Journal of Physics
Condensed Matter

Highlights 2010
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If you have a high-quality short article of new and important research, then you can submit this as a fast track communication (FTC).

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To be considered as a FTC your work must be:

- Reporting new and timely developments in condensed matter research.
- Excellent quality and of interest to the community.
- Written in a clear and concise style.

When submitting your FTC for publication please provide a written justification to the editors explaining why your article meets our stringent quality and novelty criteria. For more information contact the publishing team at jpcm@iop.org.

We invite you to visit our dedicated FTC webpage on the JPCM website at iopscience.org/jpcm to read some of the FTCs published in the journal.

**Cover image:** A graphene antidot. Occupational probabilities on carbon atoms of a state near the Dirac point. Park *et al* 2010 J. Phys.: Condens. Matter 22 375302.
Dear Colleagues,

This has been another successful year for *Journal of Physics: Condensed Matter* (JPCM) with our increased readership enjoying issues of high quality and exciting research. 2010 saw the launch of ‘LabTalk’, an online feature displaying author-written news items highlighting the key achievements of their recent work. We are pleased to announce that JPCM is now indexed in PubMed, and biomedical papers will also appear in Medline; great news for authors publishing in our liquids, soft matter and biological physics section.

This collection of highlights displays some of the best articles published in the journal over the course of 2010. All of these were chosen primarily for their excellent science, and they also received endorsements from referees, board members and readers. Topics featured in this collection are diverse and display the broad scope of the journal.

Fast track communications (FTCs) feature strongly in this showcase, with many researchers taking advantage of the many benefits of FTCs to display their most significant and timely work. FTCs are open access and the average receipt-to-web publication time is just 40 days. In addition, authors of FTCs can benefit from promotion of their work via LabTalk and our recommended reader service, where free electronic offprints are sent to readers of the author’s choice.

The journal continues to publish work at the forefront of condensed matter. Keep an eye out for our special issues in 2011, which will focus on a number of exciting, fast-moving areas. Topics to feature include: geometrically frustrated magnetism, domain wall dynamics in magnetic nanostructures, strongly correlated electron systems and nanoscale ferroelectrics. An area where the journal has been strong this year is graphene, and a number of top papers feature in this collection. Among these is a paper studying the electronic properties of a biased graphene bilayer, with authors including 2010 Nobel Prize® winners Andre Geim and Konstantin Novoselov.

We hope that you will find this latest collection informative and interesting. Thank you to all the authors, referees and readers who have contributed to the journal, and we look forward to working with you during 2011.

David Ferry
Editor-in-Chief

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**SEM image of FIB fabricated disks from the Co/Cu/Py/Cu(001).** Wu *et al* 2010 *J. Phys. Condens. Matter* **22** 342001.

**Five unit cells of a (4, 4) single-wall CNT (consisting of 80 atoms) as the channel, in the presence of two and four vacancies on a ring of carbon atoms.** Farghadan and Saffarzadeh 2010 *J. Phys. Condens. Matter* **22** 255301.
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Journal scope

Journal of Physics: Condensed Matter covers the whole of condensed matter physics, including soft condensed matter and nanostructures. Papers may report experimental, theoretical and simulation studies.

Papers are published under the following subject sections:
- Surface, interface and atomic-scale science
- Liquids, soft matter and biological physics
- Nanostructures and nanoelectronics
- Solid structure and lattice dynamics
- Electronic structure
- Correlated electrons
- Superconductors and metals
- Semiconductors
- Dielectrics and ferroelectrics
- Magnetism and magnetic materials

More information on each of these areas can be found at iopscience.org/jpcm.

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Our dedicated team at IOP Publishing is here to ensure that the peer-review process runs as smoothly as possible for our authors.

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2010 Special issues

The journal’s authoritative special issue programme aims to cover the most exciting and most rapidly developing areas of condensed matter, with experts in the field contributing to high-quality issues of original research. Below are some highlights from our special issue programme for 2010.

**Carbon and related nanomaterials**

**Guest Editors:** Milton W Cole, Vincent H Crespi, Gene F Dresselhaus, Mildred S Dresselhaus, Gerald D Mahan and Jorge O Sofo

*2010 J. Phys.: Condens. Matter 22 issue 33*

This special issue contains a selection of articles providing new insights into the fascinating and challenging science behind nanomaterials. Among the materials considered in this issue are graphene, nanotubes, nanopores and fullerenes. The reader will find studies into the magnetic behaviour, optics, structure, adsorption and transport properties of such materials.

**New developments in nanopore research**

**Guest Editors:** Tim Albrecht, Joshua B Edel and Mathias Winterhalter

*2010 J. Phys.: Condens. Matter 22 issue 45*

Biological and solid-state nanopores are an exciting field of research, which has seen a rapid development over the last 10 to 20 years. Activities in this area range from theoretical and experimental work on the underlying fundamental (bio)physics to applications in single-molecule biosensing. This is a very active area and these articles aim to inspire researchers active in the field, to liberate inherent synergies, and not least, to demonstrate to the outside world the current state-of-the-art and future opportunities.

**Time-resolved scanning tunnelling microscopy**

**Guest Editor:** Harold J W Zandvliet and Nian Lin

*2010 J. Phys.: Condens. Matter 22 issue 26*

Scanning tunnelling microscopy (STM) has revolutionized our ability to image, manipulate, and investigate solid surfaces on the length scale of individual atoms and molecules. This issue reports progress in the rapidly emerging field of time-resolved STM, and highlights the potential of this powerful technique. Although the majority of studies that have been performed so far focus on simple systems it is anticipated that time-resolved scanning tunneling microscopy will also be applied in other research areas, such as biology and soft condensed matter, where the experimental conditions are often less ideal.

**New trends in simulating colloids and self-assembling systems**

**Guest Editors:** Giuseppe Foffi and Gerhard Kahl

*2010 J. Phys.: Condens. Matter 22 issue 10*

Interest in colloidal physics has grown at an incredible pace over the past few decades. To a great extent this remarkable development is due to the fact that colloidal systems are highly relevant in everyday applications as well as in basic research. This issue presents theoretical and simulation-based papers and aims to further understanding of many phenomena in soft and bio-related physics, such as phase behaviour, self-assembly strategies, and rheological properties. These insights might help to guide experiments and the design of new colloid-based materials with desired properties.
Topical reviews

Topical reviews in *Journal of Physics: Condensed Matter* (JPCM) bring you an authoritative, up-to-date overview of the latest hot topics in the field of condensed matter. Typically commissioned by the Editorial Board they often deal with subjects that are still developing rapidly and may provide an indication of the future direction of the field.

