially disordered suspension in the $v_N$ plane at high $P_0$ number. The arrows on the FFT indicate the compressional axis and the extensional axis of the flow field; the velocity vectors are shown as well.

Familiar colloidal dispersions include paints, inks, cosmetics, pharmaceuticals and food. The macroscopic properties of suspensions are determined by the spatial organization of the particles, i.e. the microstructure. J. Vermaart (Leuven) and M.J. Solomon (Michigan) review the sequences of structural states that can be induced in colloidal suspensions by the application of flow. Structure formation during flow is strongly affected by the delicate balance among interparticle forces, Brownian motion and hydrodynamic interactions. The resulting non-equilibrium microstructure determines the rheology. Colloidal suspensions with near-hard-sphere interactions develop an anisotropic, amorphous structure at low dimensionless shear rates. At high rates, clustering due to strong hydrodynamic forces leads to shear thickening rheology. Application of steady-shear flow to suspensions with repulsive interactions induces a rich sequence of transitions to one-, two- and three-dimensional order. Oscillatory-shear flow generates metastable ordering in suspensions with equilibrium liquid structure. However, short-range attractive interactions can lead to a fluid-gel transition under quiescent suspensions. Application of flow leads to orientation, breakup, densification and spatial reorganization of aggregates. Using a non-Newtonian suspending medium leads to additional possibilities for organization. Vermaart and Solomon examine the extent to which theory and simulation have yielded mechanistic understanding of the observed microstructural transitions. For fluid-like and ordered suspensions, the effects of flow are fairly well understood, and even quantitative predictions exist between microstructure and macroscopic properties have been established. For weakly aggregated suspensions and for suspensions of particles in rheologically more complex fluids, more work is needed for mechanistic understanding. New experimental methods such as in situ CSLM microscopy and measurements on two-dimensional model suspensions may contribute to this development.

For numerical simulations, inclusion of hydrodynamic interactions helps develop understanding of the physical mechanisms involved and leads to prediction of macroscopic properties. Simulation methods that can accommodate either the non-ergodicity of aggregated suspensions or the non-Newtonian nature of the suspending media are difficult but necessary next steps.

Quantum phase transitions

Heavy fermion systems, with quasiparticle mass over a hundred times the bare electron mass, are interesting for studying strongly correlated Fermi liquids and superconductors. The large mass reflects the Kondo screening of the magnetic moments, which is necessary to overcome magnetism. Heavy fermions are of interest for both experimental and theoretical studies of quantum critical points (QCP). Magnetic QCP in heavy fermion metals are reviewed by Qiunao Si of Rice University and co-workers. The interplay between Kondo screening and magnetic interactions in Kondo lattice systems has been re-examined theoretically. A local quantum critical point has emerged, in which magnetic interactions suppress Kondo screening precisely at the magnetic QCP. The Fermi surface undergoes a large reconstruction across the QCP and the coherence scale of the Kondo lattice vanishes there. The dynamical spin susceptibility exhibits $\omega/T$ scaling and non-trivial exponents describe the temperature and frequency dependences of various physical quantities, in contrast with the conventional Fermi liquid theory. Heavy fermion systems are of interest for both experimental and theoretical studies of quantum critical points (QCP).

S. et al discuss recent microscopic studies of Kondo lattices within an extended dynamical mean field theory (EDMFT). Beyond the initial studies based on an $M$-expansion renormalization group method, Kondo lattice models with Ising anisotropy have been investigated, which have allowed the study of both the destruction of Kondo screening and the concomitant fractional exponent and $\omega/T$ scaling in the magnetic dynamics. They also discuss the magnetic phase diagram and summarize the evidence for the second-order nature of the magnetic quantum phase transition.

These microscopic approaches show that critical modes beyond the order parameter fluctuations exist associated with the destruction of Kondo screening. Consequences of this – in magnetic dynamics and also in the Fermi surface properties and thermodynamics – are supported by experiments. The insights will also help find a field theory that describes quantum critical heavy fermions, and they may be relevant to the exotic quantum critical behaviour in other strongly correlated systems such as doped Mott insulators.
Electrowetting

Electrowetting is widely used to manipulate tiny amounts of liquids on surfaces in applications from 'lab-on-a-chip' devices to adjustable lenses and new kinds of electronic displays. Frieder Mugele and Jean-Christophe Baret of University of Twente review both fundamental and applied aspects of electrowetting.

