Journal of Physics:
Condensed Matter
TOP PAPERS 2006 SHOWCASE

Professor David Ferry
Editor-in-Chief
from 2007

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Editor-in-Chief
2002- 2006

Research journals are only worth reading if the quality of the science in them is good enough. Top Papers 2006 is our annual attempt to give an impression of the diversity, range and scientific quality of papers in Journal of Physics: Condensed Matter (JPCM). Choosing these examples is one of the hardest but most pleasurable tasks for the Editors, Board Members and Publishing staff.

The choice is difficult because JPCM has succeeded in attracting many excellent and innovative authors. Our very fair but rigorous referees have also ensured a consistently high standard of papers in the journal. Many more papers were singled out with the support of referees (identifying work of the very highest importance), of readers (through high numbers of full-text downloads) and of our Board members (through recommending articles they found especially valuable) than could be featured here. The final choice by us as Editors in Chief can only give an indication of papers that seemed to us to be exciting and of especial interest.

These papers give a flavour of the exciting work published in JPCM, showing just how vigorous and lively the condensed matter field is at present. They also reflect the highly international nature of our authorship. Perhaps your paper will be one chosen for Top Papers 2007.

Marshall Stoneham and David Ferry

In this issue

From molecular elevator…

State 0 ⇌ State 1
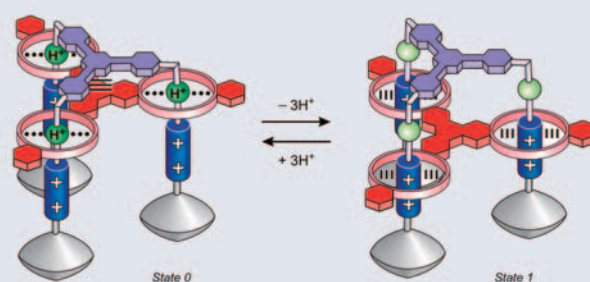
A two-component molecular device, $4H_3^{9+}$, that behaves like a nanometre-scale elevator. It consists of a tripod component containing two different notches at different levels in each leg. The latter are interlocked by the tritopic host, which plays the role of a platform that can be made to stop at the two different levels.

See Artificial nanomachines page 17.

…to space elevator
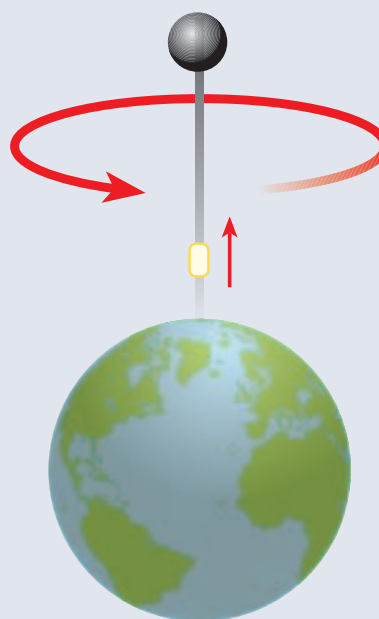
Will it break?

See Space elevator: not all it's cracked up to be? page 11.

Full contents overleaf

REVIEW ARTICLES

Molecular motors for lithography

A molecular motor consisting of a self-assembled monolayer of 'chemical fuel' may offer a route to molecular lithography

A molecular motor produces a controlled displacement of matter at the molecular scale, under the influence of a suitable energy-supplying process (e.g. a chemical reaction).

Vincent Huc of Université de Paris-Sud has suggested that some transition-metal-based catalysts can be converted to molecular motors. The molecules to be used by the catalyst as 'chemical fuel' can be grafted onto a surface as a self-assembled monolayer (SAM), resulting in a periodic 2D molecular array. The catalytic motor may move along this array by jumping from one molecule to the next.

One possibility is to introduce an electric charge to the catalytic motor and to control the motion by using an electric field to change the direction of the catalyst's displacement.

Another possibility is to place a liquid crystalline phase above the SAM of 'fuel' molecules (see figure).

Another approach is to induce a change in the favoured direction of motion by reversibly modifying the organization of the 'fuel' molecules on the surface, for example by irradiating the surface with a laser.

This 'molecular chessboard' approach
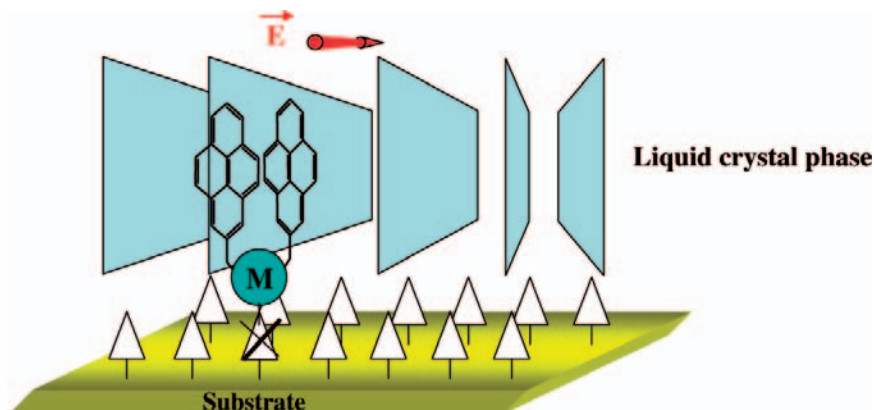
Controlling the motion of the catalyst with a liquid crystalline phase; this has a highly anisotropic orientation of molecules which can be easily tuned using an electric field or polarized light, inducing a preferential direction for the motion of the catalyst.

may open the possibility to build complex molecular objects on a surface in a very precise way (at the sub-nanometre scale) under the influence of a macroscopic control, opening the way to a true 'molecular lithography'.

Transition metal catalysts for molecular motors: towards molecular lithography
Vincent Huc
J. Phys.: Condens. Matter **18** (2006) S1909–S1926

This article is part of a special section on molecular nanomachines. To find out more about molecular nanomachines, see Journal of Physics: Condensed Matter Vol 18, No 33.

New route to spintronic materials

Magnetic semiconductor materials can be produced in a controllable way by inducing oxygen vacancies in TiO_2 films

Magnetically ordered semiconductor materials are sought because of their potential new applications in spintronics devices (e.g. spin diodes and spin-FETs).

Vincent Harris of Northeastern University and co-workers have induced magnetism in films of TiO_{2-d}. The amount of induced moment is systematically controlled by the oxidation pressure employed during PLD growth and by defects generated at the film–substrate interface.

Stoichiometric TiO_2 is a wide bandgap semiconductor and contains only Ti^{4+} ions so it is non-magnetic. Oxygen vacancies create a charge imbalance and unpaired 3d electrons in Ti^{3+} and Ti^{2+} ions can potentially cause magnetism. The formation of Ti^{3+} and Ti^{2+} requires the Ti ions to be stripped of electrons from the s band rather than the 3d band, so Ti^{3+} and Ti^{2+} ions have $3d^1$ and $3d^2$ electronic configurations, respectively.

Harris *et al* demonstrate the ability to control the concentration of oxygen defects
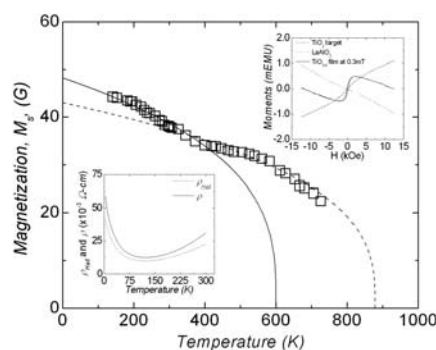
Temperature dependence of the magnetization for the $TiO_{2-\delta}$ film deposited at 0.3mTorr of oxygen pressure, The kink around 450K shows a second transition at a lower temperature. The data was fitted to two functions with magnetic ordering temperature of 880K and a second transition temperature of ~600K.

and to explore their relationship to magnetism and transport in the oxide semiconductor. Magnetism scales with conductivity, suggesting that a double

exchange interaction is active. Films having the highest moments have magnetic transition temperatures near 880 K. Furthermore, they demonstrate a dependence of both conductivity and magnetization with sample thickness where thin films have the strongest magnetization, thus confirming the role of interfacial defects in inducing magnetism in these films.

This represents a new approach in the design and refinement of magnetic semiconductor materials for spintronics device applications above room temperature.

Oxygen-defect-induced magnetism to 880 K in semiconducting anatase TiO_2 films
Soack Dae Yoon, Yajie Chen, Aria Yang, Trevor L Goodrich, Xu Zuo, Dario A Arena, Katherine Ziemer, Carmine Vittoria and Vincent G Harris
J. Phys.: Condens. Matter **18** (2006) L355–L361

Coherence of spin qubits in silicon

P donors in isotopically pure ^{28}Si have sufficiently long spin relaxation times to be candidates for qubits in a quantum computer

Semiconducting systems are obvious candidates for quantum computers because of the huge base of knowledge and experience built up through their use in classical electronics. Many different states inside a semiconductor have been proposed as qubits. One possible approach is to use spins as qubits: of nuclei, of electrons, or both in combination.

A recent paper by S A Lyon (Princeton) and co-workers reviews progress in understanding spin relaxation for P donors in natural and ^{28}Si-purified silicon. In natural Si the spin relaxation is strongly affected by spectral diffusion due to presence of 4.7% ^{29}Si magnetic nuclei which decohere the electron spin in less than 0.5 ms. Very long relaxation times (extrapolating to $T_{2e} = 60$ ms) have been found in isotopically pure ^{28}Si. They have also demonstrated that the spin states of both the electron and nucleus of a ^{31}P donor can be effectively controlled using resonant microwave and RF pulses.

The bang-bang decoupling pulse protocol has been successfully implemented through

(A) Free Rabi nutation of the ^{31}P nuclear spin driven by a long RF pulse at ν_{n1} can be stopped at will and locked into a particular spin state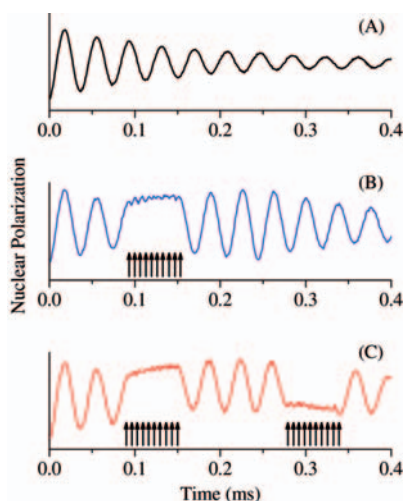 (B) by applying a burst of the closely spaced 2π microwave pulses (ν_{e1}) to the electron spin. The position of the microwave pulses is schematically shown with vertical arrows. The nuclear spin nutation can then be released for further evolution to be locked later on in the opposite state (C) with a second burst of microwave pulses.

the advantage of having coupled electron and nuclear spins in the donor. There are still many questions remaining to be answered. The implementation of two-qubit gates will require advanced processing, but the effects on spin coherence of this processing and of locating the spins in device structures is not yet known, for example. However, work on donor spins in silicon has established that this system can be considered a promising candidate for a future solid state quantum information processing technology.