Visit our dedicated topical review page at [iopscience.iop.org/jpcm](http://iopscience.iop.org/jpcm) to view some of the best recent reviews. All reviews in this collection are free to read.

JPCM topical reviews continue to prove popular with readers, and here we highlight some of the best from 2010.

**Magnetic nanostructures**
K Bennemann
2010 *J. Phys.: Condens. Matter* **22** 243201

**Charge transport through molecular switches**
Sense Jan van der Molen and Peter Liljeroth
2010 *J. Phys.: Condens. Matter* **22** 133001

**Magnetism in Fe-based superconductors**
M D Lumsden and A D Christianson
2010 *J. Phys.: Condens. Matter* **22** 203203

**Disorder and electronic transport in graphene**
E R Mucciolo and C H Lewenkopf
2010 *J. Phys.: Condens. Matter* **22** 273201

**Magnetism of solids resulting from spin polarization of p orbitals**
O Volnianska and P Boguslawski
2010 *J. Phys.: Condens. Matter* **22** 073202

**Jamming of soft particles: geometry, mechanics, scaling and isostaticity**
M van Hecke
2010 *J. Phys.: Condens. Matter* **22** 033101

**A perspective on the Fe-based superconductors**
John A Wilson
2010 *J. Phys.: Condens. Matter* **22** 203201

**Sensing gases with carbon nanotubes: a review of the actual situation**
A Goldoni, L Petaccia, S Lizzit and R Larciprete
2010 *J. Phys.: Condens. Matter* **22** 013001

**Electronic phenomena at complex oxide interfaces: insights from first principles**
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Grant van Riessen, Zheng Wei, Rajendra S Dhaka, Carsten Winkler, Frank O Schumann and Jürgen Kirschner

Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany

2010 J. Phys.: Condens. Matter 22 092201

We have measured the correlated electron pair emission from a Cu(001) surface by both direct and core-resonant channels upon excitation with linearly polarized photons of energy far above the 3p threshold. As expected for a single-step process mediated by electron correlation in the initial and final states, the two electrons emitted by the direct channel continuously share the sum of the energy available to them. The core-resonant channel is often considered in terms of successive and independent steps of photoexcitation and Auger decay. However, electron pairs emitted by the core-resonant channel also share their energy continuously to jointly conserve the energy of the complete process. By detecting the electron pairs in parallel over a wide range of energy, evidence of the core-resonant double photoemission proceeding by a coherent single-step process is most strikingly manifested by a continuum of correlated electron pairs with a sum energy characteristic of the process but for which the individual electrons have arbitrary energies and cannot meaningfully be distinguished as a photoelectron or Auger electron.

Modified bimodal growth mechanism of pentacene thin films at elevated substrate temperatures

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The growth of pentacene thin films at elevated temperatures was studied. We observed decreased grain size and crystallinity with increasing substrate temperature in 30 nm films, despite the increased grain size of the submonolayer films. These were attributed to a two-dimensional to three-dimensional growth transition and a pronounced desorption of the first monolayer molecules. The observed coarsening-like behavior and the dendritic to compact grain geometry transition with temperature were explained by classic growth theories. A modified bimodal growth mechanism at elevated temperatures was proposed by analyzing both the out-of-plane and the in-plane grazing incidence x-ray diffraction patterns of the same films.

Structural characterization of thin layered materials using x-ray standing wave enhanced elastic and inelastic scattering measurements

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By measuring the intensities of the x-ray standing wave induced elastic and inelastic x-ray scattering from thin multilayer structures, we show that structural characterizations of the high and low z (atomic number) material layers can be performed independently. The method has been tested by analyzing the structural properties of an Nb/C/Nb trilayer and a Mo/Si periodic multilayer structure. The results of the x-ray scattering measurements have been compared with those obtained using x-ray reflectivity and conventional x-ray standing wave fluorescence techniques. It has been demonstrated that the present approach is especially suitable for studying multilayer structures comprising low atomic number layers, as it eliminates the requirement of a fluorescence signal, which is very weak in the case of low z materials.
Thermodynamic instability at the stoichiometric LaAlO$_3$/SrTiO$_3$(001) interface

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Stoichiometric epitaxial LaAlO$_3$ grown on TiO$_2$-terminated SrTiO$_3$(001) by off-axis pulsed laser deposition is shown to exhibit strong cation intermixing. This result is corroborated by classical and quantum mechanical calculations of the relative stabilities of abrupt and intermixed interface configurations. The valence band offset was measured to be 0.16 ± 0.10 eV, and this value cannot be accounted for theoretically without including intermixing in the physical description of the interface.

High-pressure behaviour of GeO$_2$: a simulation study

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In this work we study the high-pressure behaviour of liquid and glassy GeO$_2$ by means of molecular dynamics simulations. The interaction potential, which includes dipole polarization effects, was parametrized using first-principles calculations. Our simulations reproduce the most recent experimental structural data very well. The character of the pressure-induced structural transition in the glassy system has been a matter of controversy. We show that our simulations and the experimental data are consistent with a smooth transition from a tetrahedral to an octahedral network with a significant number of pentacoordinated germanium ions appearing over an extended pressure range. Finally, the study of high-pressure, liquid germania confirms that this material presents an anomalous behaviour of the diffusivity as observed in analogous systems such as silica and water. The importance of pentacoordinated germanium ions for such behaviour is stressed.

