Highlights
A compilation of some of the best papers published during 2012
How to submit

Submission to JPCM is via our online portal, available from iopscience.org/jpcm.

*Journal of Physics: Condensed Matter (JPCM)* covers the whole of condensed matter physics including soft condensed matter and nanostructures. Papers may report experimental, theoretical and simulation studies. To be publishable in JPCM papers must fit the scope of the journal and meet the highest scientific quality standards. In addition, they should contain significant and original new science and make a substantial advance within a particular area of condensed matter physics. Note that papers must contain fundamental condensed matter science: papers reporting methods of materials preparation or properties of materials without novel condensed matter content will not be considered.

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

As well as regular research papers the journal offers the option of fast track communications (FTCs). These short, outstanding papers report new and timely developments in condensed matter physics. These articles will be of importance to readers of JPCM, but are not expected to meet any requirement of ‘general interest’. To facilitate a fast review process, we advise authors to restrict the length of their article to eight journal pages (5000 words). Authors submitting fast track communications should provide reasons why the work is urgent and requires rapid publication. They will be refereed by a member of the Editorial Board who will check that they have the necessary urgency.

If you have any questions about submitting your next paper to the journal, please contact us at jpcm@iop.org.

To help early career researchers prepare their papers for publication, we have published a digital brochure ‘Introductory guide for authors’ available at iopscience.org/author-guide.
Welcome

Jason S Gardner
Editor-in-Chief

The papers in this collection represent just a small selection of the high quality and interesting work that has been published in the journal over the course of 2012. Papers were chosen by the editors based on a number of criteria, including referee comments, downloads from our readers and scientific impact.

This year has been another successful one for the journal. Our impact factor rose again to 2.546 reflecting the high quality of our articles. In addition, readership of the current year’s papers is at its highest ever level. JPCM boasts very fast publication times with median receipt-to-web-publication times of just 95 days for regular papers and 46 days for fast track communications (FTCs).

For 2013 we plan to expand the number of our popular collections pages. These feature a selection of the best JPCM papers in particular subject areas. Among the topics in our first set of compilations are multiferroics and frustrated magnetism.

From the Publisher

Lucy Smith
Publisher

JPCM is one of a number of IOP Publishing journals to host article level metrics. These were recently introduced and most significantly allow authors and readers to view the number of downloads a paper has received. Citation data and social networking shares are also available. The display and functionality of these article metrics will be improved and enhanced during the course of 2013 so please do visit our website to catch up with the latest developments.

We look forward to working with many of you this year and hope that you will consider JPCM for your next paper.

## Contents

<table>
<thead>
<tr>
<th>Category</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>Surface, interface and atomic-scale science</td>
<td>5</td>
</tr>
<tr>
<td>Liquids, soft matter and biological physics</td>
<td>8</td>
</tr>
<tr>
<td>Nanostructures and nanoelectronics</td>
<td>11</td>
</tr>
<tr>
<td>Solid structure and lattice dynamics</td>
<td>14</td>
</tr>
<tr>
<td>Electronic structure</td>
<td>16</td>
</tr>
<tr>
<td>Correlated electrons</td>
<td>19</td>
</tr>
<tr>
<td>Superconductors and metals</td>
<td>21</td>
</tr>
<tr>
<td>Semiconductors</td>
<td>23</td>
</tr>
<tr>
<td>Dielectrics and ferroelectrics</td>
<td>25</td>
</tr>
<tr>
<td>Magnetism and magnetic materials</td>
<td>28</td>
</tr>
<tr>
<td>Fast track communications</td>
<td>31</td>
</tr>
<tr>
<td>Topical reviews</td>
<td>35</td>
</tr>
<tr>
<td>Editorial board</td>
<td>36</td>
</tr>
<tr>
<td>Contact us</td>
<td>38</td>
</tr>
</tbody>
</table>
The preceding year has been an exciting and successful year for *Journal of Physics: Condensed Matter*. The impact factor and immediacy index have exhibited a steady increase over the last few years. The most recent impact factor (2.546) and immediacy index (0.667) are even the highest values ever.

Over the course of 2012 the surface, interface and atomic-scale science section of the journal included many outstanding fast track communications, topical reviews, regular papers and special issues covering a broad range of topics including cutting-edge developments in emerging areas such as graphene, oxide interfaces, low-dimensional electron systems and topological insulators. The papers selected as highlights here represent some of the best of those articles.

In 2013 we aim to further strengthen the position of the journal by adding more features to the journal’s website, selecting attractive and thorough topical reviews, inviting the best authors to submit their work as fast track communications to our journal and publishing a number of special issues on cutting-edge topics. For critical and thorough articles of the rapidly developing fields that constitute modern condensed matter physics we are convinced that *Journal of Physics: Condensed Matter* is, and will be, an excellent choice.

**Did you know?**

JPCM articles received 1.4 million downloads in 2012.

**E-mail alerts?**

Get the latest JPCM research sent straight to you. Sign up for free e-mail alerts at iopscience.org/jpcm.
Three-dimensional topological insulator in a magnetic field: chiral side surface states and quantized Hall conductance

Yan-Yang Zhang, Xiang-Rong Wang and X C Xie

2012 J. Phys.: Condens. Matter 24 015004

Low energy excitation of surface states of a three-dimensional topological insulator (3DTI) can be described by Dirac fermions. By using a tight-binding model, the transport properties of the surface states in a uniform magnetic field are investigated. It is found that chiral surface states parallel to the magnetic field are responsible for the quantized Hall (QH) conductance \((2n + 1)\frac{e^2}{h}\) multiplied by the number of Dirac cones. Due to the two-dimensional nature of the surface states, the robustness of the QH conductance against impurity scattering is determined by the oddness and evenness of the Dirac cone number. An experimental setup for transport measurement is proposed.

Atomic imaging and direct phase retrieval using anomalous surface x-ray diffraction

S A Pauli, S J Leake, M Björck and P R Willmott

2012 J. Phys.: Condens. Matter 24 305002

The application of multi-wavelength anomalous diffraction to thin films, interfaces and surface structures is presented. The method directly determines the amplitudes and phases of the complex surface structure factors from surface x-ray diffraction data, measured at three different energies around the absorption edge of one of the elements present in the film. Thereby, one is able to directly Fourier transform the data, which immediately provides meaningful and unambiguous electron-density distributions. These serve as a starting point for subsequent structural refinement.

The robustness of the algorithm was evaluated on simulated data as a proof of principle. The experimental limitations and their effect on the method will be discussed as well as stability tests for the algorithm, such as the positions of the anomalous scatterers and the interfacial roughness.