The basis of electrowetting is a change of contact angle between an electrode and electrode on applying a voltage. In an external electric field, the charge carriers on the droplet surface of a conductive liquid redistribute, changing the surface morphology. The equilibrium surfaces remain surfaces of constant mean curvature because the electric field vanishes along the liquid–vapour interface, so capillarity determines the morphology. Electrowetting is then equivalent to conventional wetting on a surface with an identical distribution of local contact angles. This description is sufficient for most practical applications but breaks down under certain conditions.

Mugele and Baret compare the various approaches used to derive the basic electrowetting equation and discuss in detail the origin of the electrostatic forces that induce both contact angle reduction and the motion of entire droplets. They present some recent extensions to the theory accounting for distortions of the liquid surface by local electric fields, for the finite penetration depth of electric fields into the liquid, and for finite conductivity effects under an AC voltage. They also discuss the most prominent failure of the electrowetting equation, namely the saturation of the contact angle at high voltage, which recent work indicates is due to several distinct physical effects. With suitable electrode patterns or topographic structures on the substrate surface, variations of the contact angle can give rise not only to continuous changes of the droplet shape, but also to discontinuous morphological transitions between distinct liquid morphologies.

They briefly discuss the dynamics of electrowetting and finally give an overview of recent work aimed at commercial applications, in particular in the fields of adjustable lenses, display technology, fibre optics, and biotechnology-related microfluidic devices.

Moving molecules with the STM

Single-molecule manipulation and chemistry with the STM

N Lorente, R Riculari and H Tang

J. Phys.: Condens. Matter

17 (2005) S1049–S1074

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Potential energy surface of NH3 along the Cu(100) surface calculated with the generalized gradient approximation using plane waves, and a 3x3 supercell where there is an ammonia molecule every three Cu atoms in the x and y directions of the surface. The plane axes are a Å, and the perpendicular axis in mV. The bridge site is at 1.29 Å along the [011] direction. It is a saddle point 301 mV in height. The hollow site is at (1.29, 1.29) Å A maximum. The barriers from top to hollow is 4.56 meV. The molecule needs less energy to go from top to top through the bridge site.

The scanning tunnelling microscope (STM) consists of a metallic tip, a tip manipulator and sophisticated electronics that record the tip–substrate electron current, bias voltage and manipulator motion. It is used to detect, analyse and modify adsorbed molecules. N Lorente et al from Toulouse review single-adsorbate manipulation from a theoretical point of view. They review both mechanical manipulations, where the interaction exerted by the probe’s tip on the adsorbate is used to initiate its motion, and recent work in the modelling and computation of inelastic effects localized at molecular adsorbates.

The aim is to account for the processes that permit controlled manipulation of matter at the atomic scale in adsorbed molecular systems. Simulations rely on total energy and electronic structure calculations where a trade-off is made between the size of the system and accuracy. This yields the basic quantities used for the next stage: the evaluation of the coupled electron–nuclear dynamics. This is a formidable task involving many approximations.

This review presents some of the customary approximations for the theoretical study of mechanical and inelastic manipulations. Mechanical manipulations use the interaction between the acting probe (usually a metallic tip) and the targeted adsorbate. The article reviews recent results in adsorbate mechanical manipulation and explains how manipulations can be effected by using the interaction between the probe’s tip and certain molecular groups of complex chemisorbed molecular systems. On the other hand, inelastic manipulations use the tunnelling current to convey energy with sub-angstrom precision. This current can excite localized vibrations that can induce measurable variations of the tunnelling conductance, hence providing a means of detecting single molecule vibrations. This current can also inject energy in a few reaction coordinates. Recently, the possibility of vibrational selective manipulations of NH3/Cu(100) has been experimentally demonstrated. The theory presented here addresses the actual pathways accessed when the molecule is excited by the tunnelling current from an STM.

TIO2 and ZnO for spintronics

Transition metal-doped TiO2 and ZnO - present status of the field

Rebecca Janisch, Priya Gopal and Nicola A Spaldin

J. Phys.: Condens. Matter

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There is much current interest in ‘spintronics’ which uses the spin of electrons in addition to their charge in electronic devices. The study of spin-polarized transport also reveals new and fascinating fundamental physics in its own right.

Magnetic semiconductors are materials that will allow signal amplification and be compatible with standard semiconductor growth techniques. Of particular interest are the so-called diluted magnetic semiconductors (DMS) in which non-magnetic semiconductor are doped with magnetic atoms. DMS based on II–VI semiconductors such as CdTe or ZnSe have interesting magneto-optical properties but the magnetic interaction in II–VI semiconductors is dominated by the antiferromagnetic exchange between the Mn spins and it is difficult to create p- or n-type carriers to mediate ferromagnetic interactions.