A density functional study of the adsorption of methane-thiol on the (111) surfaces of the Ni-group metals: I. Molecular and dissociative adsorption

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The molecular and dissociative adsorption of methane-thiol (CH$_3$SH) in the high-coverage limit on the (111) surfaces of the Ni-group metals has been investigated using ab initio density functional techniques. In molecular form, methane-thiol is bound to the surface only by weak polarization-induced forces in a slightly asymmetric configuration with the C–S axis tilted by 35–60° relative to the surface normal. On Ni and Pd surfaces the S atom occupies a position close to a bridge site; on Pt it is located close to an on-top position. The length of the S–H bond is only slightly stretched relative to its value in the gas phase, indicating only a very modest degree of activation for dehydrogenation. A strong covalent adsorbate/substrate bond is formed upon adsorption of a methane-thiolate (CH$_3$S) radical. On Ni(111) in the energetically most favorable configuration the S atom occupies a position in a threefold hollow, slightly displaced towards a bridge site. The C–S axis is tilted by about 35° across the bridge. On Pd(111) and Pt(111) the S atom of thiolate occupies a position between a hollow and a bridge site, with the C–S axis tilted even more strongly across a neighboring threefold hollow. On all three surfaces our calculations demonstrate the existence of multiple metastable adsorption configurations, including upright CH$_3$S bound in the center of a threefold hollow as reported in some earlier studies. Dehydrogenation of the adsorbed methane-thiol to form co-adsorbed methane-thiolate and atomic hydrogen is an exothermic process, which is not activated on Ni(111) but activated on Pd(111) and Pt(111).

Simulated diffusion coefficients on liquid (T ~ 4000 K) germania and percentage of GeO$_2$ units as a function of increasing pressure.
Modulation of electronic structures of bases through DNA recognition of protein

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The effects of environmental structures on the electronic states of functional regions in a fully solvated DNA·protein complex were investigated using combined ab initio quantum mechanics/molecular mechanics calculations. A complex of a transcriptional factor, PU.1, and the target DNA was used for the calculations. The effects of solvent on the energies of molecular orbitals (MOs) of some DNA bases strongly correlate with the magnitude of masking of the DNA bases from the solvent by the protein. In the complex, PU.1 causes a variation in the magnitude among DNA bases by means of directly recognizing the DNA bases through hydrogen bonds and inducing structural changes of the DNA structure from the canonical one. Thus, the strong correlation found in this study is the first evidence showing the close quantitative relationship between recognition modes of DNA bases and the energy levels of the corresponding MOs. Thus, it has been revealed that the electronic state of each base is highly regulated and organized by the DNA recognition of the protein. Other biological macromolecular systems can be expected to also possess similar modulation mechanisms, suggesting that this finding provides a novel basis for the understanding for the regulation functions of biological macromolecular systems.

Structural origin of dynamic heterogeneity in three-dimensional colloidal glass formers and its link to crystal nucleation

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The physical understanding of glass transition remains a major challenge of physics and materials science. Among various glass-forming liquids, a colloidal liquid interacting with hard-core repulsion is now regarded as one of the most ideal model systems. Here we study the structure and dynamics of three-dimensional polydisperse colloidal liquids by Brownian dynamics simulations. We reveal that medium-range crystalline bond orientational order of the hexagonal close packed structure grows in size and lifetime with increasing packing fraction. We show that dynamic heterogeneity may be a direct consequence of this transient structural ordering, which suggests its origin is thermodynamic rather than kinetic. We also reveal that nucleation of crystals preferentially occurs in regions of high medium-range order, reflecting the low crystal–liquid interfacial energy there. These findings may shed new light not only on the fundamental nature of the glass transition, but also the mechanism of crystal nucleation.

NEW FOR 2011

JPCM is now indexed in PubMed. Biomedical papers will also be indexed and included in Medline.
Biomimetic structures for fluid drag reduction in laminar and turbulent flows

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Biomimetics allows one to mimic nature to develop materials and devices of commercial interest for engineers. Drag reduction in fluid flow is one of the examples found in nature. In this study, nano, micro, and hierarchical structures found in lotus plant surfaces, as well as shark skin replica and a rib patterned surface to simulate shark skin structure were fabricated. Drag reduction efficiency studies on the surfaces were systematically carried out using water flow. An experimental flow channel was used to measure the pressure drop in laminar and turbulent flows, and the trends were explained in terms of the measured and predicted values by using fluid dynamics models. The slip length for various surfaces in laminar flow was also investigated based on the measured pressure drop. For comparison, the pressure drop for various surfaces was also measured using air flow.

Modelling the self-assembly of virus capsids

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We use computer simulations to study a model, first proposed by Wales (2005 Phil. Trans. R. Soc. A 363 357), for the reversible and monodisperse self-assembly of simple icosahedral virus capsid structures. The success and efficiency of assembly as a function of thermodynamic and geometric factors can be qualitatively related to the potential energy landscape structure of the assembling system. Even though the model is strongly coarse-grained, it exhibits a number of features also observed in experiments, such as sigmoidal assembly dynamics, hysteresis in capsid formation and numerous kinetic traps. We also investigate the effect of macromolecular crowding on the assembly dynamics. Crowding agents generally reduce capsid yields at optimal conditions for non-crowded assembly, but may increase yields for parameter regimes away from the optimum. Finally, we generalize the model to a larger triangulation number \( T = 3 \), and observe assembly dynamics more complex than that seen for the original \( T = 1 \) model.

Mechanical properties of ternary lipid membranes near a liquid–liquid phase separation boundary

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We study the mechanical properties of ternary lipid bilayers assembled in giant vesicles, formed from a saturated and an unsaturated phosphocholine (in equal proportions) and cholesterol. As a function of temperature, these systems can undergo in-plane phase separation. Using image analysis we identify the vesicle contour, and quantify the vesicle shape and the amplitude of membrane thermal fluctuations. The two lipid compositions chosen show different thermotropic behaviours. At 60 mol% cholesterol the membrane is in a uniform liquid state over the entire temperature range investigated (10–50 °C), but vesicles containing 30 mol% cholesterol undergo phase separation into two immiscible liquid phases at around 28 °C. Upon cooling below this transition temperature we observe a marked increase in the measured bending elastic modulus. Phase separation proceeds over a long time (tens of minutes), and we measure the properties of vesicles both during the domain coarsening phase and in the fully phase separated condition. Fluorescence microscopy allows us to identify the coexisting phases. We can therefore measure directly the bending moduli of each of the phases as a function of temperature, showing a strong variation which is attributed to the changing phospholipid and cholesterol composition.
Electronic structure of a graphene/hexagonal-BN heterostructure grown on Ru(0001) by chemical vapor deposition and atomic layer deposition: extrinsically doped graphene

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A significant BN-to-graphene charge donation is evident in the electronic structure of a graphene/h-BN(0001) heterojunction grown by chemical vapor deposition and atomic layer deposition directly on Ru(0001), consistent with density functional theory. This filling of the lowest unoccupied state near the Brillouin zone center has been characterized by combined photoemission/\( k \) vector resolved inverse photoemission spectroscopies, and Raman and scanning tunneling microscopy/spectroscopy. The unoccupied \( \sigma^*(\Gamma_1+) \) band dispersion yields an effective mass of 0.05 \( m_e \) for graphene in the graphene/h-BN(0001) heterostructure, in spite of strong perturbations to the graphene conduction band edge placement.