It will be shown that the method can be applied to real structures. The algorithm was tested on real data from a thin film of SrTiO\(_3\) grown on NdGaO\(_3\)(110).
One-dimensional gratings evolving through high-temperature annealing: sine-generated solutions

Marcos A Madrid, Roberto C Salvarezza and Marcos F Castez

2012 J. Phys.: Condens. Matter 24 015001

Sine-generated curves (i.e. curves in which the curvature is a sine function of the arc-length parameter) have been used in the past to describe river meanders. Here we show how these curves spontaneously appear during the decay of high-aspect-ratio surfaces mediated by surface diffusion. We obtained analytical results for the kinetic evolution of such processes relevant to a wide class of initial geometries. Our theoretical results were satisfactorily compared with numerical simulations and with results from previous approaches to the same problem, and can be useful for interpreting and designing experiments related to the technologically important process of high-temperature annealing on nano/micro-structured samples.

Anchoring platinum on graphene using metallic adatoms: a first principles investigation

F G Sen, Y Qi and A T Alpas


First principles calculations based on spin-polarized density functional theory were used to identify metallic adatoms that would strengthen the Pt(111)/graphene interface (with a low work of separation of 0.009 J m⁻²), when the adatom was placed between the Pt(111) and the graphene. It was shown that the strength of the Pt–adatom bond, which had a metallic character, increased with the amount of charge transferred from the adatom to the Pt. The carbon–adatom bond, on the other hand, had a mixed ionic and covalent character and was weaker than the Pt–adatom bond for each of the 25 elements considered. Consequently, the total Pt(111)/graphene interface strength and, hence, the anchoring effect of the adatom were controlled by the carbon–adatom bond strength. Metals with unfilled \( d \) orbitals increased the Pt/graphene interface strength to above 0.5 J m⁻². The carbon–adatom bond strength was proportional to the ratio between the charge transferred from the adatom to the graphene (\( \Delta Z^p \)) and the charge transferred to the Pt surface (\( \Delta Z^p \)); i.e., the \( \Delta Z^p / \Delta Z^p \) ratio defined the ability of an adatom to anchor Pt to graphene. For Ir, Os, Ru, Rh and Re, \( \Delta Z^p / \Delta Z^p > 1.0 \), making these elements the most effective adatoms for anchoring Pt to graphene.
This New Year brings JPCM readers a new Section Editor for liquids, soft matter and biological physics. I am really pleased to serve a journal that, while duly addressing specialized topics, does not give up its standing as a common reference for the whole condensed matter community.

The four papers we selected among the most downloaded in 2012 are a manifest example of the wide range of topics covered by our journal.

• The investigation of the equilibrium concentration profile induced by gravity can provide, in a single measurement, the whole equation of state of a colloidal fluid. The paper by Luigjes et al is a first attempt to perform such a measurement on a suspension of particles interacting via magnetic dipole forces.

• Confining a liquid generates new theoretically challenging effects that are of primary interest for nanofluidics. The experimental study of thin polymer liquid films by Bäumchen et al provides novel clues on interfacial boundary conditions and on the dynamics of dewetting in macromolecular fluids.

• When surrounded by a viscoelastic liquid, molecular motors may perform very differently as well. A theoretical model by Nam and Epureanu shows, for instance, that the mobility of kinesin in the macromolecular crowding of the cytoplasm may show very distinctive features.

• Active motion is also the subject of the numerical simulations by Costanzo et al concerning the behavior of self-propelled organisms in micro-channel flow, where several fascinating effects, such as upstream swimming or aggregation near the channel walls, are extensively scrutinized.

**Did you know?**
JPCM is indexed in PubMed. Biomedical papers are also indexed and included in Medline.

**Did you know?**
JPCM’s impact factor is 2.546*

*As listed in 2011 Journal Science Citation reports (Thomson Reuters 2012)*.
Transport of self-propelling bacteria in micro-channel flow

A Costanzo, R Di Leonardo, G Ruocco and L Angelani

2012 J. Phys.: Condens. Matter 24 065101

Understanding the collective motion of self-propelling organisms in confined geometries, such as that of narrow channels, is of great theoretical and practical importance. By means of numerical simulations we study the motion of model bacteria in 2D channels under different flow conditions: fluid at rest, steady and unsteady flow. We find aggregation of bacteria near the channel walls and, in the presence of external flow, also upstream swimming, which turns out to be a very robust result. Detailed analysis of bacterial velocity and orientation fields allows us to quantify the phenomenon by varying cell density, channel width and fluid velocity. The tumbling mechanism turns out to have strong influence on velocity profiles and particle flow, resulting in a net upstream flow in the case of non-tumbling organisms. Finally we demonstrate that upstream flow can be enhanced by a suitable choice of unsteady flow pattern.

The effects of viscoelastic fluid on kinesin transport

Woochul Nam and Bogdan I Epureanu

2012 J. Phys.: Condens. Matter 24 375103

Kinesins are molecular motors which transport various cargoes in the cytoplasm of cells and are involved in cell division. Previous models for kinesins have only targeted their in vitro motion. Thus, their applicability is limited to kinesin moving in a fluid with low viscosity. However, highly viscoelastic fluids have considerable effects on the movement of kinesin. For example, the high viscosity modifies the relation between the load and the speed of kinesin. While the velocity of kinesin has a nonlinear dependence with respect to the load in environments with low viscosity, highly viscous forces change that behavior. Also, the elastic nature of the fluid changes the velocity of kinesin. The new mechanistic model described in this paper considers the viscoelasticity of the fluid using subdiffusion. The approach is based on a generalized Langevin equation and fractional Brownian motion. Results show that a single kinesin has a maximum velocity when the ratio between the viscosity and elasticity is about 0.5. Additionally, the new model is able to capture the transient dynamics, which allows the prediction of the motion of kinesin under time varying loads.
LIQUIDS, SOFT MATTER AND BIOLOGICAL PHYSICS

Sedimentation equilibria of ferrofluids: I. Analytical centrifugation in ultrathin glass capillaries

Bob Luigjes, Dominique M E Thies-Weesie, Albert P Philipse and Ben H Erné

2012 J. Phys.: Condens. Matter 24 245103

Analytical centrifugation is used for the first time to measure sedimentation equilibrium concentration profiles of a ferrofluid, a concentrated colloidal dispersion of strongly absorbing magnetic nanoparticles. To keep the optical absorbance from becoming too strong, the optical path length is restricted to 50 μm by placing the dispersion in a flat glass capillary. The concentration profile is kept from becoming too steep, despite the relatively high buoyant mass of the nanoparticles, by making novel use of a low-velocity analytical centrifuge that was not designed to measure equilibrium profiles. The experimental approach is validated by comparison with profiles obtained using an analytical ultracentrifuge. At concentrations of a few hundred grams per liter, the osmotic pressures calculated from the equilibrium profiles are lower than expected for hard spheres or non-interacting particles, due to magnetic dipolar interactions. By following the presented experimental approach, it will now also be possible to characterize the interparticle interactions of other strongly absorbing colloidal particles not studied before by analytical centrifugation.