An important class of DMS is transition-metal-doped oxides. Co-doped TiO2 is ferromagnetic with Tc up to 650 K reported. The magnetic interaction is controversial but may result from the presence of Co clusters (Tc = 1180 K). Studies of ZnO doped with the whole range of 3d transition metal ions have variously shown high room-temperature ferromagnetism, spin-glass and paramagnetic behaviour.

Rebecca Janisch, Priya Gopal and Nicola Spaldin from University of California, Santa Barbara review the properties of Co-doped TiO2 and Mn- and Co-doped ZnO to elucidate the origin and optimization of the magnetic properties. They also discuss the effect of other transition metal dopants, including V, Cr, Mn, Fe and Ni, in both oxides to compare the magnetism in ZnO- and TiO2-based systems, and to evaluate the theoretical models for both.

They summarize the theoretical models that have been proposed to explain ferromagnetism in diluted magnetic semiconductors in general, and in oxide-based DMS in particular. Finally, they review the proposed mechanisms for the experimentally observed ferromagnetism and compare the predictions with the range of available data, outlining the experimental conditions that promote large magnetization and high ferromagnetic Curie temperature.
Surface roughness
On the nature of surface roughness with application to contact mechanics, scaling, rubber friction and adhesion
B N J Persson, O Albohr, U Tartaglino, A I Volokitin and E Tosatti

Computing nanostructures
Carbon-based nanotechnology on a supercomputer
David Tománek

Self-healing process within a (3, 3) nanotube with a monatomic vacancy, induced by illumination. (a) Time evolution of the geometry. The three atoms adjacent to the vacancy and the new C–C bond, which forms ~200 fs after the electronic excitation, are emphasized by colour and shading. (b) Time evolution of the partial charge density associated with the excited electron state. The lowest contour lines are common to the three panels.

Carbon nanostructures, particularly C60 and carbon nanotubes, are candidates for components of future nanoscale devices. They show unusual mechanical, thermal, electronic and optical properties.

Surface roughness and adhesion.

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Institute of Physics Publishing, c/o American Institute of Physics, PO Box 303294, St Louis, MO 63150-3284, USA. Tel: (303) 544-6901 Fax: (516) 349-9574 E-mail: subs@aip.org

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China National Publications Import & Export (Group) Corporation. Periodicals Department, 16 Gongti East Road, Beijing 100020, People’s Republic of China. Tel: +86 (010) 6508 6953 Fax: +86 (010) 6386 0970

JAPAN
Maruzen Co. Ltd, 3-10 Nihonbashi, 2-Chome, Chuo-ku, Tokyo 103, Japan. Tel: +81 (0)3 3275 6591 Fax: +81 (0)3 3275 0657 E-mail: journal@maruzen.co.jp

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A schematic picture of the lizard adhesive system. The skin of the lizard is covered by a dense layer of thin fibers or hairs (outer length ~100 µm and thickness of fiber ~4 µm). Each of these fibers branches into about 1000 thinner fibers (length = 10 µm and width = 0.1 µm). Each of the thin fibers ends with a thin (1–10 nm) leaf-like plate (spatula).

B N J Persson (Jülich) and co-workers in Germany and Italy present a review of surface roughness, which has a huge influence on many common phenomena. It is the main reason why macroscopic bodies usually do not adhere to each other with any measurable strength.

As the size of a solid object decreases, its surface to volume ratio increases, so surface roughness becomes more important. Miniaturization of mechanical systems, e.g., microelectromechanical systems, requires a better understanding of the role of surface roughness in, e.g., contact mechanics and adhesion.

Surface roughness is also of great importance in many biological systems. Flies, bugs, crickets and lizards have very soft layers on their feet which allow them to attach and move on both very smooth and rough vertical solid walls. Another example is non-wetting coatings on plant surfaces based on surface roughness.

The roughness of surfaces can be studied over a wide range of length scales using optical methods (~1 µm to kilometers) and cantilever methods, e.g., the atomic force microscope (~1 nm to 100 µm). For randomly rough surfaces, the most important quantity is the roughness power spectrum. It determines the contact mechanics and adhesion for solid objects in direct contact, and also governs rubber friction on rough substrates, e.g., friction of tyres on a road surface, and influences other phenomena of technological importance, e.g., the roughness induced leaking of sealings.

The study of surface roughness is important for understanding many natural and biological phenomena and also for many technological processes. The present drive toward miniaturization and the design of optimal systems by transfer of ideas from biology to materials science, is likely to accelerate efforts to study and predict the influence of surface roughness on many phenomena.