Thermoelectric properties of graphene nanoribbons, junctions and superlattices

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Using model interaction Hamiltonians for both electrons and phonons and Green’s function formalism for ballistic transport, we have studied the thermal conductance and the thermoelectric properties of graphene nanoribbons (GNR), GNR junctions and periodic superlattices. Among our findings we have established the role that interfaces play in determining the thermoelectric response of GNR systems both across single junctions and in periodic superlattices. In general, increasing the number of interfaces in a single GNR system increases the peak \( ZT \) values that are thus maximized in a periodic superlattice. Moreover, we proved that the thermoelectric behavior is largely controlled by the width of the narrower component of the junction. Finally, we have demonstrated that chevron-type GNRs recently synthesized should display superior thermoelectric properties.

Graphene based quantum dots

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Laterally localized electronic states are identified on a single layer of graphene on ruthenium by low temperature scanning tunneling spectroscopy (STS). The individual states are separated by 3 nm and comprise regions of about 90 carbon atoms. This constitutes a highly regular quantum dot-array with molecular precision. It is evidenced by quantum well resonances (QWRs) with energies that relate to the corrugation of the graphene layer. The \( dI/dV \) conductance spectra are modeled by a layer height dependent potential-well with a delta-function potential that describes the barrier for electron penetration into graphene. The resulting QWRs are strongest and lowest in energy on the isolated ‘hill’ regions with a diameter of 2 nm, where the graphene is decoupled from the surface.
The conduction gap in double gate bilayer graphene structures

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Using the nonequilibrium Green function method, the electrical behavior of a double gate bilayer graphene structure is investigated. Due to energy bandgap opening when potential energies in the layers are different, a clear gap of electrical current is observed. The sensitivity of this phenomenon to device parameters (gate length, temperature) has been considered systematically. It appears that the threshold voltage can be controlled by tuning the gate voltages and/or the Fermi energy. Our obtained results may be useful and provide new suggestions for further experimental investigations.

Local density of states for a double gate bilayer graphene structure.

Curvature-induced D-band Raman scattering in folded graphene

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Micro-Raman scattering from folds in single-layer graphene sheets finds a D-band at the fold for both incommensurate and commensurate folding, while the parent single-layer graphene lacks a D-band. A coupled elastic-continuum/tight-binding calculation suggests that this D-band arises from the spatially inhomogeneous curvature around a fold in a graphene sheet. The polarization dependence of the fold-induced D-band further reveals that the inhomogeneous curvature acts as a very smooth, ideal one-dimensional defect along the folding direction.

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Selective D₂ adsorption enhanced by the quantum sieving effect on entangled single-wall carbon nanotubes

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The quantum sieving effect of D₂ over H₂ is examined at 40 and 77 K by means of experiments and GCMC simulations, for two types of single-wall carbon nanotubes that are distinguishable by their unique entangled structures; (1) a well-bundled SWCNT and (2) loosely-assembled SWCNT produced by the super growth method (SG-SWCNT). Oxidized SWCNT samples of which the so-called internal sites are accessible for H₂ and D₂, are also studied. Experimental H₂ and D₂ adsorption properties on the well-bundled SWCNTs are compared with the simulated ones, revealing that pore-blocking and restricted diffusion of the molecules suppress the high selectivity of D₂ over H₂. The non-oxidized SG-SWCNT assembly shows the highest selectivity among the SWCNT samples, both at 40 and 77 K. The high selectivity of the SG-SWCNT assembly, which is pronounced even at 77 K, is ascribed to their unique assembly structure.

Brillouin spectra have been collected in situ at temperatures up to ~1000 K for different crystallographic directions from two single crystal plates of LaAlO₃ perovskite. Elastic moduli derived from these, together with heat capacity, spontaneous strain and Raman data from the literature, have then been used to calibrate the coefficients in a classical Landau free energy expansion for the second order Pm3m ↔ R3c phase transition at T_c = 817 K. The static strain/order parameter coupling model provides a quantitative description of elastic softening between room temperature and ~700 K, but from ~700 K up to T_c additional elastic softening correlates with the development of a central peak in the Brillouin spectra. The presence of quasi-elastic scattering, which reaches maximum intensity ~5–15 K below T_c, implies a strong dynamical component to the phase transition. Relaxation times estimated from the width of the central peak are of the order of ~10–100 ps and appear to be more or less constant between ~700 and 800 K, which is consistent with an intrinsic origin associated with phonon density fluctuations. Central peak width variations and an irregular pattern of acoustic velocity variations in a 20 K temperature interval below T_c are interpreted in terms of flipping of clusters of tilted octahedra between different 〈111〉, 〈011〉 and 〈001〉 tilt axes. The additional softening beyond that expected from the classical strain/order parameter coupling model can be understood in terms of coupling of acoustic modes with the central peak mode(s).

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A mixed-space approach to first-principles calculations of phonon frequencies for polar materials

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2010 J. Phys.: Condens. Matter 22 202201

IOP Fast Track Communications

We propose a mixed-space approach using the accurate force constants calculated by the direct approach in real space and the dipole–dipole interactions calculated by linear response theory in reciprocal space, making the accurate prediction of phonon frequencies for polar materials possible using the direct approach as well as linear response theory. As examples, by using the present approach, we predict the first-principles phonon properties of the polar materials \(\alpha\)-Al\(_2\)O\(_3\), MgO, c-SiC, and h-BN, which are in excellent agreement with available experimental data.