Slippage and nanorheology of thin liquid polymer films

Oliver Bäumchen, Renate Fetzer, Mischa Klos, Matthias Lessel, Ludovic Marquant, Hendrik Hähl and Karin Jacobs

2012 J. Phys.: Condens. Matter 24 325102

Thin liquid films on surfaces are part of our everyday life; they serve, e.g., as coatings or lubricants. The stability of a thin layer is governed by interfacial forces, described by the effective interface potential, and has been the subject of many studies in recent decades. In recent years, the dynamics of thin liquid films has come into focus since results on the reduction of the glass transition temperature raised new questions on the behavior of especially polymeric liquids in confined geometries. The new focus was fired by theoretical models that proposed significant implication of the boundary condition at the solid/liquid interface on the dynamics of dewetting and the form of a liquid front. Our study reflects these recent developments and adds new experimental data to corroborate the theoretical models. To probe the solid/liquid boundary condition experimentally, different methods are possible, each bearing advantages and disadvantages, which will be discussed.
Nanostructures and nanoelectronics

This section provides a venue for papers in the field of nanoscience reporting novel fundamental physics phenomena. Many papers also relate this fundamental work to applications and devices.

The journal has a strong history in the field of nanostructures and nanoelectronics. A wealth of regular papers were published during the course of 2012 and special issues on ‘domain wall dynamics in nanostructures’ (iopscience.org/jpcm/domain-wall-dynamics) and ‘ultrathin layers of graphene, h-BN and other honeycomb structures’ (iopscience.org/jpcm/ultrathin-graphene) proved popular with readers.

Look out for our nanoscience-related special issues in 2013, including ultrafast and nonlinear optics in carbon nanomaterials.

---

Large RF susceptibility of transverse domain walls

O Rousseau, S Petit-Watelot and M Viret

2012 J. Phys.: Condens. Matter 24 024211

Changes in domain wall resistance under radio-frequency (RF) irradiation are experimentally studied for transverse walls. An original experimental technique is applied to the measurement in a permalloy nano-stripe with a notch, where the walls are found to provide a largely enhanced resistive response as compared to saturated domains. Their susceptibility is found to be an order of magnitude larger than that of the domains in a frequency range between 5 and 20 GHz. We argue that the RF fields induce an internal distortion of the magnetization profile that depends on the shape of the domain wall.
Roles of the magnetic field and electric current in thermally activated domain wall motion in a submicrometer magnetic strip with perpendicular magnetic anisotropy

Satoru Emori and Geoffrey S D Beach

2012 J. Phys.: Condens. Matter 24 024214

We have experimentally studied micrometer-scale domain wall (DW) motion driven by a magnetic field and an electric current in a Co/Pt multilayer strip with perpendicular magnetic anisotropy. The thermal activation energy for DW motion, along with its scaling with the driving field and current, has been extracted directly from the temperature dependence of the DW velocity. The injection of DC current resulted in an enhancement of the DW velocity independent of the current polarity, but produced no measurable change in the activation energy barrier. Through this analysis, the observed current-induced DW velocity enhancement can be entirely and unambiguously attributed to Joule heating.

Bilayer graphene on h-BN substrate: investigating the breakdown voltage and tuning the bandgap by electric field

José Eduardo Padilha, Renato Borges Pontes and Adalberto Fazzio

2012 J. Phys.: Condens. Matter 24 075301

By performing density functional theory calculations we show that it is possible to make the electronic bandgap in bilayer graphene supported on hexagonal boron nitride (h-BN) substrates tunable. We also show that, under applied electric fields, it is possible to insert states from h-BN into the bandgap, which generates a conduction channel through the substrate making the system metallic. In addition, we verify that the breakdown voltage strongly depends on the number of h-BN layers. We also show that both the breakdown voltage and the bandgap tuning are independent of the h-BN stacking order.
NANOSTRUCTURES AND NANOELECTRONICS

Graphene-based one-dimensional photonic crystal

Oleg L Berman and Roman Ya Kezerashvili

2012 J. Phys.: Condens. Matter 24 015305

A novel type of one-dimensional (1D) photonic crystal formed by an array of periodically located stacks of alternating graphene and dielectric stripes embedded into a background dielectric medium is proposed. The wave equation for the electromagnetic wave propagating in such a structure is solved in the framework of the Kronig–Penney model. The frequency band structure of the 1D graphene-based photonic crystal is obtained analytically as a function of the filling factor and the thickness of the dielectric between the graphene stripes. The photonic frequency corresponding to the electromagnetic wave localized by a defect of the photonic crystal formed by an extra dielectric placed in the position of one stack of alternating graphene and dielectric stripes is obtained.

Back-to-back Schottky diodes: the generalization of the diode theory in analysis and extraction of electrical parameters of nanodevices

Adenilson J Chiquito, Cleber A Amorim, Olivia M Berengue, Luana S Araujo, Eric P Bernardo and Edson R Leite

2012 J. Phys.: Condens. Matter 24 225303

We report on the analysis of nonlinear current–voltage characteristics exhibited by a set of blocking metal/SnO₂/metal. Schottky barrier heights in both interfaces were independently extracted and their dependence on the metal work function was analyzed. The disorder-induced interface states effectively pinned the Fermi level at the SnO₂ surface, leading to the observed Schottky barriers. The model is useful for any two-terminal device which cannot be described by a conventional diode configuration.
Understanding of the structure of solids and lattice dynamics is important for many branches of solid state physics as well as earth and mineral sciences.

This section reports experimental, theoretical and simulation studies of the structural, mechanical and thermal properties of solids. The three papers selected here represent just some of the high quality work published during 2012. Lee et al have developed two new modified embedded-atom potentials for elemental iron which offer an advance on existing potentials. De Koker has studied the melting of cubic BN at high pressures via first-principles molecular dynamics. Finally, Abd el All et al performed an EXAFS study of CdTe.