Coherence of spin qubits in silicon
A M Tyryshkin, J J L Morton,
S C Benjamin, A Ardavan, G A D Briggs,
J W Ager and S A Lyon.
J. Phys.: Condens. Matter **18** (2006) S783–S794

Complementary media of electrons

The concept of complementary media, analogous to negative refractive index materials, for electron waves is feasible

Pendry and Ramakrishna introduced the concept of a complementary medium - a material with permittivity $\varepsilon_c = -\varepsilon$ and permeability $\mu_c = -\mu$, where ε and μ are the permittivity and permeability of the original medium - which reproduces the information of amplitude and phase of electromagnetic waves in the original medium. This is the origin of negative refraction and perfect lenses.

Katsuyoshi Kobayashi of Ochanomizu University, Japan, has extended the formulation of complementary media to electron waves. He defines the complementary medium as having a transfer matrix which is the inverse of that of the original medium.

He describes an application to subsurface imaging in scanning tunneling microscopy. He simulates the impurity images for a simple subsurface impurity and an impurity hindered from imaging by an obstacle and shows that the resolution can be improved using complementary media.

He extends the formulation of complementary media to include interface scattering. Because the electron wavelength is of the order of atomic distances, the atomic structure of the interface is important. The
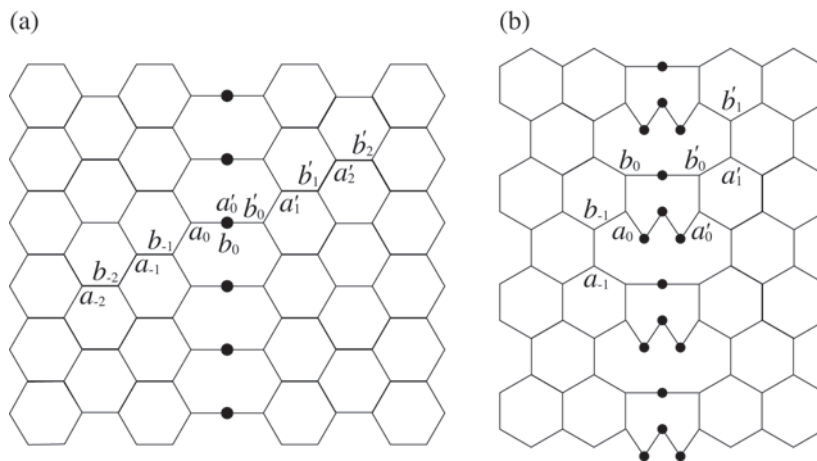
Interface structures forming complementary systems of the graphitic lattice. They either interchange the A and B sublattices of the graphitic lattice while keeping the waves at points K and K_0 in the Brillouin zone or vice versa. Closed circles show sites with only two π bonds.

extended formulation makes it possible to form effectively complementary systems only by tuning transmission properties at interfaces.

Practical realization of complementary media for electrons is a difficult problem to be solved in future, but Kobayashi has shown that it is theoretically possible.

Complementary media of electrons
Katsuyoshi Kobayashi
J. Phys.: Condens. Matter **18** (2006) 3703–3720

Negative refraction in multilayers

Metal-insulator multilayer systems can show negative refractive index behaviour

There is currently much interest in left-handed and negative refractive index materials. In left-handed materials the direction of energy flow of an electromagnetic wave is opposite to the wavevector. In negative refractive index material the component of the average Poynting vector of an electromagnetic wave tangential to the interface changes sign after refraction.

S T Chui (University of Delaware) and co-workers have investigated multilayer structures as negative refractive index and left-handed materials. Multilayer structures have two advantages: firstly, the propagation of electromagnetic waves can be calculated exactly, allowing assessment of different approximations. Secondly, metal-insulator multilayers are highly anisotropic, acting as a metal along the planes and an insulator perpendicular to the planes, so providing a wide range of incident angle within which negative refraction will occur.

A condition for negative refraction is that the interlayer spacing is much less than the wavelength, so the wave is not confined in a single insulating region confined by the

The geometry of refraction from the multilayer.

metallic layers. This condition can be easily satisfied at both microwave and infrared frequencies.

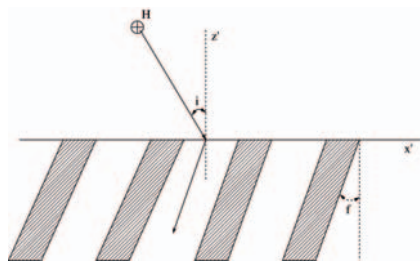Negative refraction comes about because the group velocity and the Poynting vector have a large component parallel to the layers, no matter what the angle of incidence of the incoming radiation is. This behaviour in turn comes from the large anisotropy of the phase velocities. If one of the components is a ferromagnetic metal, the system can be a left-handed material above the ferromagnetic resonance frequency.

Multilayer structures as negative refractive and left-handed materials
S T Chui, C T Chan and Z F Lin
J. Phys.: Condens. Matter **18** (2006) L89-L95

Another new class of negative refractive-index metamaterials made of metallic spheres arranged in a three-dimensional lattice of helicoidal symmetry is reported by Vassilios Yannopapas (Patras).

The studied metamaterial possesses several frequency bands which give rise to negative refraction. The proposed structures constitute a viable solution to realizing optical metamaterials since they can exhibit negative refraction in the frequency region of the surface-plasmon excitations of noble metals.

Negative index of refraction in artificial chiral materials
Vassilios Yannopapas
J. Phys.: Condens. Matter **18** (2006) 6883–6890

How life (un)folds?

This paper explores how networks of molecular interactions can have given rise to life

A recent paper by Timothy R Lezon, Jayanth R Banavar (Penn State) and Amos Maritan (Padova) ties together the biology of proteins with a novel phase of matter that protein structures are housed in. The key idea is that living matter is governed by physical law and understanding the underlying physics is vital for progress.

All living organisms rely upon networks of molecular interactions to carry out their vital processes. In order for a molecular system to display the properties of life, its constituent molecules must themselves be endowed with several features: stability, specificity, self-organization, functionality, sensitivity, robustness, diversity, and adaptability. The authors reflect upon how these molecular needs are met by known organisms, and they discuss properties of conventional phases of matter that make them poorly suited for
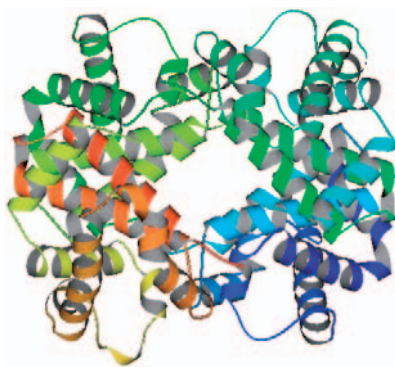
Ribbon views of haemoglobin, which contains four chains folded into α helical domains.

supporting life. They postulate a novel molecular phase of matter and demonstrate

that proteins, the functional molecules of terrestrial life, are perfectly suited to this phase. They explore, through an understanding of this phase of matter, the physical principles that govern the operation of living matter. The new ideas presented in this paper pertain to how advances in nanoscience and supramolecular chemistry can be harnessed for powerful applications and indeed for the ultimate development of physically-based artificial life itself.

This paper is a clear tutorial that is easily accessible to a broad audience and is specially suited to condensed matter physicists.

The origami of life
Timothy R Lezon, Jayanth R Banavar and Amos Maritan
J. Phys.: Condens. Matter **18** (2006) 847–888

Nucleation of nano-domains

A new defect-free model of nucleation in ferroelectrics and ferromagnets has significant implications for the ultimate switching speed in thin-film memory devices

A skyrmion is a quasiparticle corresponding to topological twists or kinks in a spin space. M Dawber (Geneva), A Gruverman (North Carolina State University) and J F Scott (Cambridge) have used skyrmions to model high-field nucleation in ferroelectrics and ferromagnets and test predictions regarding nucleation sites with new experimental data.

This nonlinear, defect-free model is qualitatively different from all known models of ferroelectric nucleation and propagation; nucleation in ferroelectrics has been viewed as inhomogeneous, initiated at static impurity or defect sites that are fixed in space; the present model is also inhomogeneous but involves nucleation at existing domain walls, which are dynamic and not fixed in space. This defect-free ferroelectric nucleation model contrasts with the frequently invoked mechanism in thin-film switching of nucleation at electrode–dielectric interfaces and thus has significant implications for the ultimate switching speed in thin-film memory devices.
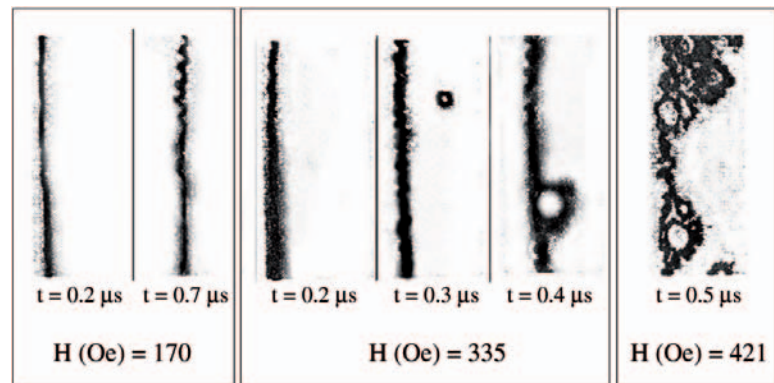
Nucleation of ferroelectric domains in other systems has been shown to strongly favour nucleation sites on existing antiphase boundaries rather than at impurity sites or electrode interfaces. The rapid nucleation of nano-domains in front of an advancing macroscopic domain wall will produce a snow-plough effect that at high fields could

Nano-domains ejected from the ferromagnetic domain wall in iron garnet at different fields H and times t.

mimic supersonic domain wall velocities, whereas real phase velocities of domain walls can remain subsonic.

Atomic force microscopy experiments have supported the basic prediction of the skyrmion model, that nucleation, albeit inhomogeneous, does not occur at reproducible sites and hence is not defect initiated.

Skyrmion model of nano-domain nucleation in ferroelectrics and ferromagnets
M Dawber, A Gruverman and J F Scott
J. Phys.: Condens. Matter **18** (2006) L71–L79

J F Scott has also published a topical review of the physics of submicron ferroelectrics, describing the application considerations for memory devices (both as switching memory elements for ferroelectric nonvolatile random access memories, FRAMs, and as passive capacitors for volatile dynamic random access memories, DRAMs) as well as the fundamental physics questions regarding both the thickness and lateral size of present interest.

Nanoferroelectrics: statics and dynamics
J F Scott
J. Phys.: Condens. Matter **18** (2006) R361–R386

Wetting problem solved?

A new coarse-grained description of wetting in the 3D Ising model accounts for missing physics in the original interfacial description

The nature of the wetting transition of the Ising model is a long-standing unsolved problem. This phase transition occurs when one of two coexisting phases (think liquid and vapour) is energetically preferred by the confining walls of the system. The wetting transition has deep implications since it is intrinsically linked to the vanishing of the contact angle formed by the drop of one of the phases (liquid, say). The hard question is 'Does the wetting transition occur continuously or abruptly?' or 'What is the order of the wetting transition for the three dimensional Ising model?'. This problem is particularly appealing since the dimension $d = 3$ is the marginal case separating the mean-field regime ($d > 3$) from the fluctuation dominated regime ($d < 3$), and the influence of fluctuations is not an easy matter to assess.

An exact solution of the 3D Ising model is

prohibitively difficult and theorists have resorted to coarse-grained descriptions based on 'interfacial models' characterized by a surface tension and an effective potential W. The predictions of this coarse-grained treatment are, however, completely at odds with simulation studies of the Ising model.