Polymeric forms of carbon in dense lithium carbide

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IOP Fast Track Communications

The immense interest in carbon nanomaterials continues to stimulate intense research activities aimed at realizing carbon nanowires, since linear chains of carbon atoms are expected to display novel and technologically relevant optical, electrical and mechanical properties. Although various allotropes of carbon (e.g., diamond, nanotubes, graphene, etc) are among the best-known materials, it remains challenging to stabilize carbon in the one-dimensional form because of the difficulty of suitably saturating the dangling bonds of carbon. Here, we show through first-principles calculations that ordered polymeric carbon chains can be stabilized in solid Li\(_2\)C\(_2\) under moderate pressure. This pressure-induced phase (above 5 GPa) consists of parallel arrays of twofold zigzag carbon chains embedded in lithium cages, which display a metallic character due to the formation of partially occupied carbon lone-pair states in sp\(^2\)-like hybrids. It is found that this phase remains the most favorable one in a wide range of pressures. At extreme pressure (larger than 215 GPa) a structural and electronic phase transition towards an insulating single-bonded threefold-coordinated carbon network is predicted.

An efficient computational method for use in structural studies of crystals with substitutional disorder

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We present a computationally efficient semi-empirical method, based on standard first-principles techniques and the so-called virtual crystal approximation, for determining the average atomic structure of crystals with substitutional disorder. We show that, making use of a minimal amount of experimental information, it is possible to define convenient figures of merit that allow us to recast the determination of the average atomic ordering within the unit cell as a minimization problem. We have tested our approach by applying it to a wide variety of materials, ranging from oxynitrides to borocarbides and transition-metal perovskite oxides. In all the cases we were able to reproduce the experimental solution, when it exists, or the first-principles result obtained by means of much more computationally intensive approaches.
Electronic properties of a biased graphene bilayer

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We study, within the tight-binding approximation, the electronic properties of a graphene bilayer in the presence of an external electric field applied perpendicular to the system—a biased bilayer. The effect of the perpendicular electric field is included through a parallel plate capacitor model, with screening correction at the Hartree level. The full tight-binding description is compared with its four-band and two-band continuum approximations, and the four-band model is shown to always be a suitable approximation for the conditions realized in experiments. The model is applied to real biased bilayer devices, made out of either SiC or exfoliated graphene, and good agreement with experimental results is found, indicating that the model is capturing the key ingredients, and that a finite gap is effectively being controlled externally. Analysis of experimental results regarding the electrical noise and cyclotron resonance further suggests that the model can be seen as a good starting point for understanding the electronic properties of graphene bilayer. Also, we study the effect of electron–hole asymmetry terms, such as the second-nearest-neighbour hopping energies $t'$ (in-plane) and $\gamma_4$ (inter-layer), and the on-site energy $\Delta$.

Electronic structure

Chemical accuracy for the van der Waals density functional

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The non-local van der Waals density functional (vdW-DF) of Dion et al (2004 Phys. Rev. Lett. 92 246401) is a very promising scheme for the efficient treatment of dispersion bonded systems. We show here that the accuracy of vdW-DF can be dramatically improved both for dispersion and hydrogen bonded complexes through the judicious selection of its underlying exchange functional. New and published exchange functionals are identified that deliver much better than chemical accuracy from vdW-DF for the S22 benchmark set of weakly interacting dimers and for water clusters. Improved performance for the adsorption of water on salt is also obtained.

Electronic properties of a biased graphene bilayer

Screened $V$ versus $n$ for a bilayer graphene system. Three different chemical dopings have been considered.

Forthcoming JPCM special issues for 2011:

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An *ab initio* study of xenon retention in \(\alpha\)-quartz

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2010 J. Phys.: Condens. Matter 22 025501

It has recently been suggested that a significant amount of Xe can be absorbed in \(\alpha\)-quartz and that this might be a significant process in the recycling of Xe from the atmosphere to the interior of the Earth. This suggestion is tested by *ab initio* calculations of Xe in \(\alpha\)-quartz using DFT. Three distinct candidate sites for Xe absorption are identified—substitutional at the silicon vacancy (Xe@V\(\text{Si}\)), at the oxygen vacancy (Xe@V\(\text{O}\)) and at an interstitial site (Xe@I)—and each is shown to be mechanically stable at both \(P = 0\) and 2 GPa. The energetics and electronic properties of these defect structures are analysed and it is shown that there is an energy barrier to the absorption at all sites at \(T = 0\). If the Xe absorption is a single-stage process in a perfect crystal then the lowest formation energy barrier (at both \(P = 0\) and 2 GPa) is for Xe@I at the interstitial site. If absorption is a two-stage process due to vacancies being already present at finite temperatures, then the subsequent barrier to Xe absorption is much lower and Xe@V\(\text{Si}\) has the lowest formation energy. However, it should be expected that there will be a much higher density of oxygen vacancies available for Xe absorption under realistic Earth core conditions and so in this scenario it is to be expected that all three candidate sites should be occupied.

Energy spectrum and density of states for a graphene quantum dot in a magnetic field

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In this paper, we determine the spectrum and density of states of a graphene quantum dot in a normal quantizing magnetic field. To accomplish this, we employ the retarded Green function for a magnetized, infinite-sheet graphene layer to describe the dynamics of a tightly confined graphene quantum dot subject to Landau quantization. Considering a \(\delta^2(\mathbf{r})\) potential well that supports just one subband state in the well in the absence of a magnetic field, the effect of Landau quantization is to ‘splitter’ this single energy level into a proliferation of many Landau-quantized states within the well. Treating the graphene sheet and dot as a closed system subject to a fully Hermitian Hamiltonian (including boundary conditions), there is no indication of decay of the Landau-quantized graphene dot states into the quantized states of the host graphene sheet for ‘tight’ confinement by the \(\delta^2(\mathbf{r})\) potential well, notwithstanding extension of the dot Green function (and eigenfunctions) outside the \(\delta^2(\mathbf{r})\) potential well.