### Atomistic modeling of thermodynamic equilibrium and polymorphism of iron

**Tongsik Lee, Michael I Baskes, Steven M Valone and J D Doll**

2012 *J. Phys.: Condens. Matter* **24** 225404

We develop two new modified embedded-atom method (MEAM) potentials for elemental iron, intended to reproduce the experimental phase stability with respect to both temperature and pressure. These simple interatomic potentials are fitted to a wide variety of material properties of bcc iron in close agreement with experiments. Performance at finite temperatures of these models has also been examined using Monte Carlo simulations. We attempt to reproduce the experimental iron polymorphism at finite temperature similar to the procedure previously pursued by Müller et al (2007 *J. Phys.: Condens. Matter* **19** 326220), and re-examine the adequacy of the conclusion drawn in the study. The MEAM potentials developed in this study correctly predict the self-interstitial in the $\langle 110 \rangle$ orientation to be the most stable configuration, and the screw dislocation to have a non-degenerate core structure, in contrast to many embedded-atom method potentials for bcc iron in the literature.
Melting of cubic boron nitride at extreme pressures

Nico de Koker

2012 J. Phys.: Condens. Matter 24 055401

Due to its large pressure range of stability and inert nature, cubic boron nitride has been proposed as a potential pressure standard for high pressure experiments. It is extremely refractive upon compression, although its melting temperature is not known beyond 10 GPa. We apply first-principles molecular dynamics to evaluate the thermodynamics of zincblende structured (cubic) and liquid boron nitride at extreme temperatures and pressures, and compute the melting curve up to 1 TPa by integration of the Clapeyron equation. The resulting equations of state reveal that liquid boron nitride becomes denser than the solid phase at pressures of around 0.5 TPa. This is expressed as a turnover in the melting curve, which reaches a maximum at 510 GPa and 6550 ± 700 K. The origin of this density crossover is explained in terms of the underlying liquid structure, which diverges from that of the zincblende structured solid as the phases are compressed.

Negative thermal expansion in crystals with the zincblende structure: an EXAFS study of CdTe

N Abd el All, G Dalba, D Diop, P Fornasini, R Grisenti, O Mathon, F Rocca, B Thiodjio Sendja and M Vaccari

2012 J. Phys.: Condens. Matter 24 115403

The extended x-ray absorption fine structure (EXAFS) has been measured at both the K edges of cadmium and tellurium in CdTe, from liquid helium to room temperature, in order to investigate the local thermodynamic behaviour. The temperature dependences of the structural parameters obtained from the separate analysis of the two edges are perfectly consistent. The positive contribution to the thermal expansion due to the bond stretching and the negative contribution due to the tension effects are disentangled and quantified in terms of the bond thermal expansion and the perpendicular mean square relative displacement. The comparison with previous EXAFS results for Ge and CuCl shows that relevant correlations can be established between a number of local parameters measured by means of EXAFS and the properties of the lattice negative thermal expansion of tetrahedrally bonded semiconductors.
Throughout its history JPCM has published key papers which have contributed significantly to the development of electronic structure theory.

In 1994 Kresse and Hafner published their work on norm-conserving and ultrasoft pseudopotentials and the journal has continued to be a venue for seminal works in the field, as evidenced by the reports on CASTEP and SIESTA, and, more recently, QUANTUM ESPRESSO, all of which are available from iopscience.org/jpcm.

The four papers selected below are superb examples of the application of electronic structure codes to materials of great current interest. The papers shed further light on the properties of the topological insulator Bi$_2$Te$_2$Se, superhard F-carbon and TiO$_2$.
ELECTRONIC STRUCTURE

Improved semiconductor lattice parameters and band gaps from a middle-range screened hybrid exchange functional

M J Lucero, T M Henderson and G E Scuseria

2012 J. Phys.: Condens. Matter 24 145504

We show that the middle-range exchange–correlation hybrid of Henderson, Izmaylov, Scuseria and Savin (HISS) performs extremely well for elemental and binary semiconductors with narrow or visible spectrum band gaps, as well as some wider gap or more ionic systems used in devices. The lattice parameters are superior to those predicted by the screened hybrid functional of Heyd, Scuseria and Ernzerhof (HSE), and provide a significant improvement over the geometries predicted by typical semilocal functionals, yielding results competitive with PBEsol, which was specially tuned for solids. HISS also yields band gaps superior to those produced by functionals developed specifically for the solid state. Timings indicate that HISS is more computationally efficient than HSE, implying that the high quality lattice constants coupled with improved optical band gap predictions render HISS a useful adjunct to HSE in the modeling of geometry-sensitive semiconductors.

The electronic structure and optical response of rutile, anatase and brookite TiO₂

M Landmann, E Rauls and W G Schmidt

2012 J. Phys.: Condens. Matter 24 195503

In this study, we present a combined density functional theory and many-body perturbation theory study on the electronic and optical properties of TiO₂ brookite as well as the tetragonal phases rutile and anatase. The electronic structure and linear optical response have been calculated from the Kohn–Sham band structure, applying (semi)local as well as nonlocal screened hybrid exchange–correlation density functionals. Single-particle excitations are treated within the GW approximation for independent quasiparticles. On this methodological basis, gap data and optical spectra for the three major phases of TiO₂ are provided. The common characteristics of brookite with the rutile and anatase phases, which have been discussed more comprehensively in the literature, are highlighted. Furthermore, comparison of the present calculations with measured optical response data of rutile indicates that discrepancies discussed in numerous earlier studies are due to the measurements rather than related to an insufficient theoretical description.
**ELECTRONIC STRUCTURE**

**Robust surface state of intrinsic topological insulator Bi$_2$Te$_2$Se thin films: a first-principles study**

Xian-Qi Dai, Bao Zhao, Jian-Hua Zhao, Yan-Hui Li, Ya-Nan Tang and Ning Li

2012 *J. Phys.: Condens. Matter* **24** 035502

Bi$_2$Te$_2$Se, a ternary tetradymite compound, has recently been identified as a three-dimensional topological insulator. In this paper, we theoretically study the electronic structures of bulk and thin films of Bi$_2$Te$_2$Se employing spin–orbit coupling (SOC) self-consistently with density-functional theory. It is found that SOC plays an important role in determining the electronic properties of Bi$_2$Te$_2$Se. A finite bandgap opens up in the surface states of Bi$_2$Te$_2$Se thin films due to the hybridization of the top and bottom surface states of films. The intrinsic Bi$_2$Te$_2$Se thin films of three or more quintuple layers exhibit a robust topological nature of electronic structure with the Fermi energy intersecting the Dirac cone of the surface states only once between time-reversal-invariant momenta. These characteristics of Bi$_2$Te$_2$Se are similar to the topological behavior of Bi$_2$Te$_3$, promising a variety of potential applications in nanoelectronics and spintronics.

**Superhard F-carbon predicted by ab initio particle-swarm optimization methodology**

Fei Tian, Xiao Dong, Zhisheng Zhao, Julong He and Hui-Tian Wang


A simple (5 + 6 + 7)–sp$^3$ carbon (F-carbon) with eight atoms per unit cell predicted by a newly developed *ab initio* particle-swarm optimization methodology on crystal structure prediction is proposed. F-carbon can be seen as the reconstruction of AA-stacked or 3R-graphite, and is energetically more stable than 2H-graphite beyond 13.9 GPa. Band structure and hardness calculations indicate that F-carbon is a transparent superhard carbon with a gap of 4.55 eV at 15 GPa and a hardness of 93.9 GPa at zero pressure. Compared with the previously proposed Bct-, M- and W-carbons, the simulative x-ray diffraction pattern of F-carbon also well matches the superhard intermediate phase of the experimentally cold-compressed graphite. The possible transition route and energy barrier were observed using the variable cell nudged elastic band method. Our simulations show that the cold compression of graphite can produce some reversible metastable carbons with energy barriers close to diamond or lonsdaleite.
Correlated electrons

A number of special issues related to the field of strongly correlated materials are planned for publication in 2013.