A O Parry (Imperial College London) and co-workers in Madrid and Seville derive a coarse-grained description which appears to consistently resolve this, and other controversies.

$$W = a_1 \; \rightthreetimes \; + \; b_1 \; \leftthreetimes \; +$$

In this theory, the potential W has the above elegant diagrammatic representation which accounts for missing physics in the original interfacial description and allows one to 'see' the shape of a free-energy.

The model also opens the door to more

systematic studies of wetting at micropatterned and sculpted substrates, relevant to nanofluidics, which were not possible in previous descriptions.

A Viewpoint article based on this article appears in the same issue (*J. Phys.: Condens. Matter* **18** (2006) V11).

Parry *et al* expect to submit part II of this work to *Journal of Physics: Condensed Matter* in 2007.

Derivation of a non-local interfacial Hamiltonian for short-ranged wetting: I. Double-parabola approximation
A O Parry, C Rascón, N R Bernardino and J M Romero-Enrique
*J. Phys.: Condens. Matter* **18** (2006) 6433–6451

In situ measurement of ZnO nanowires

A TEM method enables *in situ* measurement of mechanical properties of ZnO nanowires

Zinc oxide nanowires, being structurally uniform and single crystalline, have potential use as nanocantilevers and nanoresonators in nanoelectromechanical systems (NEMS), so it is important to study their mechanical resonance behaviour, especially their elastic bending modulus.

Measurement of the elastic bending modulus of a nanowire object with a length of a few micrometres is challenging because its small size prevents the use of established techniques. A new experimental approach, based on electric-field-induced resonant excitation, has recently been developed for direct measurement of the mechanical properties of individual nano-objects such as carbon nanotubes, silicon nanowires, silicon carbide–silica composite nanowires, and ZnO nanobelts by *in situ* transmission electron microscopy (TEM).

Yue Zhang of State Key Laboratory for Surface Physics in Beijing and co-workers have studied individual ZnO nanowires, grown by a solid–vapour phase thermal sublimation process. They studied the mechanical resonances induced by an alternating electric field, by an *in situ* TEM
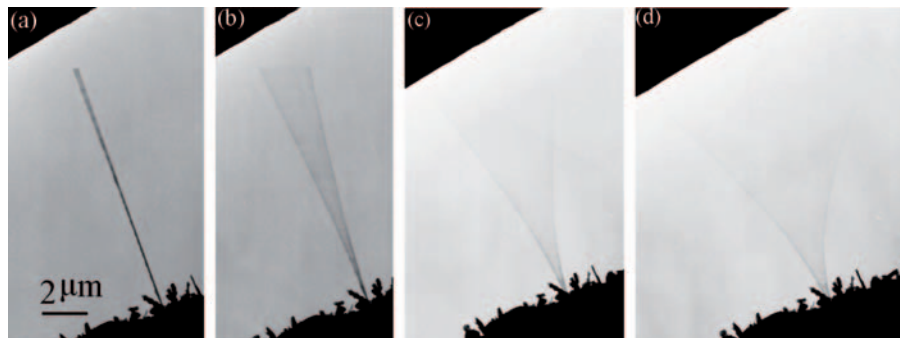
Images showing mechanical resonances of nanowire of length 11.40 Tm, diameter 77 nm, fundamental frequency 269 kHz, bending modulus 59.7 GPa.

method and characterized the mechanical properties, including elastic properties and damping dissipation. They also built a nanobalance and used it to measure the mass of the nanoparticle attached at the tip of a nanowire.

They concluded that the single crystalline, structurally controlled nanowires could be used as a new type of nanoresonator and nanocantilever, which is useful in NEMS and highly functional nanodevices. The ZnO nanowires could also be used as functional

tips for scanning probe microscopy.

A TEM method enables *in situ* measurement of mechanical properties of ZnO nanowires.

***In situ* mechanical properties of individual ZnO nanowires and the mass measurement of nanoparticles**
Yunhua Huang, Xuedong Bai and Yue Zhang
*J. Phys.: Condens. Matter* **18** (2006) L179–L184

Testing DFT for surfaces

Monte Carlo simulations test different approximation schemes in DFT for metal and oxide surfaces and for desorption

Density functional theory (DFT) is widely used in surface science, but its predictions can depend strongly on the approximation used for exchange-correlation energy. D Alfé and M J Gillan (University College London) have tested recent suggestions that the generalized gradient approximation (GGA) is inferior to the local density approximation (LDA) for the surface formation energy σ of transition metals and oxides.

Their quantum Monte Carlo calculations of σ for the MgO(001) surface support the accuracy of LDA, and indicate that GGA is ~30% too low. This has important implications for nanoscience modelling.

In a further paper they present a technique for computing the absolute desorption rate σ of adsorbate molecules from a surface for any coverage and temperature. The technique is based on an exact expression for σ in terms of the difference of non-configurational chemical potentials of gas-phase and adsorbed molecules. This
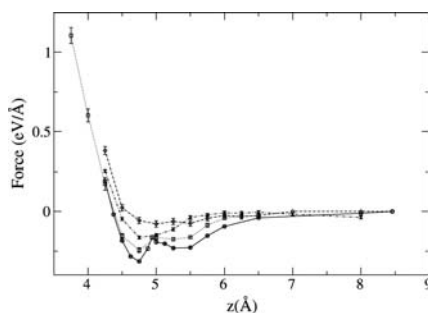
Mean force on water O atom against its height (relative to a fixed atom in the centre of the slab) above the surface at 100, 300, 600 and 800 K (solid, dotted, chain and dashed curves, respectively). Bars show statistical errors.

difference is expressed in terms of a potential of mean force, which is computed by constrained first-principles molecular dynamics.

They applied the technique to D_2O on the MgO(001) surface at low coverage, using the GGA. Comparisons with experimental data

allow an assessment of the accuracy of the GGA.

This scheme can provide calculated values of frequency prefactors, which are important in interpreting experimental results, and provides a way of testing DFT exchange-correlation functionals against experiment. These methods also provide a way of calculating adsorption isotherms by DFT simulation, which should provide another way of probing the accuracy of DFT.

The energetics of oxide surfaces by quantum Monte Carlo.
D Alfé and M J Gillan
J. Phys.: Condens. Matter **18** (2006) L435–L440

Absolute rate of thermal desorption from first-principles simulation
D Alfé and M J Gillan
*J. Phys.: Condens. Matter* **18** (2006) L451–L457

Coherent phonons in semimetals

At a high level of excitation, phonons in semimetals show interesting quantum interference effects

O V Misochko (Institute of Solid State Physics, Moscow), K Ishioka and M Kitajima (NIMS, Tsukuba) and Muneaki Hase (Tsukuba University) have performed a comprehensive investigation of the coherent phonons of different symmetry in the semimetals bismuth and antimony under various temperature and excitation conditions.

Decreasing temperature can increase the number of phonon modes observed in time-domain since at low temperature and any excitation level, both A_{1g} and E_g coherent phonons appear in time-resolved reflectivity. The fact that E_g coherent phonons disappear at room temperature, whereas A_{1g} phonons do not, can be explained by a smaller thermal population of the latter mode.

The relative initial phase of the A_{1g} and E_g oscillations in bismuth testifies that the fully symmetric mode is excited for the most part displacively, whereas the doubly degenerate mode is driven impulsively, suggesting that the A_{1g} and E_g phonons respectively couple to real and virtual charge-density fluctuations.
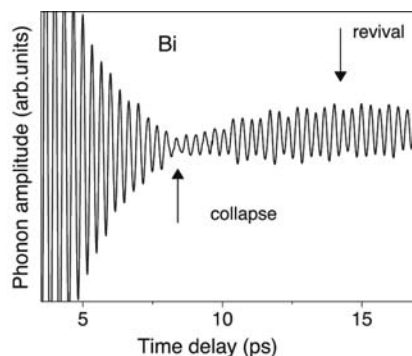
Coherent oscillations in bismuth (after the removal of non-oscillating background) demonstrating collapse and revival in Bi at $T = 7$ K and $F = 9.5$ mJ/cm².

At high excitation level, both modes are coupled and behave in a similar way: an initial fast decay of oscillations is followed by weak recurrence with much slower decay, but the characteristic times of the recurrence are shorter for the doubly degenerate phonons.
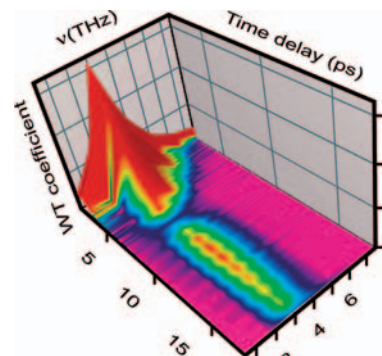
Wavelet transform of the collapsing and reviving oscillations in bismuth.

Fully symmetric and doubly degenerate coherent phonons in semimetals at low temperature and high excitation: Similarities and differences

O V Misochko, K Ishioka, Muneaki Hase and M Kitajima
*J. Phys.: Condens. Matter* **18** (2006) 10571–10584

A new relaxor ferroelectric

Barium substitution enhances the properties of a relaxor ferroelectric for applications

Pb-based perovskites with the general formula $Pb(B'_xB''_{1-x})O_3$ are typical relaxor ferroelectrics and have important applications in optical modulators and information storage.

V Marinova (Hamburg) and co-workers have synthesized single crystals of a new relaxor compound with chemical formula $Pb_{0.78}Ba_{0.22}Sc_{0.5}Ta_{0.5}O_3$ (PBST). Its frequency dependence of the dielectric constant shows a strong dielectric dispersion over a wide temperature range and a dielectric-constant maximum near 200 K at 10 kHz.

They probed the local atomic environment by Raman scattering and optical absorption spectroscopy. The results show that the incorporation of Ba deforms the BO_6 octahedra adjoining the BaO_{12} polyhedra along the <111> direction and shortens the Pb-O bond lengths next to the BaO_{12} polyhedra within the {111} planes. The random substitution of Ba for Pb leads to a wider distribution in the size and shape of the ferroic species in PBST compared with stoichiometric $PbSc_{0.5}Ta_{0.5}O_3$. As a result, the non-ergodic 'true-relaxor' state is enhanced on account of the proper long-range ordered ferroelectric state, which considerably
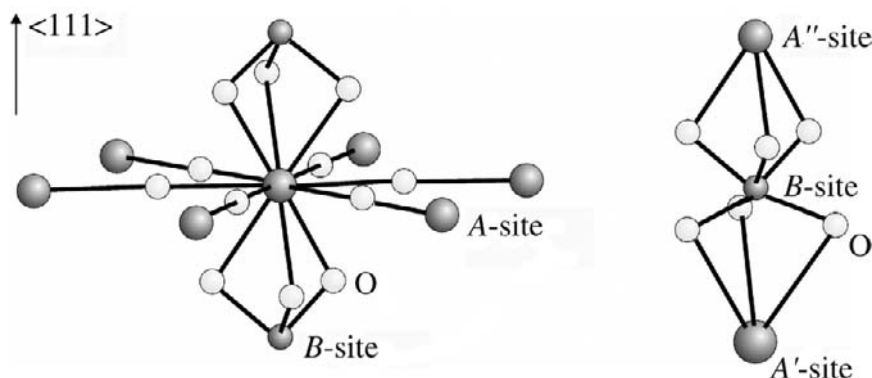
The atomic environment of an A-site cation and of a B-site cation neighbouring two different A-site cations. The swelling of the AO_{12} polyhedron when Ba substitutes for Pb should result in a shortening of the adjacent Pb–O bonds in the plane perpendicular to the <111> direction as well as to a deformation of the adjacent BO_6 octahedra along the <111> direction.

broadens the dielectric-constant maximum and modifies the optical absorption edge.