![Energy spectrum and density of states for a graphene quantum dot subject to Landau quantization for the K node as a function of the square root of the magnetic field.](image)

Preferred functionalization on zigzag graphene nanoribbons: first-principles calculations

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We investigate the functionalization of functional groups to graphene nanoribbons with zigzag and armchair edges using first-principles calculations. We find that the formation energy for the configuration of the functional groups functionalized to the zigzag edge is \(~0.2\) eV per functional group lower than that to the armchair edge. The formation energy difference arises from a structural deformation on the armchair edge by the functionalization whereas there is no structural deformation on the zigzag edge. Selective functionalization on the zigzag edge takes place at a condition of the temperature and the pressure of \(~25\) °C and \(10^{-5}\) atm. Our findings show that selective functionalization can offer the opportunity for an approach to the separation of zigzag graphene nanoribbons with their solubility change.

![The charge density difference between the O atom and the H atom or the zigzag-edged graphene nanoribbons (ZGNR) when two hydroxyl groups are attached to the edge of the ZGNR.](image)
Evidence of superconductivity on the border of quasi-2D ferromagnetism in Ca$_2$RuO$_4$ at high pressure

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The layered perovskite Ca$_2$RuO$_4$ is a spin-one Mott insulator at ambient pressure and exhibits metallic ferromagnetism at least up to ~80 kbar with a maximum Curie temperature of 28 K. Above ~90 and up to 140 kbar, the highest pressure reached, the resistivity and ac susceptibility show pronounced downturns below ~0.4 K in applied magnetic fields of up to ~10 mT. This indicates that our specimens of Ca$_2$RuO$_4$ are weakly superconducting on the border of a quasi-2D ferromagnetic state.

Antiferro-quadrupolar structures in UPd$_3$ inferred from x-ray resonant Bragg diffraction

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A systematic analysis of resonant x-ray Bragg diffraction data for UPd$_3$, with signal enhancement at the U M$_{IV}$ edge, including possible structural phase transitions leads to a new determination of the space groups of the material in the phases between $T_0 = 7.8$ K and $T_1 = 6.9$ K, as $P_{222}$, and between $T_1 = 6.7$ K and $T_2 = 4.4$ K, as $P_2_1$. In addition, the quadrupolar order parameters, $\langle Q_{xy} \rangle$ and $\langle Q_{yz} \rangle$, inferred from diffraction data for the phase between $T_1$ and $T_2$, are $\langle Q_{yz} \rangle$ and $\langle Q_{xy} \rangle$ at the (103) Bragg reflection and $\langle Q_{xy} \rangle$ at the (104) reflection.

Antiferro-quadrupolar orderings of $\langle Q_{xy} \rangle$ and $\langle Q_{yz} \rangle$ observed in the (104) and (103) reflections at $T = 5.2$ K.
Magnetic susceptibility, magnetization, specific heat, and electrical resistivity studies on single crystals of Ce$_4$Pt$_{12}$Sn$_{25}$ reveal an antiferromagnetic transition at $T_N = 0.19$ K, which develops from a paramagnetic state with a very large specific heat coefficient ($C/T$) of 14 Joule mol$^{-1}$ K$^{-2}$-Ce just above $T_N$. On the basis of its crystal structure and these measurements, we argue that a weak magnetic exchange interaction in Ce$_4$Pt$_{12}$Sn$_{25}$ is responsible for its low ordering temperature and a negligible Kondo-derived contribution to physical properties above $T_N$. The anomalous enhancement of specific heat above $T_N$ is suggested to be related, in part, to weak geometric frustration of $f$-moments in this compound.

Three-dimensional representation of the crystal structure of Ce$_4$Pt$_{12}$Sn$_{25}$. The pressure inhomogeneity ($\Delta p$) for each of the different pressure media as a function of pressure, as calculated from the width of the superconducting transition of the pressure gauge. The pressure media in order of highest hydrostaticity are pentane–isopentane, Daphne oil 7373, and steatite. We investigate the evolution of the electrical resistivity of BaFe$_2$As$_2$ single crystals with pressure. The samples used were from the same batch, grown using a self-flux method, and showed properties that were highly reproducible. Samples were pressurized using three different pressure media: pentane–isopentane (in a piston–cylinder cell), Daphne oil (in an alumina anvil cell) and steatite (in a Bridgman cell). Each pressure medium has its own intrinsic level of hydrostaticity, which dramatically affects the phase diagram. An increasing uniaxial pressure component in this system quickly reduces the spin density wave order and favours the appearance of superconductivity, which is similar to what is seen in SrFe$_2$As$_2$. The pressure inhomogeneity ($\Delta p$) for each of the different pressure media as a function of pressure, as calculated from the width of the superconducting transition of the pressure gauge. The pressure media in order of highest hydrostaticity are pentane–isopentane, Daphne oil 7373, and steatite.
A comparative study on the thermoelectric effect of parent oxypnictides LaTAsO (T = Fe, Ni)

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The thermopower and Nernst effect were investigated for undoped parent compounds LaFeAsO and LaNiAsO. Both the thermopower and Nernst signal in iron-based LaFeAsO are significantly larger than those in nickel-based LaNiAsO. Furthermore, abrupt changes in both the thermopower and Nernst effect are observed below the structural phase transition temperature and spin-density wave (SDW) type antiferromagnetic (AFM) order temperature in Fe-based LaFeAsO. On the other hand, the Nernst effect is very small in the Ni-based LaNiAsO and it is weakly temperature-dependent, reminiscent of the case in normal metals. We suggest that the effect of SDW order on the spin scattering rate should play an important role in the anomalous temperature dependence of the Hall effect and Nernst effect in LaFeAsO. The contrasting behaviour between the LaFeAsO and LaNiAsO systems implies that the LaFeAsO system is fundamentally different from the LaNiAsO system and this may provide clues to the mechanism of high $T_c$ superconductivity in Fe-based systems.