These issues include:
- correlation and many-body effects at surfaces
- condensed matter analogues of cosmology
- rare-earth replacement permanent magnets

Keep an eye on our homepage iopscience.org/jpcm for the release of these special issues and other regular correlated electron content.

A self-consistent DFT + DMFT scheme in the projector augmented wave method: applications to cerium, Ce$_2$O$_3$ and Pu$_2$O$_3$ with the Hubbard I solver and comparison to DFT + U

B Amadon

2012 J. Phys.: Condens. Matter 24 075604

An implementation of full self-consistency over the electronic density in the DFT + DMFT framework on the basis of a plane wave–projector augmented wave (PAW) DFT code is presented. It allows for an accurate calculation of the total energy in DFT + DMFT within a plane wave approach. In contrast to frameworks based on the maximally localized Wannier function, the method is easily applied to f electron systems, such as cerium, cerium oxide (Ce$_2$O$_3$) and plutonium oxide (Pu$_2$O$_3$). In order to obtain a correct and physical calculation of the energy terms, we find that the calculation of the self-consistent density is mandatory. The formalism is general and does not depend on the method used to solve the impurity model. Calculations are carried out within the Hubbard I approximation, which is fast to solve, and gives a good description of strongly correlated insulators. We compare the DFT + DMFT and DFT + $U$ solutions, and underline the qualitative differences of their converged densities. We emphasize that in contrast to DFT + $U$, DFT + DMFT does not break the spin and orbital symmetry. As a consequence, DFT + DMFT implies, on top of a better physical description of correlated metals and insulators, a reduced occurrence of unphysical metastable solutions in correlated insulators in comparison to DFT + $U$. 
CORRELATED ELECTRONS

High pressure transport properties of the topological insulator Bi$_2$Se$_3$

J J Hamlin, J R Jeffries, N P Butch, P Syers, D A Zocco, S T Weir, Y K Vohra, J Paglione and M B Maple

We report x-ray diffraction, electrical resistivity, and magnetoresistance measurements on Bi$_2$Se$_3$ under high pressure and low temperature conditions. Pressure induces profound changes in both the room temperature value of the electrical resistivity as well as the temperature dependence of the resistivity. Initially, pressure drives Bi$_2$Se$_3$ toward increasingly insulating behavior and then, at higher pressures, the sample appears to enter a fully metallic state coincident with a change in the crystal structure. Within the low pressure phase, Bi$_2$Se$_3$ exhibits an unusual field dependence of the transverse magnetoresistance $\Delta \rho_{xx}$ that is positive at low fields and becomes negative at higher fields. Our results demonstrate that pressures below 8 GPa provide a non-chemical means to controllably reduce the bulk conductivity of Bi$_2$Se$_3$.

Single crystal study of the heavy-fermion antiferromagnet CePt$_2$In$_7$

Paul H Tobash, F Ronning, J D Thompson, B L Scott, P J W Moll, B Batlogg and E D Bauer

We report the synthesis, structure, and physical properties of single crystals of CePt$_2$In$_7$. Single crystal x-ray diffraction analysis confirms the tetragonal $I4/mmm$ structure of CePt$_2$In$_7$, with unit cell parameters $a = 4.5886(6)$ Å, $c = 21.530(6)$ Å and $V = 453.32(14)$ Å$^3$. The magnetic susceptibility, heat capacity, Hall effect and electrical resistivity measurements are all consistent with CePt$_2$In$_7$ undergoing an antiferromagnetic order transition at $T_N = 5.5$ K, which is field independent up to 9 T. Above $T_N$, the Sommerfeld coefficient of specific heat is $\gamma \approx 300$ mJ mol$^{-1}$ K$^{-2}$, which is characteristic of an enhanced effective mass of itinerant charge carriers. The electrical resistivity is typical of heavy-fermion behavior and gives a residual resistivity $\rho_0 \sim 0.2 \mu\Omega$ cm, indicating good crystal quality. CePt$_2$In$_7$ also shows moderate anisotropy of the physical properties that is comparable to structurally related CeMIn$_5$ (M = Co, Rh, Ir) heavy-fermion superconductors.
Superconductors and metals

A century after the discovery of superconductivity, the field remains incredibly active with the emergence of new materials continuing to drive progress.

The pages of this section have been dominated by iron-based superconductors for the past few years. The papers selected for the highlights this year prove that there are a wealth of different superconducting materials which are of great interest to the community. Zhang et al explore phase transitions and superconductivity of platinum hydride under pressure using DFT. Casaca et al study the transport properties of CuS single crystals via electrical resistivity, transverse magnetoresistance and thermoelectric power measurements. Zaleski-Ejgierd et al present an observation of the formation of WHn under pressure.

Electrical transport properties of CuS single crystals

A Casaca, E B Lopes, A P Gonçalves and M Almeida

2012 J. Phys.: Condens. Matter 24 015701

Electrical resistivity, transverse magnetoresistance and thermoelectric power measurements were performed on CuS high quality single crystals in the range 1.2–300 K and under fields of up to 16 T. The zero field resistivity data are well described below 55 K by a quasi-2D model, consistent with a carrier confinement at lower temperatures, before the transition to the superconducting state. The transverse magnetoresistance develops mainly below 30 K and attains values as large as 470% for a 16 T field at 5 K, this behaviour being ascribed to a band effect mechanism, with a possible magnetic field induced DOS change at the Fermi level. The transverse magnetoresistance shows no signs of saturation, following a power law with field $\Delta \rho/\rho(0) \propto H^{1.4}$, suggesting the existence of open orbits for carriers at the Fermi surface. The thermoelectric power shows an unusual temperature dependence, probably as a result of the complex band structure of CuS.
Phase transitions and electron–phonon coupling in platinum hydride

Chao Zhang, Xiao-Jia Chen and Hai-Qing Lin

2012 J. Phys.: Condens. Matter 24 035701

Structural phase transitions and superconducting properties of platinum hydride under pressure are explored through first-principles calculations based on density functional theory. Three new low-pressure phases (Pm̅3m, Cmmm and P4/nmm) are predicted, and all of them are metallic and stable relative to the decomposed cases. The superconducting critical temperature of the two high-pressure phases correlates with the electron–phonon coupling. The presence of soft modes induced by Kohn anomalies and the hybridization between H and Pt atoms result in the strong electron–phonon coupling. Our results have major implications for other transition metal hydrides under pressure.