The addition of Ba shifts the optical absorption edge to lower energies and gives rise to extra absorption peaks at 460 and 730 nm. The latter peak is related to polar atomic rearrangements in the vicinity of the Ba ions embedded into the $PbSc_{0.5}Ta_{0.5}O_3$ matrix.

Structural, optical and dielectric properties of relaxor-ferroelectric $Pb_{0.78}Ba_{0.22}Sc_{0.5}Ta_{0.5}O_3$

V Marinova, B Mihailova, T Malcherek, C Paulmann, K Lengyel, L Kovacs, M Veleva, M Gospodinov, B Güttler, R Stosch and U Bismayer
*J. Phys.: Condens. Matter* **18** (2006) L385–L393

Theory of glasses in transition?

Experiments at extremely high pressure are proposed to resolve the controversy over the driving force behind the glass transition

The driving force behind the glass transition is very controversial. It could be mainly a free-volume (or density, or pressure) phenomenon, since glass formers are typically dense liquids where core-repulsion effects are large, or it could be a dominantly energetic (temperature-driven) phenomenon, as it clearly is in bonding-driven network-forming glasses such as silica. This question is now being addressed in high-pressure experiments but the results are far from equivocal.

Th Voigtmann and Wilson Poon (University of Edinburgh) have suggested that conventional molecular glasses and colloidal glasses have in common the physical interpretation of the way their glass transition changes with pressure and temperature. This opens a connection between the two kinds of systems that has received little attention: it suggests that one
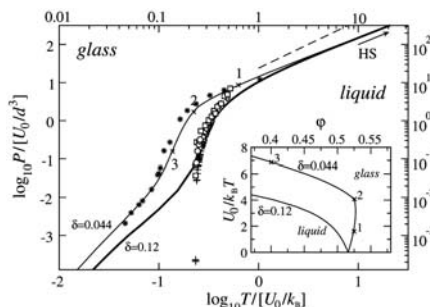
The glass transition in the pressure–temperature plane for hard spheres with square-well attraction: * experimental data from colloid–polymer mixtures (the hard-sphere data point is indicated by an arrow to $T \infty$); other symbols are experimental data for small-molecular and polymeric glass formers. Lines are mode-coupling theory predictions for the square-well system. The dashed line indicates the soft-sphere asymptote, $P \propto T^{5/4}$. Inset: MCT lines in the usual density–attraction-strength representation. Points 1–3 correspond in the two plots.

can use colloidal systems, taking advantage of the fine control they offer over the interaction potential, to gain insight into some open questions in the field of molecular glasses. As a first example, they estimate the minimum pressure needed to reveal a properly density- or pressure-driven glass transition in molecular glass formers. Their estimate is 10 GPa, higher than the pressures reached in previous dynamic experiments at high viscosities, explaining why the controversy is still alive. Extremely-high-pressure experiments on molecular glass-forming liquids, accessing this regime, would be of great value.

Glasses under high pressure: a link to colloidal science?
Th Voigtmann and Wilson C K Poon
J. Phys.: Condens. Matter **18** (2006) L465–L469
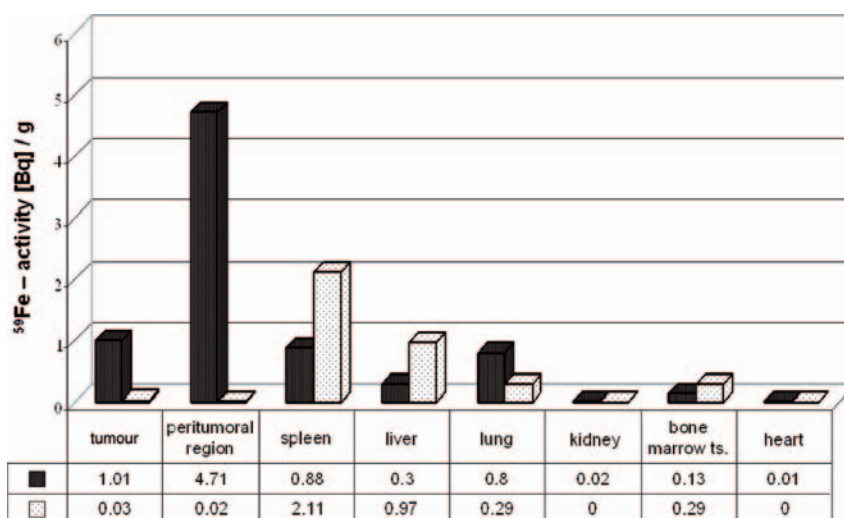
Fighting cancer with nanoparticles

Magnetic nanoparticles can be used in cancer therapy either for drug delivery or for destroying the tumour by heating

Two recent papers describe the use of magnetic nanoparticles in treating cancer, either as magnetic targetable carriers for drug delivery systems or for local hyperthermia.

Biocompatible nanosized drug delivery systems for specific targeting of therapeutics are being developed, especially for the treatment of cancer and diseases of the vascular system. In an experimental cancer model, R Jurgons (Erlangen) and co-workers performed targeted drug delivery and used magnetic iron oxide nanoparticles, bound to a chemotherapeutic agent, which were attracted to an experimental tumour in rabbits by an external magnetic field (magnetic drug targeting). Complete tumour remission could be achieved. An important advantage of these carriers is the possibility for detecting these nanoparticles after treatment with common imaging techniques (i.e., x-ray-tomography, magnetorelaxometry, magnetic resonance imaging), which can be correlated to histology.

Rudolf Hergt and co-workers in Jena have studied loss processes in several types of magnetic iron oxide nanoparticles to optimize the specific loss power (SLP) for application in tumour hyperthermia. In magnetically mediated hyperthermia, magnetic material is deposited in the tumour and heated by an external alternating magnetic field.

They studied the dependence of the SLP on the mean particle size over a broad range

	tumour	peritumoral region	spleen	liver	lung	kidney	bone marrow ts.	heart
■	1.01	4.71	0.88	0.3	0.8	0.02	0.13	0.01
▨	0.03	0.02	2.11	0.97	0.29	0	0.29	0

Radioactive ^{59}Fe-distribution 60 min after intra-arterial ^{59}Fe-ferrofluid application; with (dark) and without (light) external magnetic field. 114 times more activity could be detected in the tumour region after magnetic drug targeting than without a magnetic field.

from superparamagnetic up to multidomain particles. Particles with mean size 18 nm and a narrow size distribution proved most useful. In particular, very high heating power may be delivered by bacterial magnetosomes. Even higher power may be achievable by metallic magnetic particles.

These papers are part of a special issue on ferrofluids. For more information on other medical applications and all other aspects of ferrofluids, see Journal of Physics: Condensed Matter Vol 18, No 38.

Drug loaded magnetic nanoparticles for cancer therapy
R Jurgons, C Seliger, A Hilpert, L Trahms, S Odenbach and C Alexiou
J. Phys.: Condens. Matter **18** (2006) S2893–S2902

Magnetic particle hyperthermia: nanoparticle magnetism and materials development for cancer therapy
Rudolf Hergt, Silvio Dutz, Robert Müller and Matthias Zeisberger
*J. Phys.: Condens. Matter* **18** (2006) S2919–S2934

Space elevator: not all it's cracked up to be?

It is argued that a proposed space elevator cable made of carbon nanotubes would contain enough defects to cause it to break

A space elevator has been proposed consisting of a cable about 105 km long fixed geosynchronously to the Earth's surface as a revolutionary method of carrying payloads into space.

The cable requires a material with very high strength and low density. The maximum stress at the geosynchronous orbit for a material with the density of carbon is 63 GPa. Only recently, since the discovery of carbon nanotubes, has such a large strength been experimentally observed: ropes composed of single- or multiwalled carbon nanotubes are expected to have an ideal strength of about 100 GPa.

Nicola M Pugno of Turin Polytechnic argues that the presence of even a few vacancies in a single nanotube play a dramatic role. In such a huge cable pre-existing defects are expected both for statistical reasons and as a consequence of damage nucleation, e.g. due to micrometeorite or low Earth orbit object
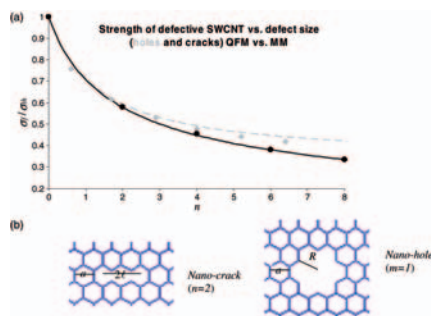
(a) Strength of defective SWCNT versus hole size (QFM, dashed line; rhombi, atomistic simulations), or versus crack length (QFM, continuous line; points, atomistic simulations). (b) Defect and fracture quantum sizes: n = 2 denotes a nanocrack formed on removing two adjacent chemical bonds, m = 1 denotes a nanohole formed on removing the first carbon atom perimeter (six atoms); the applied tensile load is vertical.

impacts and atomic oxygen erosion. He reviews the mechanics of the cable, and considers the effect on the strength of the types of damage mentioned. He predicts that

the strength of a megacable is reduced by a factor of at least 70% compared with the theoretical nanotube strength, sufficient to place in doubt the feasibility of the space elevator which he claims would break. This is confirmed by experiments and atomistic simulations based on molecular or quantum mechanics.

On the strength of the carbon nanotube-based space elevator cable: from nanomechanics to megamechanics

Nicola M Pugno
J. Phys.: Condens. Matter **18** (2006) S1971–S1990

This article is part of a special section on nanoscience and nanotechnology; see Journal of Physics: Condensed Matter Vol 18, No 33 for more papers in this area.

Quantitative description of exchange bias

Taking into account spin disorder at the interface accounts for experimental results for exchange bias

The exchange bias system refers to the shift of the ferromagnetic (F) hysteresis loop to positive or negative values when the F system is in contact with an antiferromagnetic (AF) system and cooled in an applied magnetic field through the Néel temperature of the AF system. Exchange bias is associated with the interfacial exchange coupling between F and AF spin structures, resulting in a unidirectional magnetic anisotropy, but the origin of the enhanced coercive field is not yet well understood. The details of the exchange bias effect depend crucially on the AF/F combination chosen and on the structure and thickness of the films.

Florin Radu and co-workers at Ruhr University, Bochum show that interface spin disorder is the main reason for the discrepancy between model calculations and experimental results. Taking into account spin disorder at the interface between the AF and F layers, they achieved a compelling agreement between the azimuthal dependence of the coercivity and exchange bias field in the IrMn/FeCo systems.