Superconductivity at 23 K in Pt doped BaFe$_{2-x}$Pt$_x$As$_2$ single crystals

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We report superconductivity in single crystals of the new iron-pnictide system BaFe$_{1.90}$Pt$_{0.10}$As$_2$ grown by a self-flux solution method and characterized via x-ray, transport, magnetic and thermodynamic measurements. The magnetic ordering associated with a structural transition at 139 K present in BaFe$_2$As$_2$ is completely suppressed by substitution of 5% Fe with Pt and superconductivity is induced at a critical temperature $T_c = 23$ K. Full diamagnetic screening in the magnetic susceptibility and a jump in the specific heat at $T_c$ confirm the bulk nature of the superconducting phase. All properties of the superconducting state—

including the transition temperature $T_c$, the lower critical field $H_{c1} = 200$ mT, the upper critical field $H_{c2} = 65$ T, and the slope $\partial H_{c2}/\partial T$—are comparable in value to those found in other transition metal-substituted BaFe$_2$As$_2$ series, indicating the robust nature of superconductivity induced by substitution of Group VIII elements.

Vortex properties of two-dimensional superconducting Pb films

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Using low temperature scanning tunnelling microscopy/spectroscopy (STM/STS) we have investigated the vortex behaviours of two-dimensional superconducting Pb films at different thicknesses. STS at the vortex core shows an evolution of electronic states with film thickness. Transition from the clean limit to the dirty limit of superconductivity is identified, which can be ascribed to the decreased electronic mean free path induced by stronger scattering from the disordered interface at smaller thicknesses. A magnetic field dependent vortex core size is observed even for such a low-κ superconductor. The weak pinning induced by surface defects leads to the formation of a distorted hexagonal vortex lattice.

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**Semiconductors**

**Native defects in oxide semiconductors: a density functional approach**

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We report a semilocal and hybrid Hartree–Fock density functional study of native defects in three oxide semiconductors: ZnO, SrTiO₃, and SnO. The defect that is responsible for the n-type conductivity of ZnO has been debated, in which the O vacancy, Zn interstitial, their complexes, and residual H impurity are considered candidates. Our results indicate that the O vacancy induces a deep and localized in-gap state, whereas the Zn interstitial is a shallow donor and hence can be a source of the carriers. In view of the formation energies, the O vacancy is likely to form with a substantial concentration under O-poor conditions, but the Zn interstitial is unlikely. We thus propose that the O vacancy is relevant to the nonstoichiometry of ZnO and that a source other than the native defects, such as the H impurity, needs to be considered for the n-type conductivity. For SrTiO₃, the O vacancy and its complexes have been regarded as the origins of some of the remarkable electrical and optical properties. We suggest significant roles of the Ti antisite for a new insight into the defect-induced properties. Two types of Ti antisite, both of which are off-centered from the Sr site but toward different directions, exhibit low formation energies under Ti-rich conditions as does the O vacancy. They can explain optical properties such as visible-light emission, deep-level absorption, and the ferroelectricity observed in reduced SrTiO₃.

**Determination of the absolute chirality of tellurium using resonant diffraction with circularly polarized x-rays**

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Many proteins, sugars and pharmaceuticals crystallize into two forms that are mirror images of each other (enantiomers) like our right and left hands. Tellurium is one enantiomer having a space group pair, P₃121 (right-handed screw) and P₃21 (left-handed screw). X-ray diffraction with dispersion correction terms has been playing an important role in determining the handedness of enantiomers for a long time. However, this approach is not applicable for an elemental crystal such as tellurium or selenium. We have demonstrated that positive and negative circularly polarized x-rays at the resonant energy of tellurium can be used to absolutely distinguish right from left tellurium. This method is applicable to chiral motifs that occur in biomolecules, liquid crystals, ferroelectrics and antiferroelectrics, multiferroics, etc.

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First principles study of the optical contrast in phase change materials

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We study from first principles the optical properties of the phase change materials Ge2Sb2Te5 (GST), GeTe and Sb2Te3 in the crystalline phase and in realistic models of the amorphous phase generated by quenching from the melt in ab initio dynamics simulations. The calculations reproduce the strong optical contrast between the crystalline and amorphous phases measured experimentally and exploited in optical data storage. It is demonstrated that the optical contrast is due to a change in the optical matrix elements across the phase change in all the compounds. It is concluded that the reduction of the optical matrix elements in the amorphous phases is due to angular disorder in p-bonding which dominates the amorphous network in agreement with previous proposals (Huang and Robertson 2010 Phys. Rev. B 81 081204) based on calculations on crystalline models.

Low temperature magnetothermoelectric effect and magnetoresistance in Te vapor annealed Bi2Te3

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The electrical properties of single crystals of p-type Bi2Te3 are shown to be tuned by annealing as-grown crystals in elemental Te vapor at temperatures in the range of 400–420 °C. While as-grown nominally stoichiometric Bi2Te3 has p-type conductivity below room temperature, Te vapor annealed Bi2Te3 shows a cross over from p- to n-type behavior. The temperature dependent resistivity of the Te annealed crystals shows a characteristic broad peak near 100 K. Applied magnetic fields give rise to a large low temperature magnetothermoelectric effect in the Te annealed samples and enhance the low temperature peak in the resistivity. Further, Te annealed Bi2Te3 shows a large positive magnetoresistance, ~200% at 2 K, and ~15% at room temperature. The annealing procedure described can be employed to optimize the properties of Bi2Te3 for study as a topological insulator.
Invariant lattice strain and polarization in BaTiO$_3$–CaTiO$_3$ ferroelectric alloys

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We report the lattice strain and polarization of the BaTiO$_3$–CaTiO$_3$ solid solution. We found that the lattice strain evaluated by the tetragonality of the tetragonal phase at room temperature is nearly independent of the composition within the limit of the solid solution. In association with this variation, the saturation polarization remains nearly unchanged. Such invariant lattice strain associated with the ionic displacement in ferroelectrics is considered to be responsible for the nearly compositional independence of the polarization and the observed ferroelectric Curie temperature. Its relatively stable polarization compared with that of pure BaTiO$_3$ is very interesting for technological applications, such as in ferroelectric memory.