WH_n under pressure

Patryk Zaleski-Ejgierd, Vanessa Labet, Timothy A Strobel, Roald Hoffmann and N W Ashcroft

2012 J. Phys.: Condens. Matter 24 155701

An initial observation of the formation of WH under pressure from W gaskets surrounding hydrogen in diamond anvil cells led to a theoretical study of tungsten hydride phases. At \( P = 1 \) atm no stoichiometry is found to be stable with respect to separation into the elements, but as the pressure is raised \( WH_n (n = 1–6, 8) \) stoichiometries are metastable or stable. WH and \( WH_4 \) are calculated to be stable at \( P > 15 \) GPa, \( WH_2 \) becomes stable at \( P > 100 \) GPa and \( WH_6 \) at \( P > 150 \) GPa. In agreement with the experiment, the structure computed for WH is anti-NiAs. \( WH_2 \) shares with WH a hexagonal arrangement of tungsten atoms, with hydrogen atoms occupying octahedral and tetrahedral holes. Prodded by these theoretical studies, experiments were then undertaken to seek phases other than WH, exploring a variety of experimental conditions that would favor further reaction.
Semiconductors

Studies on bulk semiconductors, semiconductor surfaces and microstructures are covered in this section of the journal. Papers have been published on a wide variety of topics including LEDs and photovoltaics, plasmonics and metamaterials, and topological insulators. Reports into the electronic and structural properties of these materials also feature strongly.

Papers from JPCM’s semiconductors section are included in the IOP Publishing subject collections on:
- graphene [iopscience.org/graphene]
- semiconductors [iopscience.org/semiconductors]

As well as these webpage compilations, brochures may be found at relevant conferences this year.

The four papers selected for this highlights collection represent some of the best papers published during the course of 2012 and demonstrate the diversity of research in this field.

**Signatures of $\Gamma_1 - \Gamma_5$ mixed-mode polaritons in polarized reflectance spectra of ZnO**

Ayako Takagi, Atsushi Nakamura, Akira Yoshikaie, So-ichiro Yoshioka, Satoru Adachi, Shigefusa F Chichibu and Takayuki Sota

2012 J. Phys.: Condens. Matter 24 415801

Theoretical and experimental studies were carried out on exciton-polaritons excited in ZnO. Polaritons in which both $\Gamma_1$ and $\Gamma_5$ excitons couple to electromagnetic waves simultaneously are shown to exist, and their signatures are observed in polarized reflectance spectra measured under $k \perp a$ and $E \parallel c$ configurations for an $m$-plane sample.

Theoretical calculations reveal that the mixed-mode polaritons consist of one $\Gamma_1$ transverse mode and two $\Gamma_5$ longitudinal modes. It is also shown that the signatures are sensitive to the valence band ordering.
Amorphous Ge$_{15}$Te$_{85}$: density functional, high-energy x-ray and neutron diffraction study

J Kalikka, J Akola, R O Jones, S Kohara and T Usuki

2012 J. Phys.: Condens. Matter 24 015802

The structure and electronic properties of amorphous Ge$_{15}$Te$_{85}$ have been studied by combining density functional (DF) simulations with high-energy x-ray and neutron diffraction measurements. Three models with 560 atoms have been constructed using reverse Monte Carlo methods constrained to (1) agree with the experimental structure factors $S(Q)$, and have (2) energies close to the DF minimum and (3) a semiconducting band structure. The best structure is based on the melt-quenched DF structure and has a small number of Ge–Ge bonds. It shows interlocking networks of Te and GeTe with a significant fraction (22–24%) of voids (cavities). Ge occurs with both tetrahedral and $3 + 3$ defective octahedral configurations, and the coordination of Te is slightly higher than indicated by the ‘8 – $N$ rule’ ($N$ is the number of valence electrons).

Current transport across the pentacene/CVD-grown graphene interface for diode applications

K Berke, S Tongay, M A McCarthy, A G Rinzler, B R Appleton and A F Hebard

2012 J. Phys.: Condens. Matter 24 255802

We investigate the electronic transport properties across the pentacene/graphene interface. Current transport across the pentacene/graphene interface is found to be strikingly different from transport across pentacene/HOPG and pentacene/Cu interfaces. At low voltages, diodes using graphene as a bottom electrode display Poole–Frenkel emission, while diodes with HOPG and Cu electrodes are dominated by thermionic emission. At high voltages conduction is dominated by Poole–Frenkel emission for all three junctions. We propose that current across these interfaces can be accurately modeled by a combination of thermionic and Poole–Frenkel emission. The results presented not only suggest that graphene provides low resistive contacts to pentacene where a flat-laying orientation of pentacene and transparent metal electrodes are desired, but also provides further understanding of the physics at the organic semiconductor/graphene interface.
Dielectrics and ferroelectrics

Look out for the launch of the JPCM multiferroics collection webpage that aims to provide a history of the seminal works published in the journal from 1998 onwards.

The four papers selected here provide experimental and theoretical insights into a fascinating collection of materials. Schiemer et al use a variety of techniques to study BiFeO$_3$ ceramics, looking at magnetic, mechanical and correlated electrical behaviour. Girshberg and Yacoby develop a theoretical model of the ferroelectric phase transitions of perovskite crystals under hydrostatic pressure. Sardar et al investigate the crystal structure and physical properties of multiferroic polycrystalline Ca$^{2+}$-doped BiFeO$_3$ samples, while Maczka et al report on work on lattice dynamics calculations and Raman scattering experiments on RbNbWO$_6$ and CsTaWO$_6$.

LabTalk
Find out what our authors have to say about their work at iopscience.iop.org/jpcm/labtalk

Did you know?
On average a JPCM article will be published online within 95 days of receipt. For a fast track communication this figure is just 46 days.
Temperature-dependent electrical, elastic and magnetic properties of sol–gel synthesized Bi$_{0.9}$Ln$_{0.1}$FeO$_3$ (Ln = Nd, Sm)

J Schiemer, R L Withers, M A Carpenter, Y Liu, J L Wang, L Norén, Q Li and W Hutchison

2012 J. Phys.: Condens. Matter 24 125901

This report details correlated electrical, mechanical and magnetic behaviour in BiFeO$_3$ ceramics doped with 10% Ln (Ln = Sm, Nd) ions on the Bi, or perovskite A, site and synthesized by a sol–gel method. The ceramics exhibit bulk piezoelectric and ferroelectric properties and clear ferroelectric domain patterns through piezoresponse force microscopy. Resonant ultrasound spectroscopy, dielectric spectroscopy and magnetometry studies show correlated magnetoelectromechanical behaviour and the existence of weak ferromagnetism for both compositions. An anomaly with simultaneous mechanical and magnetic signatures is discovered in both materials near room temperature, while previously reported transitions and anomalies are found to exhibit electro- and/or magnetomechanical coupling. Magnetism is significantly enhanced in the Sm doped sample, which is a promising multiferroic material.