The new key physical concept is a realistic state of the interface characterized by a reduced AF anisotropy. This disorder governs the enhanced coercivity in the ferromagnetic layer and reduces the exchange bias field to realistic values. They
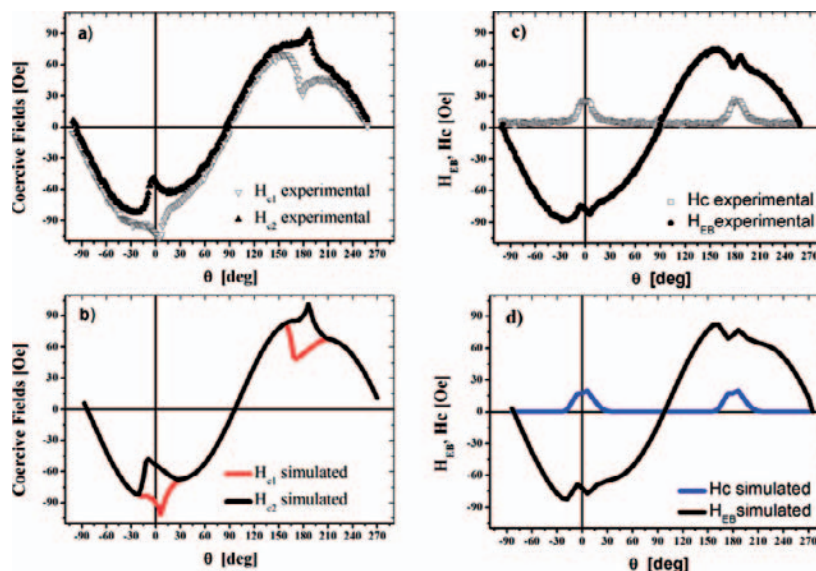
Azimuthal dependence of the coercive fields H_{c1} and H_{c2} (a) from the experimental hysteresis loops and (b) calculated. The coercive field and exchange bias field as a function of the azimuthal angle θ (c) experimental and (d) simulated.

believe that this is a general feature of exchange bias systems. By controlling the degree of spin disorder and the thickness of the interfacial layer, better control over the exchange bias of magnetic heterostructures could be achieved.

Quantitative description of the azimuthal dependence of the exchange bias effect

Florin Radu, Andreas Westphalen, Katharina Theis-Bröhl and Hartmut Zabel
J. Phys.: Condens. Matter **18** (2006) L29–L36

Stretching proteins in a force-clamp

Stretching proteins in a force-clamp yields information on the statistics of unfolding events

Atomic force microscopy (AFM) is used to probe biomolecules by stretching at a constant speed. The force of resistance to stretching yields information about their elastic structure. A new variant of AFM, a force-clamp, allows one to maintain a constant pulling force on the protein while monitoring the end-to-end distance as a function of time. For polyubiquitin, the length of the protein increased in a step-wise manner with each step corresponding to unwinding of a single ubiquitin chain in agreement with a simple, i.e., two-state all-or-none, model of unfolding. The ensemble-averaged length of a protein is well described by a single exponential with a characteristic time whose logarithm depends linearly on the force.

P Szymczak and Marek Cieplak (Warsaw) have investigated the generality of these results. They show that the average unfolding time needs not be exponential (especially at large forces) and they provide an example of a protein with more than two steps of unfolding at low force. A coarse-grained model of ubiquitin has log-normal statistics above a threshold force and exponential statistics below it.
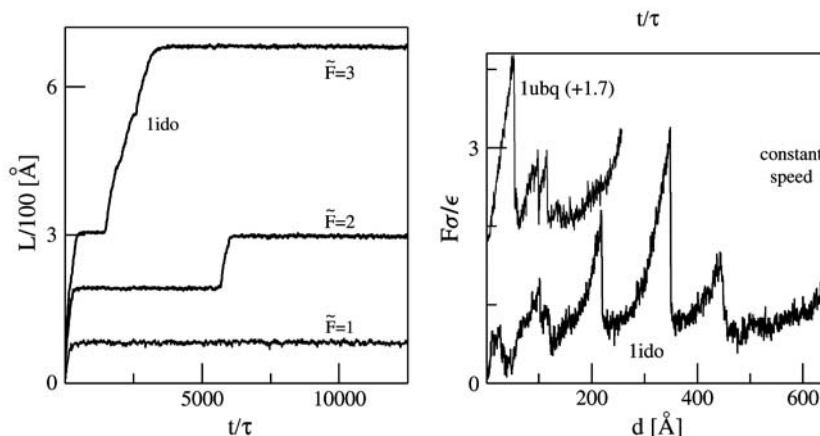
Left: three trajectories for integrin at various forces. The lower two trajectories lead to full unfolding at much longer time than the scale in the figure. Right: force versus displacement traces for stretching at constant speed for ubiquitin (shifted upward by 1.7 to avoid overlap) and integrin. For this trace, $\tilde{F}_{max}$ is near 2.45.

Correspondingly, the mean unfolding time is slowly varying and decreases exponentially with the force. The time dependences of the end-to-end distances are also distinct. The time sequence of unfolding events depends weakly on force and much of it resembles that for stretching at constant speed. A more complicated time dependence is found for integrin.

Stretching proteins in a force-clamp yields information on the statistics of unfolding events

P Szymczak and Marek Cieplak
*J. Phys.: Condens. Matter* **18** (2006) L21–L28

Light damage in a-Si:H

Structural changes from exposure of a-Si:H to intense light have been successfully simulated

Hydrogenated amorphous silicon (a-Si:H) is an important material for solar photovoltaic (PV) devices. It is inexpensive and serves an important niche in energy markets. An impediment to its use is the so-called Staebler–Wronski effect (SWE) (the light-induced creation of carrier traps causing reduced energy conversion efficiency). Exposure of a-Si:H to intense light leads to structural changes, with a serious impact on the performance of a-Si:H cells.

T A Abtew and D A Drabold (Ohio University) have used *ab initio* molecular dynamics to simulate the SWE. They obtain improved microscopic understanding of photovoltaic operation, compute the motion of H atoms, and modes of light-induced degradation of photovoltaics.

Highly accurate simulations in a light-induced state lead to the formation of a class of new configurations, consistent with (a) recent NMR experiments and the authors' previous studies, and (b) the hydrogen collision model of Branz and other paired-H models. In contrast, simulations in the electronic ground state do not exhibit the tendency to paired-H final states. For the first
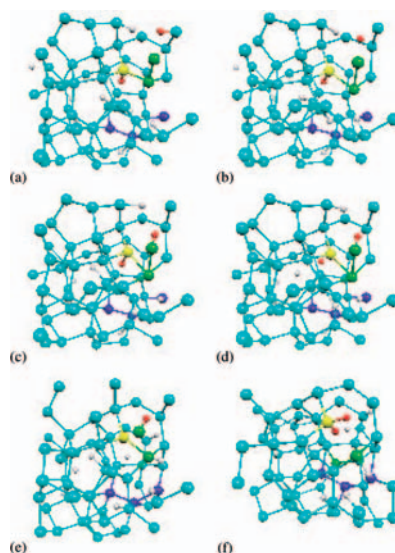
Motion of key atoms from photo-excited ab initio MD simulation of a-Si:H. Small atoms depict H and large atoms represent Si. (light blue: 'typical' Si atoms; white: 'typical' H atoms; red: H atoms that eventually pair; green: initial Si DB sites; dark blue: Si atoms that end as DB.) (a) Initial conformation, (b) one H dissociates and forms a DB, (c) mobile H attaches to a Si DB, (d) the other (red) H becomes mobile, (e) atomic rearrangements near defect sites, (f) SiH$_2$ is formed.

time, they show the detailed dynamic pathways that arise from light-induced occupation changes, and provide one explicit example (see figure) of defect creation and paired-H formation.

This work should be extended in a number of ways, including: exploration of longer time scales, large models, and a thorough study of possible photo-excitations and the statistics of associated events.

Atomistic simulation of light-induced changes in hydrogenated amorphous silicon

T A Abtew and D A Drabold
J. Phys.: Condens. Matter **18** (2006) L1-L6

Landau theory corrected

The phase behaviour of certain polymers depends crucially on certain non-local terms in the Landau free energy expansion that have been neglected before

Landau theory is commonly used to describe the thermodynamic behaviour of polydisperse heteropolymer systems. All calculations up to now have retained only the fourth-order non-local term in the free energy expansion. S I Kuchanov and S V Panyukov (Moscow) have shown that the neglect of some non-local terms of sixth order is responsible for the erroneous results reported.

In particular they have shown that the addition of two such terms, ignored in all preceding publications, is indispensable. This assertion stems from the inspection of the phase diagram they calculated for the melt of binary Markovian multiblock copolymers. It differs markedly from the phase diagram constructed earlier disregarding these terms (see figure).

Key results they obtained for Markovian heteropolymers can be verified for other polydisperse multiblock copolymers, since their formulae hold at arbitrary values of the parameters of the vertex functions in expansion of the Landau free energy.

The central idea of Kuchanov and Panyukov far exceeds the limits of the
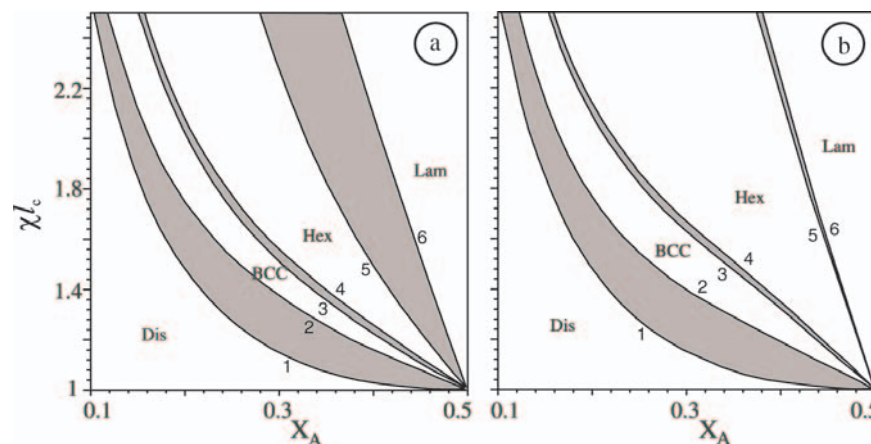
Phase diagram of the melt of binary Markovian copolymers: (a) calculated by Kuchanov and Panyukov and (b) reported earlier. Lines separate homophase regions (coloured white) from two-phase ones (coloured grey).

construction of the phase diagram of heteropolymer liquids. This idea may well find application when considering the thermodynamic behaviour of various systems with 'quenched' structural disorder in terms of the Landau theory of phase transitions.

A correct account of the non-local terms in the Landau theory of phase transitions in polydisperse heteropolymers
S I Kuchanov and S V Panyukov
J. Phys.: Condens. Matter **18** (2006) L43–L48

Separating particles by their surface properties.

Particles, proteins and DNA may be separated by their surface properties using a liquid crystal as solvent

Electrophoresis and sedimentation are powerful means for separating particles, proteins, and DNA, via differences in particle charge, mass, and size. Surface properties of colloids and proteins are closely related to their physical, chemical, and biological functions, so the selection of particles by their surface properties is highly desirable.

Takeaki Araki and Hajime Tanaka (Tokyo) report a new principle of surface-sensitive particle selection by using nematic liquid crystal as a solvent. When colloidal particles are immersed in a nematic liquid crystal, the director field of the nematic solvent around them is distorted due to the anchoring on the particle surface. The elastic coupling between particles and nematic liquid crystal leads to rich static and dynamic behaviour which may be used for surface-sensitive
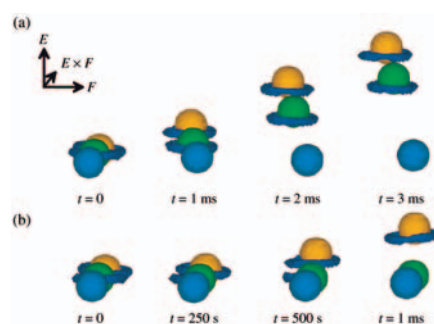
Surface-sensitive particle separation. Particles with different anchoring strengths are dragged by an external force $F = 6\,pN$ (a) and $F = 20\,pN$ (b) in a nematic liquid crystal aligned such that $E \perp F$. The anchoring strengths of the blue, green, and red particles (bottom to top) are $W = 1.5, 2.0$ and $2.5 \times 10^{-4}\,N\,m^{-1}$, respectively.

particle separation. Using a special type of lyotropic liquid crystal that is water-based but non-surfactant and non-toxic, it may be possible to disperse colloidal particles or biological molecules in a liquid crystal homogeneously.