Polarization and magnetization dynamics of a field-driven multiferroic structure

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We consider a multiferroic chain with a linear magnetoelectric coupling induced by electrostatic screening at the ferroelectric/ferromagnet interface. We study theoretically the dynamic ferroelectric and magnetic response to external magnetic and electric fields by utilizing an approach based on coupled Landau–Khalatnikov and finite-temperature Landau–Lifshitz–Gilbert equations. Additionally, we make comparisons with Monte Carlo calculations. It is demonstrated that for material parameters corresponding to BaTiO$_3$/Fe the polarization and the magnetization are controllable by external magnetic and electric fields, respectively.
Artificial magnetism and left-handed media from dielectric rings and rods

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It is shown that artificial magnetism with relatively large frequency bandwidth can be obtained from periodic arrangements of dielectric rings. Combined with dielectric rods, dielectric rings can provide 3D isotropic left-handed metamaterials which are an advantageous alternative to metallic split ring resonators (SRRs) and/or metallic wires when undetectability by low frequency external magnetic fields is desired. Furthermore it is shown that, unlike conventional SRRs, dielectric rings can also be combined with natural plasma-like media to obtain a left-handed metamaterial.

SEM images of as-grown samples of undoped and Cu-doped ZnO nanowires. The insets show magnified images of their local morphologies.

Effects of annealing on the ferromagnetism and photoluminescence of Cu-doped ZnO nanowires

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Room temperature ferromagnetic Cu-doped ZnO nanowires have been synthesized using the chemical vapor deposition method. By combining structural characterizations and comparative annealing experiments, it has been found that both extrinsic (CuO nanoparticles) and intrinsic (\(\text{Zn}_x\text{Cu}_y\text{O}\) nanowires) sources are responsible for the observed ferromagnetic ordering of the as-grown samples. As regards the former, annealing in Zn vapor led to a dramatic decrease of the ferromagnetism. For the latter, a reversible switching of the ferromagnetism was observed with sequential annealings in Zn vapor and oxygen ambience respectively, which agreed well with previous reports for Cu-doped ZnO films. In addition, we have for the first time observed low temperature photoluminescence changed with magnetic properties upon annealing in different conditions, which revealed the crucial role played by interstitial zinc in directly mediating high \(T_c\) ferromagnetism and indirectly modulating the Cu-related structured green emission via different charge transfer transitions.
Neutron diffraction study of the BiFeO$_3$ spin cycloid at low temperature

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The reported observation of two anomalies in the intensity of the magnon Raman peaks of BiFeO$_3$, at 140 and 200 K (Singh et al 2008 J. Phys.: Condens. Matter 20 252203; Cazayous et al 2008 Phys. Rev. Lett. 101 037601) led to the hypothesis that such anomalies might originate from a spin reorientation transition. In order to test this hypothesis, we have used temperature-dependent neutron diffraction to track the evolution of the magnetic configuration in single crystals of BiFeO$_3$. Our results indicate that there is no average reorientation of the spins. This suggests that the magnon anomalies may instead be related to the freezing of modes that do not alter the average projection of the spins over the plane of the cycloid, as also reported for multiferroic TbMnO$_3$ (Sentff et al 2006 J. Phys.: Condens. Matter 18 2069).

Low temperature incommensurately modulated and noncollinear spin structure in FeCr$_2$S$_4$

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FeCr$_2$S$_4$ orders magnetically at $T_N = 170$ K. According to neutron diffraction, the ordered state down to 4.2 K is a simple collinear ferrimagnet maintaining the cubic spinel structure. Later studies, however, claimed trigonal distortions below ~60 K coupled to the formation of a spin glass type ground state. To obtain further insight, muon spin rotation/relaxation ($\mu$SR) spectroscopy was carried out between 5 and 200 K together with new $^{57}$Fe Mössbauer measurements. Below ~50 K, our data point to the formation of an incommensurately modulated noncollinear spin arrangement like a helical spin structure. Above 50 K, the spectra are compatible with collinear ferrimagnetism, albeit with a substantial spin disorder on the scale of a few lattice constants. These spin lattice distortions become very large at 150 K and the magnetic state is now better characterized as consisting of rapidly fluctuating short-range ordered spins. The Néel transition is of second order, but ill defined, extending over a range of ~10 K. The Mössbauer data around 10 K confirm the onset of orbital freezing and are also compatible with the noncollinear order of iron. The absence of a major change in the quadrupole interaction around 50 K renders the distortion of crystal symmetry to be small.

Fe Mössbauer data of FeCr$_2$S$_4$. Temperature dependences of the hyperfine field $B_{hf}$ (top) and the quadrupole interaction Q (bottom).

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Stable and fast semi-implicit integration of the stochastic Landau–Lifshitz equation

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We propose new semi-implicit numerical methods for the integration of the stochastic Landau–Lifshitz equation with built-in angular momentum conservation. The performance of the proposed integrators is tested on the 1D Heisenberg chain. For this system, our schemes show better stability properties and allow us to use considerably larger time steps than standard explicit methods. At the same time, these semi-implicit schemes are also of comparable accuracy to and computationally much cheaper than the standard midpoint implicit method. The results are of key importance for atomistic spin dynamics simulations and the study of spin dynamics beyond the macro spin approximation.

Comparison of the explicit HeunP, implicit IMP and semi-implicit methods SIA and SIB for the deterministic case \( \alpha = 0 \). The trajectory of two interacting spins is shown by plotting the \( x \) components of the two spins and one \( z \) component. Solid lines indicate the analytical solution.

The paired-electron crystal in the two-dimensional frustrated quarter-filled band

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The competition between antiferromagnetic and spin-singlet ground states within quantum spin models and the \( \frac{1}{2} \)-filled band Hubbard model has received intense scrutiny. Here we demonstrate a frustration-induced transition from Néel antiferromagnetism to a spin-singlet state in the interacting \( \frac{1}{4} \)-filled band on an anisotropic triangular lattice. While the antiferromagnetic state has equal charge densities, 0.5, on all sites, the spin-singlet state is a paired-electron crystal, with pairs of charge-rich sites separated by pairs of charge-poor sites. The paired-electron crystal provides a natural description of the spin-gapped state proximate to superconductivity in many organic charge transfer solids. Pressure-induced superconductivity in these correlated-electron systems is likely a result of a transition from the \( \frac{1}{4} \)-filled band valence bond solid to a valence bond liquid.

Charge occupancies and singlet bonds for \( \kappa-(ET)_2Cu_2(CN)_3 \) in the \( T = 0 \) limit, as suggested from extension of the paired-electron crystal concept to this system.

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