Off-center displacements and hydrostatic pressure induced phase transition in perovskites

Y Girshberg and Y Yacoby

2012 J. Phys.: Condens. Matter 24 015901

Pressure has a profound effect on the paraelectric and ferroelectric properties of perovskite crystals. In this paper we theoretically investigate the effect of pressure on the cubic-to-tetragonal phase transition and on the soft mode dynamics of some classical perovskite crystals: BaTiO$_3$, PbTiO$_3$ and KNbO$_3$. We use a model consisting of three subsystems: electrons, phonons and off-center displacements treated as spins. This model accounts quantitatively for the experimentally measured nonlinear pressure dependence of the cubic-to-tetragonal phase transition temperature, up to the critical pressure where the transition temperature is zero. It also accounts quantitatively for the pressure dependence of the soft mode frequency, which is finite at the phase transition in spite of the fact that the phase transition at elevated pressures is second order, and for the pressure dependence of the electronic gap energy.
DIELECTRICS AND FERROELECTRICS

Structural, spectroscopic, magnetic and electrical characterization of Ca-doped polycrystalline bismuth ferrite, Bi$_{1-x}$Ca$_x$FeO$_{3-x/2}$ ($x \leq 0.1$)

Kripasindhu Sardar, Jiawang Hong, Gustau Catalan, P K Biswas, Martin R Lees, Richard I Walton, James F Scott and Simon A T Redfern

2012 J. Phys.: Condens. Matter 24 045905

The crystal structure and physical properties of multiferroic polycrystalline Ca$^{2+}$-doped BiFeO$_3$ samples have been investigated. The present experimental investigation suggests that Bi$_{1-x}$Ca$_x$FeO$_{3-x/2}$ ($x \leq 0.1$) can be considered as a solid solution between BiFeO$_3$ and CaFeO$_{2.5}$. For each composition, two structural phase transitions are revealed as anomalies in the variable-temperature in situ x-ray diffraction data which is consistent with the well-established high-temperature structural transformation in pure BiFeO$_3$. All compositions studied show antiferromagnetic behaviour along with a ferromagnetic component that increases with Ca$^{2+}$ doping. The resistivities of the Bi$_{1-x}$Ca$_x$FeO$_{3-x/2}$ samples at room temperature are of the order of 109 $\Omega$ cm and decrease with increasing Ca$^{2+}$ content. Arrhenius plots of the resistivity show two distinct linear regions with activation energies in the range of 0.4–0.7 and 0.03–0.16 eV. A correlation has been established between the critical temperatures associated with the structural phase transitions and the multiferroic properties.

Temperature-dependent Raman scattering study of the defect pyrochlores RbNbWO$_6$ and CsTaWO$_6$

M Maćzka, A V Knyazev, A Majchrowski, J Hanuza and S Kojima

2012 J. Phys.: Condens. Matter 24 195902

Lattice dynamics calculations and temperature-dependent Raman scattering experiments were performed on RbNbWO$_6$ and CsTaWO$_6$ pyrochlore oxides. The observed bands were assigned to the respective motions of atoms in the unit cell. The spectra showed the presence of additional Raman bands not allowed for by the Fd$ar{3}$m cubic structure. We have shown that these bands appear due to both substitutional disorder in the 16c sites and displacive disorder of the A ions. Raman studies also revealed the presence of an additional 80 cm$^{-1}$ band at room temperature for RbNbWO$_6$, not observed for CsTaWO$_6$. The presence of this band has been attributed to off-center displacement of the Nb and W ions due to structural phase transition into a tetragonal ferroelectric phase. The temperature evolution of the 80 cm$^{-1}$ band intensity revealed that it disappeared at a much higher temperature (about 650 K) than the reported phase transition temperature (about 360 K).
Magnetism and magnetic materials

Papers on magnetism and magnetic materials have traditionally featured strongly in JPCM. With such a large number of quality papers to pick from, selecting just a few for these highlights was a difficult task.

The selection here, as for the other articles in the collection, were picked on the basis of reader downloads, Board Member recommendations and referee comments.

Nechache et al report studies into Bi$_2$FeCrO$_6$ thin films and are able to explain the origins of the thickness dependence of the multiferroic properties observed. Frontzek et al present single crystal neutron diffraction measurements of multiferroic CuCrO$_2$. Carpenter et al present a simple model of macroscopic magnetic and structural order parameters with linear-quadratic coupling and test this model against experimental data for the magnetoelastic phase transitions in Fe$_{1-x}$O and MnO. Finally, Lederman et al study the magnetic anisotropy of ferromagnetic Ni, Co and Fe polycrystalline thin films grown on antiferromagnetic FeF$_2$ (110) epitaxial layers.

Did you know?
JPCM can publish open access articles under a CC-BY licence. This allows articles to be shared, adapted and made commercial use of subject to appropriate attribution.

Did you know?
If you have a high-quality short article of new and important research, you can submit this as a Fast Track Communication (FTC). All FTCs are completely free to read for one year from online publication.
MAGNETISM AND MAGNETIC MATERIALS

Multiferroic properties—structure relationships in epitaxial Bi$_2$FeCrO$_6$ thin films: recent developments

R Nechache, C Harnagea and A Pignolet

2012 J. Phys.: Condens. Matter 24 096001

We report recent developments in the growth and characterization of epitaxial Bi$_2$FeCrO$_6$ (BFCO) thin films. The body of experimental data stemming mostly from our investigations, and also considering the few available reports from other groups, allows us to explain the origin(s) of the thickness dependence of the multiferroic properties observed. A drastic reduction of the films’ magnetization is observed for film thicknesses larger than 80 nm. This decrease in magnetization is attributed to the formation of defects, such as antisites and antiphase boundaries, in the BFCO films. The change in magnetization is accompanied by a BFCO cell expansion, a consequence of the volume increase of the oxygen octahedra surrounding the Fe cations induced by the defects. BFCO films are ferroelectric for all the thicknesses investigated, ferroelectricity being only moderately affected by the film thickness.