Numerical simulations incorporating both elastic and nematohydrodynamic couplings show that the surface anchoring properties change both direction and speed of motion of a particle driven in an oriented nematic liquid crystal. This principle may be used for separating particles in terms of their surface properties.

Surface-sensitive particle selection by driving particles in a nematic solvent
Takeaki Araki and Hajime Tanaka
J. Phys.: Condens. Matter **18** (2006) L193–L203

Liquid silicon under pressure

An *ab initio* study accounts for experimentally found pressure-induced structural and dynamical changes in liquid silicon

Upon melting, silicon undergoes a semiconductor–metal transition, its local structure changing from fourfold to approximately sixfold coordination.

A Delisle and M J Stott (Queen's University, Canada) and D J González (University of Valladolid) have investigated l-Si using orbital-free *ab initio* molecular dynamics (OF-AIMD) combined with a first-principles local pseudopotential.

Their results for the static structure qualitatively follow the experimental trends when the pressure is increased from 4 to 23 GPa, namely an increase of intensity and position of the S(q)'s main peak, along with a progressive vanishing of its shoulder. The static structures of l-Si from the triple point up to 8 GPa are very similar, but between 8 and 14 GPa it transforms to a denser structure typical of a liquid simple metal.

The structural changes are also reflected in the dynamic structure factors and the
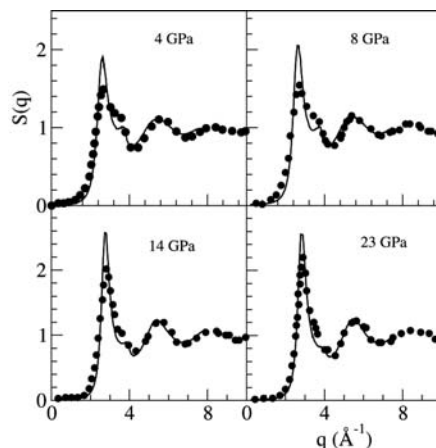
Static structure factor of l-Si at different high pressures: full circles: experimental x-ray diffraction data; continuous line: OF-AIMD simulations.

transverse current correlation. The calculated self-diffusion and shear viscosity transport coefficients are also affected by the structural changes occurring between 8 and 14 GPa.

These results for the static and dynamic properties of compressed l-Si underscore the capability of the OF-AIMD method to tackle liquid systems encompassing a range of bonding and structure which evolves from mild remnants of covalent bonding to a metallic one. Further improvements will be focused on developing more accurate electron kinetic energy functionals and local ionic pseudopotentials.

Pressure-induced structural and dynamical changes in liquid Si–an *ab initio* study
A Delisle, D J González and M J Stott
*J. Phys.: Condens. Matter* **18** (2006) 3591–3605

Decomposing food

Spinodal decomposition in a food colloid–biopolymer mixture shows evidence for a linear regime

Colloidal suspensions are ideal model systems to study fundamental issues such as liquid ordering, crystallization and glass formation. Food is a classical example of complex soft condensed matter.

Suresh Bhat and Peter Schurtenberger (University of Fribourg) and Remco Tuinier (Jülich) have investigated phase separation and structural evolution in a complex food colloid (casein micelles) and biopolymer (xanthan) mixture using small-angle light scattering. They show that phase separation is induced by a depletion mechanism, and that the resulting coexistence curve can be described by osmotic equilibrium theory for mixtures of colloids and polymer chains in a background solvent, taking into account interactions between the polymer chains in the excluded volume limit. The light scattering pattern of an unstable mixture exhibits the typical behaviour of spinodal decomposition, confirming the validity of dynamic similarity scaling.

They find three distinct regimes for the
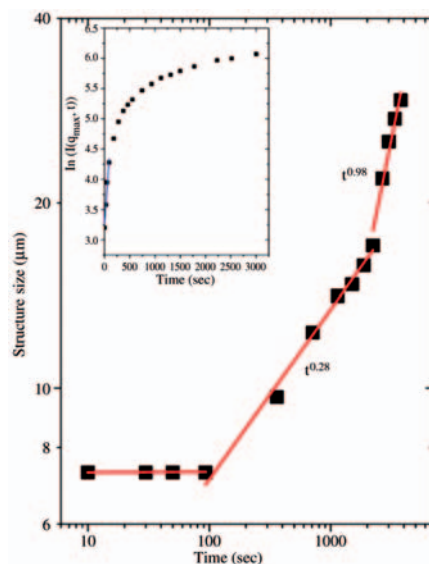
Evolution of the characteristic domain size obtained from the position $q_{max}(t)$ of the peak of the scattered intensity as a function of time. The inset shows the time evolution of the logarithm of the scattered intensity $I(q,t)$ at q_{max}.

decomposition kinetics that differ in the time dependence of the peak position of the structure factor. In the initial linear regime, the peak position remains constant and the amplitude grows. The existence of spinodal-like decomposition and the validity of universal scaling in the intermediate and transition stages have been found in previous studies, but to the authors' knowledge the initial linear regime has never been observed in colloidal suspensions. They attribute this at least partly to hydrodynamic interactions which are efficiently screened in their system as the measurements were performed at high polymer concentrations, i.e. in the semi-dilute regime.

**Spinodal decomposition in a food colloid–biopolymer mixture: evidence for a linear regime**
Suresh Bhat, Remco Tuinier and Peter Schurtenberger
J. Phys.: Condens. Matter **18** (2006) L339–L346

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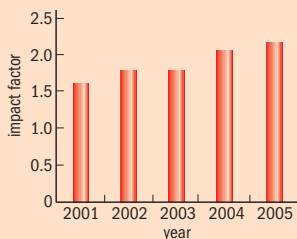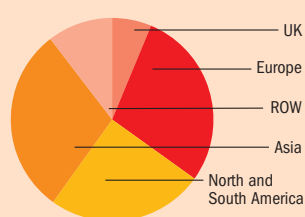
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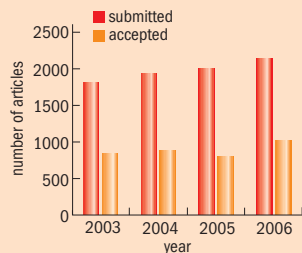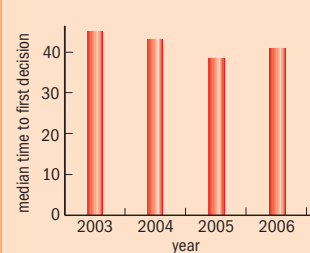
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Quantum IT clouded by uncertainty

Issues affecting how a quantum information technology industry may develop in the future are discussed

The research fields of quantum information processing and communication are now well established, although still growing and developing. A Viewpoint article by T P Spiller and W J Munro of Hewlett-Packard Laboratories, Bristol discusses how a quantum information technology (QIT) industry may develop in the future.

As electronic devices become smaller, they will suffer errors from quantum fluctuations so, unless we can control these effects, nanoscale conventional IT devices will fail to work. As a result, IT companies are researching quantum effects, and this could have a spin-off in a revolutionary new QIT, based on storing, processing and communicating information according to the laws of quantum physics, utilizing effects such as superposition, entanglement and quantum measurement.

Spiller and Munro discuss the issues to consider with regard to the start of a QIT industry, including the need for a market for
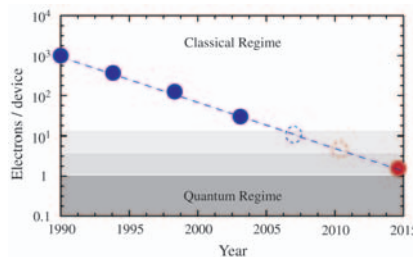
Moore's Law, illustrated through the number of electrons per operating device. This is decreasing exponentially as devices shrink in size. Quantum effects become increasingly important as the quantum regime is approached.

QIT. Building a factoring machine in order to break 'secure' communications is a much-quoted example. Other possible areas are quantum communication (key exchange, cryptography, etc), quantum(-improved) sensing and detecting (i.e. quantum metrology), and quantum simulation.

They then consider some of the candidate technologies and associated problems such as interconversion between travelling optical qubits and static (presumably matter-based) qubits, and processing qubits. They conclude that there is currently no consensus on the best route to scalable quantum computing.

There is now a growing expectation of real quantum information technology. Certainly there are some promising avenues for seeding and growing a QIT industry.

Towards a quantum information technology industry

To find out more about quantum information processing see special issue on quantum information processing, Journal of Physics: Condensed Matter Vol 18, No 21.

Ultrafast magneto-optics

The use of magneto-optical spectroscopy in investigating spin-related phenomena in (III, Mn)V ferromagnetic semiconductors is reviewed

Junichiro Kono (Rice University) and colleagues from Virginia Tech, UCSD, Florida University and Tokyo Institute of Technology have reviewed various ultrafast optical processes in ferromagnetic (III, Mn)V semiconductors induced by femtosecond laser pulses. Magneto-optical spectroscopy combined with femtosecond laser pulses provides direct time-domain information about magnetic properties of excited states with high temporal resolution and fine control.

They describe newly developed two-colour methods of MOKE and MCD spectroscopy and present experimental results on charge dynamics, phonon dynamics, and spin dynamics.

Time-resolved two-colour transient reflectivity measurements with a mid-infrared pump and a single-colour near-infrared probe yield very short carrier lifetimes (~2 ps) and multilevel charge decay dynamics. Carrier relaxation of (III, Mn)V semiconductors show some unique properties such as large-density mid-
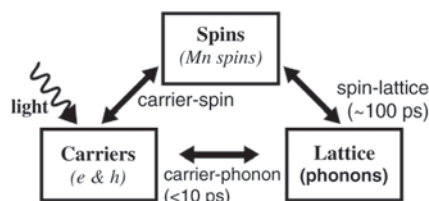
Three reservoirs (carriers, spins, lattice) taking part in the light-induced demagnetization process. The descriptions in italics are specific to the (III, Mn)V case. Spin–lattice and carrier–phonon are quite well understood and direct carrier–spin coupling is a subject of current research. In (III, Mn)V ferromagnetic semiconductors the carrier–spin mechanism is the sp–d interaction between the spins of delocalized carriers and the localized Mn spins.

bandgap states and heavy Mn p-doping.

The transient reflectivity technique also provides direct information about phonon dynamics. An oscillatory component in the transient reflectivity, whose period, amplitude and damping depend strongly on the probe laser energy, is associated with propagating coherent acoustic phonon wavepackets. The CAP in (III, Mn)Vs is similar to that in GaN/InGaN epilayers, but

its generation mechanism is via a deformation potential coupling mechanism, instead of screening of piezoelectric fields.

Both fast (<1 ps) and slow (~100 ps) demagnetization processes are observed in ferromagnetic InMnAs and GaMnAs. The fast dynamics is attributed to spin heating through sp–d exchange interaction between photo-carriers and Mn ions while the ~100 ps component is interpreted as spin–lattice relaxation.

They also give a qualitative picture of ultrafast photoinduced softening in ferromagnetic InMnAs.

Ultrafast magneto-optics in ferromagnetic III–V semiconductors
Jigang Wang, Chanjuan Sun, Yusuke Hashimoto, Junichiro Kono, Giti A Khodaparast, Łukasz Cywiński, L J Sham, Gary D Sanders, Christopher J Stanton and Hiro Munekata
*J. Phys.: Condens. Matter* **18** (2006) R501–R530

Single-molecule experiments in biological physics

Experimental techniques for manipulating and measuring single molecules and their applications are reviewed

Recent technological developments have provided the tools to design and build scientific instruments of high enough sensitivity and precision to manipulate and visualize individual molecules and measure microscopic forces. Using single-molecule experiments (SMEs) it is possible to manipulate molecules one at a time and measure distributions describing molecular properties, characterize the kinetics of biomolecular reactions and detect molecular intermediates.

SMEs provide additional information about thermodynamics and kinetics of biomolecular processes that complements information obtained in traditional bulk assays. In SMEs it is also possible to measure small energies and detect large Brownian deviations in biomolecular reactions, offering new methods and systems to scrutinize the basic foundations of statistical mechanics.

F Ritort (Barcelona) has reviewed SMEs at a very introductory level. The review discusses SMEs from an experimental perspective, first describing the most common experimental methodologies and later presenting various molecular systems where such techniques have been applied. It briefly discusses experimental techniques such as atomic-force microscopy, laser
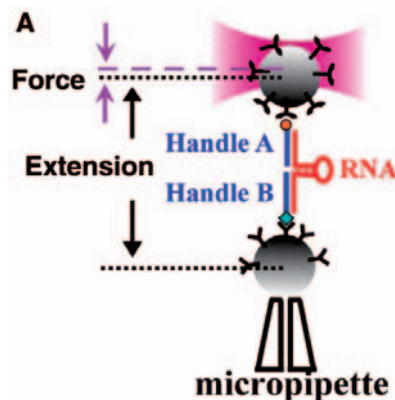
Experimental set-up for RNA pulling experiments using laser optical tweezers.

optical tweezers, magnetic tweezers, biomembrane force probes and single-molecule fluorescence. It then presents several applications of SME to the study of nucleic acids (DNA, RNA and DNA condensation) and proteins (protein–protein interactions, protein folding and molecular motors). Finally, it discusses applications of SMEs to the study of the nonequilibrium thermodynamics of small systems and the experimental verification of fluctuation theorems and concludes with a discussion of open questions and future perspectives.
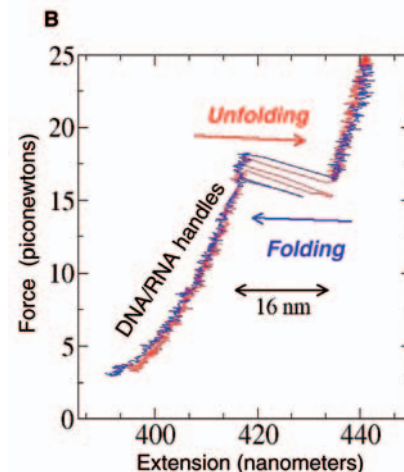
Force-extension curve of RNA hairpin in a pulling cycle. During the stretching (red) the elastic response of the handles is followed by the sudden release of extension and a drop in the force corresponding to the unfolding of the RNA molecule. During relaxation (blue) the RNA molecule folds back again.

Single-molecule experiments in biological physics: methods and applications
F Ritort
J. Phys.: Condens. Matter **18** (2006) R531–R583

Nanoemulsions: clearly superior

Nanoemulsions have quite different physical properties from microscale emulsions, which gives them great potential in a wide range of industries

Extreme emulsification methods can be used to produce nanoscale dispersions of droplets of one liquid in another immiscible liquid. These microfluidic and ultrasonic approaches of rupturing larger microscale droplets into nanoscale droplets provide interesting non-equilibrium systems of structured liquids. The physical properties of nanoemulsions can be quite different from those of microscale emulsions.

Nanoemulsions hold great promise as useful dispersions of deformable nanoscale droplets that can have flow properties ranging from liquid to highly solid and optical properties ranging from opaque to nearly transparent. They will play an increasingly important role commercially, since they can typically be formulated using significantly less surfactant than is required for nanostructured lyotropic microemulsion phases.
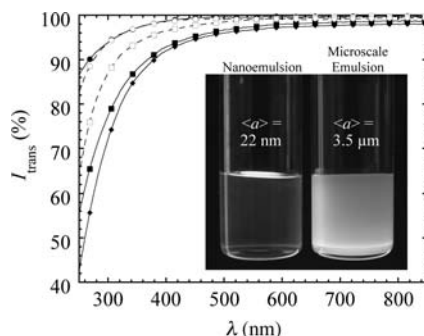
Transmitted intensity, I_{trans}, of nanoemulsions having $<a> = 40$ nm in a 0.2 mm thick cell as a function of wavelength, λ, in UV and visible for a series of volume fractions. The high I_{trans} at visible wavelengths indicates that the nanoemulsions are nearly transparent, yet they scatter significantly in the UV. Inset: 1 cm diameter glass vials contain a nanoemulsion that is nearly transparent in the visible spectrum, and a microscale emulsion that appears white and opaque due to multiple scattering of visible light.

This review by T G Mason and co-workers at UCLA summarizes procedures for producing 'nanoemulsions' comprised of nanoscale droplets, methods for controlling the droplet size distribution and composition, and interesting physical properties of nanoemulsions. In contrast to more common microscale emulsions, nanoemulsions exhibit optical transparency at high droplet volume fractions, φ, surprisingly strong elasticity at low φ, and enhanced diffusive transport and shelf stability. For these reasons, nanoemulsions have great potential in a wide range of industries including pharmaceuticals, foods, and personal care products.

Nanoemulsions: formation, structure, and physical properties
T G Mason, J N Wilking, K Meleson, C B Chang and S M Graves

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Artificial nanomachines

Recent progress in constructing simple prototypes of artificial molecular machines is reviewed

Molecular machines are supramolecular structures designed to perform a function through the mechanical movements of its components, which occur under appropriate external stimulation. They operate via nuclear rearrangements and require an energy input. Through progress in chemistry, and better understanding of biological molecular machines, it has become possible to design and construct simple prototypes of artificial molecular machines. Alberto Credi (Bologna) reviews recent progress and describes some examples based on rotaxanes, catenanes, and related interlocked molecules.

The review covers: (i) the design and construction of more sophisticated artificial molecular motors and machines; (ii) the use of such systems to do tasks such as molecular-level transportation, catalysis, and mechanical gating of molecular channels; and (iii) the possibility of exploiting their logic behaviour for information processing at the molecular level and, in the long run, for the construction of chemical computers.

Apart from more or less futuristic applications, the extension of the concept of motor and machine to the molecular level is of interest not only for the development of nanotechnology, but also for the growth of basic research. Looking at molecular and
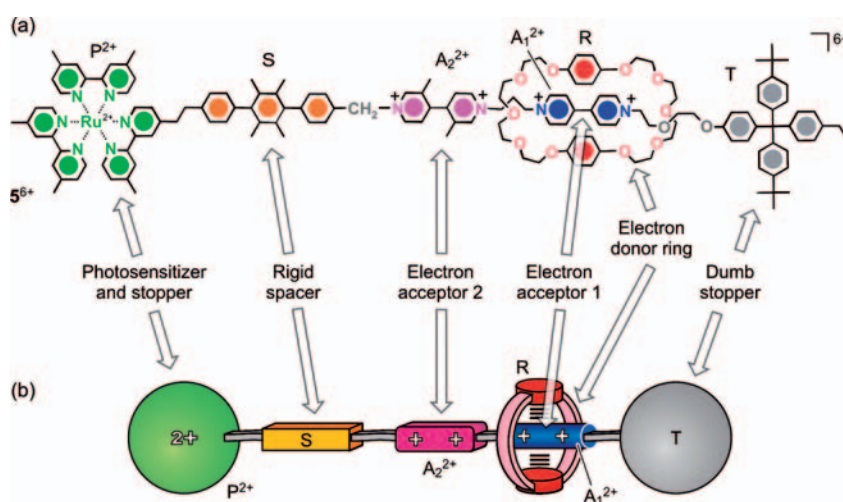
Chemical formula (a) and cartoon representation (b) of the rotaxane 5^{6+}, showing its modular structure. Molecular models show that a rotaxane molecule is approximately 5 nm long, and the diameter of the ring is about 1.3 nm.

supramolecular species from the viewpoint of functions with references to devices of the macroscopic world is indeed a very interesting exercise which introduces novel concepts into chemistry as a scientific discipline.

Artificial nanomachines based on interlocked molecules
Alberto Credi

This article is part of a special section on molecular nanomachines. To find similar related articles see Journal of Physics: Condensed Matter Vol 18, No 33.

Si-Ge nanostructures

Epitaxial growth and characterization of $Si_{1-x}Ge_x$ islands and Ge dots on (001) Si are reviewed

Semiconductor three-dimensional (3D) islands and quantum dots have potential in new electronic, photonic, or optoelectronic devices. Accurate control of the size, shape, and position of the dots is crucial.

J-M Baribeau, X Wu, N L Rowell and D J Lockwood (National Research Council Canada) review recent progress in the growth and characterization of $Si_{1-x}Ge_x$ islands and Ge dots on (001) Si. They discuss the evolution of the island morphology with $Si_{1-x}Ge_x$ coverage, and the effect of growth parameters or post-growth annealing on the shape of islands and dots. They outline some of the structural, vibrational, and optical properties of $Si_{1-x}Ge_x$ islands and review recent advances in the determination of their composition and strain distribution.

They present an analytical electron transmission microscopy study of the Ge spatial distribution in Ge dots and $Si/Si_{1-x}Ge_x$ island superlattices grown by molecular beam epitaxy and ultra-high vacuum chemical vapour deposition. They describe the use of undulated $Si_{1-x}Ge_x$ island superlattices for infrared detection at telecommunication wavelengths.

Finally, they discuss various approaches currently being investigated to engineer $Si_{1-x}Ge_x$ quantum dots and, in particular,
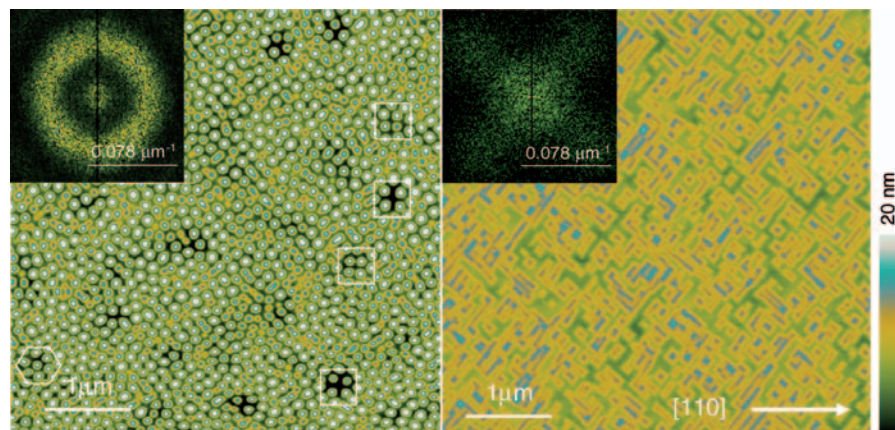
AFM images showing the surface morphology of $Si/Si_{1-x}Ge_x$ island superlattices prepared by (left) MBE and consisting of ten periods of 13 nm Si/3.4 nm $Si_{0.54}Ge_{0.46}$ and (right) UHV-CVD and consisting of ten periods of 15 nm Si/3 nm $Si_{0.50}Ge_{0.50}$. The inset is a power spectral density map of the image.

control their size, density, and spatial distribution. As examples, they show how carbon pre-deposition on Si(001) can influence nucleation and growth of Ge islands and how low-temperature Si homo-epitaxy can lead to a particular surface cusp morphology that may promote dot nucleation.

Despite all the challenges that remain in the understanding and control of semiconductor nanostructures, these

artificial materials constitute a key enabling technology leading to the development of quantum devices and eventually quantum computing.

**Ge dots and nanostructures grown epitaxially on Si**
J-M Baribeau, X Wu, N L Rowell and D J Lockwood
J. Phys.: Condens. Matter **18** (2006) R139–R174

Simulating smart biomaterials

New multiscale techniques for simulating smart biomaterials are reviewed

Biological membranes are 'smart' materials whose properties emerge from the propagation across many scales of the molecular characteristics of their constituents. Artificial smart materials, such as drug delivery vehicles and biosensors, often rely on modifying naturally occurring soft matter, such as polymers and lipid vesicles, so that they possess useful behaviour. However, the complexity of natural membranes, both in their static properties, exemplified in their phase behaviour, and in their dynamic properties, as in the kinetics of their formation and interactions, hinders their rational modification. Mesoscopic simulations, such as dissipative particle dynamics, allow *in silico* experiments to be easily performed on complex, soft materials requiring as input only the molecular structure of the constituents at a coarse-grained level. They can therefore act as a guide to experimenters prior to performing costly assays. Also, mesoscopic simulations provide the only
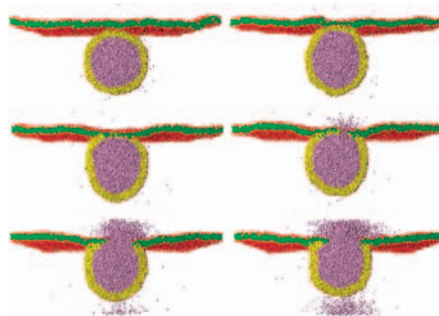
Sequence of snapshots of a 28 nm diameter vesicle fusing with a 100x100 nm² planar membrane patch.

currently feasible window on the length- and timescales relevant to important biophysical processes such as vesicle fusion.

Julian Shillcock and Reinhard Lipowsky (Max Planck Institute of Colloids and Interfaces) review the development of computational models of bilayer membranes, and in particular the use of mesoscopic simulations to follow the molecular rearrangements that occur during

membrane fusion.

It seems likely that in the future several techniques will be combined into a 'multi-scale self-parametrizing model' in which key parameters for the larger length- and timescales are continuously determined from data generated at smaller scales. This will be of immense benefit in visualizing and rationally designing the smart biomaterials of tomorrow.

The computational route from bilayer membranes to vesicle fusion
Julian C Shillcock and Reinhard Lipowsky
J. Phys.: Condens. Matter **18** (2006) S1191–S1219

This article is part of a special section on biomembranes. To find more papers on biomembranes see Journal of Physics: Condensed Matter Vol 18, No 28.
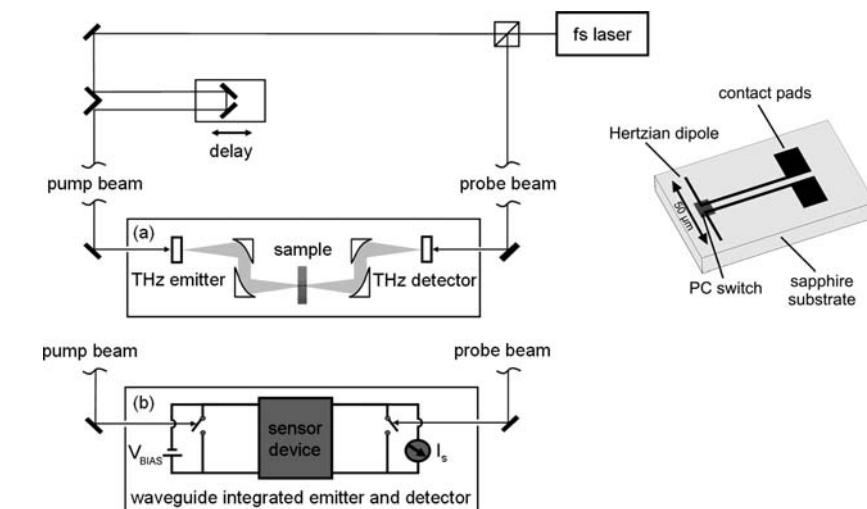
THz biosensing devices

THz devices offer marker-free biomolecule detection on functionalized surfaces in dry and fluid environments

In the last few years THz technology has become increasingly important for biological applications. It is particularly interesting for biosensing applications because numerous characteristic vibrational modes of macro-molecules, like proteins or DNA, are located in the THz part of the spectrum. The energy levels at THz frequencies are low (4 meV at 1 THz), enabling low-invasiveness probing of biological samples. THz probes have recently been applied to identify conformational states of proteins, monitor receptor binding events and for DNA analysis and imaging of cancerous tissue.

M Nagel, M Först and H Kurz of RWTH Aachen have presented different concepts of integrated THz-sensor devices for marker-free biosensing applications. They showed that functionalized resonators can detect specific DNA sequences at probe molecules immobilized on the sensor surface via a time-resolved photoconductive sampling technique with femtomole sensitivity. This principle is suitable for the parallel execution of several hybridizing experiments on a chip with an array arrangement of differently functionalized sensors.

They also introduced a compact THz transceiver device for fluidic analysis which has been applied for the characterization of

water–ethanol mixtures. The implementation of asynchronous optical sampling into the biochip reader system is an important development step that strongly increases the data throughput for this type of sensing devices.

Schematic drawing of two types of time-domain pump/probe measurement set-ups. A fs laser and a delay scanning stage are applied to facilitate generation and time-resolved detection of transmitted THz signals. (a) Quasi-optical variation using propagation of free-space THz radiation generated and detected with photoconductive antennas (see inlay). (b) Equivalent circuit diagram representing a waveguide-based scheme using integrated photoconductive switches.

Organic superconductors

Organic charge transfer salts are reviewed, especially their superconducting properties

Organic charge transfer salts are excellent model strongly correlated electron systems. Band structure suggests they should be metals at all pressures and temperatures, but observed phases include Mott insulators, Néel antiferromagnets, spin liquids, (unconventional) superconductors, Fermi liquids, a pseudogap and a 'bad metal'.

B J Powell and Ross H McKenzie (University of Queensland) review the role of strong electronic correlations in quasi-two-dimensional organic charge transfer salts. They identify two classes: one is strongly dimerized and is described by a half-filled Hubbard model; the second is not strongly dimerized and is described by a quarter-filled extended Hubbard model.

They explore the phase diagram of the half-filled quasi-two-dimensional organic charge transfer salts, focusing on the metallic and superconducting phases. The metallic phase, which has both Fermi liquid and 'bad metal' regimes, is well described by dynamical mean field theory. They critically review experimental studies of the
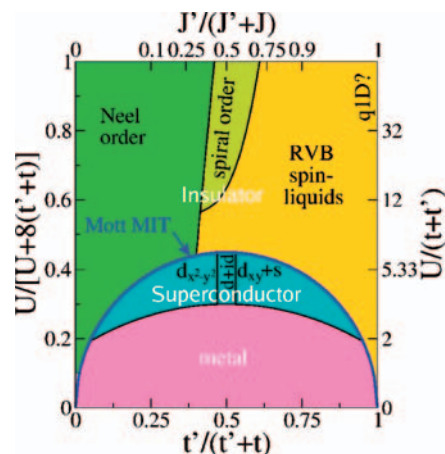
Schematic zero temperature phase diagram of the Hubbard model on the anisotropic triangular lattice at half filling, which provides an excellent qualitative description of the β, β', κ and λ phase organic charge transfer salts.

superconducting state, which is still controversial, focusing on the key results that may distinguish between rival theories of superconductivity, particularly probes of

the pairing symmetry and measurements of the superfluid stiffness. They then discuss some strongly correlated theories of superconductivity, in particular the resonating valence bond theory.

Finally they discuss some major challenges, including parameterizing minimal models, the evidence for a pseudogap from nuclear magnetic resonance experiments, superconductors with low critical temperatures and extremely small superfluid stiffnesses, the possible spin-liquid states in κ-(ET)$_2$Cu$_2$(CN)$_3$ and β-[Pd(dmit)$_2$]$_2$Z, and the need for high-quality large single crystals.

Amorphous ices

Recent experiments and computer simulations of the different phases of water are reviewed

Water has a very complex phase diagram; for example, ice exists in at least 15 different phases, including metastable phases such as cubic ice, ice IV and ice XII. In the (metastable) amorphous solid state (also called glassy water), water shows polyamorphism, i.e., the presence of more than one amorphous state. In addition to LDA (low-density amorphous ice), a second amorphous state, HDA (high-density amorphous ice), was discovered about twenty years ago. Since then, polyamorphism has been observed in many other substances such as SiO_2, GeO_2, Si, and Ge. Five years ago, experimental results suggesting the existence of a third amorphous state, VHDA (very high-density amorphous ice), were reported, opening the possibility that more than two amorphous states could be observed in other substances as well.

A consistent phase diagram of glassy water does not yet exist. Such a phase diagram is necessary if one also wants to understand the anomalous behaviour of supercooled liquid water. Since the discovery of HDA, a large amount of work based on
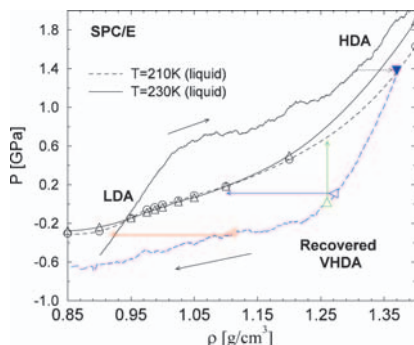
Effect of heating decompressed VHDA at constant pressure and constant volume from molecular dynamics simulations using the SPC/E model. O, Δ: liquid isotherms; thick solid line: compression curve of LDA at T = 77 K; blue thick line: decompression curve of VHDA at T = 77 K. Blue and red arrows (at P ~ 0 and ~ -0.3 GPa, respectively) show the density change upon annealing decompressed VHDA up to T ~ 170 K. Only at P ~ 0.3 GPa does VHDA seem to transform to LDA. Green arrow indicates the pressure change upon heating isochorically HDA at L ~ 1.6 g/cm³. At the present heating rate, VHDA does not transform to HDA and the system gets trapped in the liquid isotherms before reaching the pressure corresponding to HDA.

experiments and computer simulations has appeared. Thomas Loerting (Innsbruck) and Nicolas Giovambattista (Princeton) review such studies with special emphasis on comparing the experimental and simulation results. In particular, they review the recent studies concerning VHDA, its nature, and discuss the main open questions relating to the phase diagram of glassy water.

Answering these questions will require a thorough understanding of transformations between disordered states at low temperatures, which will probably require a few more decades of effort, e.g., to learn more about the effects of cooling/heating and compression/decompression rates in the glass and liquid states.