Magnetic structure of CuCrO$_2$: a single crystal neutron diffraction study

M Frontzek, G Ehlers, A Podlesnyak, H Cao, M Matsuda, O Zaharko, N Aliouane, S Barilo and S V Shiryaev

2012 J. Phys.: Condens. Matter 24 016004

This paper presents results of a recent study of multiferroic CuCrO$_2$ by means of single crystal neutron diffraction. This system has two close magnetic phase transitions at $T_N = 24.2$ K and $T_{mf} = 23.6$ K. The low temperature magnetic structure below $T_{mf}$ is unambiguously determined to be a fully three-dimensional proper screw. Between $T_N$ and $T_{mf}$ antiferromagnetic order is found that is essentially two-dimensional. In this narrow temperature range, magnetic near neighbor correlations are still long range in the $(H,K)$ plane, whereas nearest neighbors along the L direction are uncorrelated. Thus, the multiferroic state is realized only in the low temperature three-dimensional state and not in the two-dimensional state.
A linear-quadratic order parameter coupling model for magnetoelastic phase transitions in \( \text{Fe}_{1-x}\text{O} \) and \( \text{MnO} \)

Michael A Carpenter, Zhiying Zhang and Christopher J Howard

2012 J. Phys.: Condens. Matter 24 156002

The combined structural and antiferromagnetic phase transition in wüstite, \( \text{Fe}_{1-x}\text{O} \), at the Néel temperature, \( T_N \sim 195 \text{ K} \), is treated in terms of coupling between two macroscopic order parameters related to separate discrete instabilities. These each couple with a rhombohedral shear strain to give an indirect mechanism of linear (structural)—quadratic (magnetic) coupling between them. It is proposed that, with increasing pressure, there is a crossover of instability temperatures such that the structural instability occurs first at pressures above \( \sim 13 \text{ GPa} \). This would be expected to give rise to a first-order phase transition, as appears to occur, but magnetic ordering would still occur simultaneously if the coupling is sufficiently strong. Symmetry analysis and comparison with the behaviour of \( \text{MnO} \) shows that there are a number of different possible magnetically ordered structures which could be stabilized by pressure or non-hydrostatic stress to give topologically rich phase diagrams.

Interface biquadratic coupling and magnon scattering in exchange-biased ferromagnetic thin films grown on epitaxial \( \text{FeF}_2 \)

David Lederman, Prasanta Dutta, Mohindar S Seehra and Hongtao Shi

2012 J. Phys.: Condens. Matter 24 186001

The magnetic anisotropy of ferromagnetic (FM) Ni, Co, and Fe polycrystalline thin films grown on antiferromagnetic (AF) \( \text{FeF}_2(110) \) epitaxial layers was studied, as a function of temperature, using ferromagnetic resonance. In addition to an in-plane anisotropy in the FM induced by fluctuations in the AF short-range order, a perpendicular (biquadratic) magnetic anisotropy, with an out-of-plane component, was found which increased with decreasing temperature above the AF Neél temperature \( (T_N = 78.4 \text{ K}) \). This is a surprising result given that the AF’s uniaxial anisotropy axis was in the plane of the sample, but is consistent with prior experimental and theoretical work. The resonance linewidth had a strong dependence on the direction of the external magnetic field with respect to in-plane \( \text{FeF}_2 \) crystallographic directions, consistent with interface magnon scattering due to defect-induced demagnetizing fields.
Fast track communications (FTCs) in JPCM report new and timely developments in condensed matter and are of excellent quality.

The benefits to authors of FTCs include very fast publication (average receipt-to-web publication times of 46 days), high visibility (free electronic offprints sent to researchers of the author’s choice) and extra promotion.

Quantum spin fluctuations in the spin-liquid state of Tb$_2$Ti$_2$O$_7$

Hiroshi Takatsu, Hiroaki Kadowaki, Taku J Sato, Jeffrey W Lynn, Yoshikazu Tabata, Teruo Yamazaki and Kazuyuki Matsuhira

2012 J. Phys.: Condens. Matter 24 052201

Neutron scattering experiments on a polycrystalline sample of the frustrated pyrochlore magnet Tb$_2$Ti$_2$O$_7$, which does not show any magnetic order down to 50 mK, have revealed that it shows condensation behavior below 0.4 K from a thermally fluctuating paramagnetic state to a spin-liquid ground state with quantum spin fluctuations. Energy spectra change from quasielastic scattering to a continuum with a double-peak structure at energies of 0 and 0.8 K in the spin-liquid state. Specific heat shows an anomaly at the crossover temperature.

Ferromagnetic Mn-doped Si$_{0.3}$Ge$_{0.7}$ nanodots self-assembled on Si(100)

P De Padova, B Olivieri, J-M Mariot, L Favre, I Berbezler, C Quaresima, B Paci, A Generosi, V Rossi Albertini, A Cricenti, C Ottaviani, M Luce, A M Testa, D Peddis, D Fiorani, M Scarselli, M De Crescenzi, O Heckmann, M C Richter, K Hricovini and F d’Acapito

2012 J. Phys.: Condens. Matter 24 142203

Densely packed epitaxial Mn-doped Si$_{0.3}$Ge$_{0.7}$ nanodots self-assembled on Si(100) have been obtained. Their structural properties were studied using reflection high-energy electron diffraction, energy dispersive x-ray diffraction, atomic force microscopy, extended x-ray absorption fine structure measurements and high-resolution transmission electron microscopy. Mn$_5$Ge$_1$Si$_2$ crystallites embedded in Si$_{0.3}$Ge$_{0.7}$ were found. They exhibit a ferromagnetic behaviour with a Curie temperature of about 225 K.
**Direct graphene growth on Co$_3$O$_4$(111) by molecular beam epitaxy**

Mi Zhou, Frank L Pasquale, Peter A Dowben, Alex Boosalis, Mathias Schubert, Vanya Darakchieva, Rositza Yakimova, Lingmei Kong and Jeffry A Kelber

*2012 J. Phys.: Condens. Matter* 24 072201

**IOP Fast Track Communications**

Direct growth of graphene on Co$_3$O$_4$(111) at 1000 K was achieved by molecular beam epitaxy from a graphite source. Auger spectroscopy shows a characteristic sp$^2$ carbon lineshape, at average carbon coverages from 0.4 to 3 ML. Low energy electron diffraction (LEED) indicates (111) ordering of the sp$^2$ carbon film with a lattice constant of 2.5(± 0.1) Å characteristic of graphene. Sixfold symmetry of the graphene diffraction spots is observed at 0.4, 1 and 3 ML. Core level photoemission shows a characteristically asymmetric C(1s) feature, with the expected π to π* satellite feature, but with a binding energy for the 3 ML film of 284.9(± 0.1) eV, indicative of substantial graphene-to-oxide charge transfer. The ability to grow graphene directly on magnetically and electrically polarizable substrates opens new opportunities for industrial scale development of charge- and spin-based devices.

**Chiral electrostatics breaks the mirror symmetry of DNA supercoiling**

R Cortini, D J Lee and A Kornyshev

*2012 J. Phys.: Condens. Matter* 24 162203

**IOP Fast Track Communications**

DNA supercoiling plays a fundamental role in regulating cellular activity and in the packaging of genetic material. In this communication, we analyse the effect of attractive chiral forces on the conformation of a closed circular DNA molecule, arising due to the helical patterns of charges on the DNA. We propose a model for closed loop DNA which uses the results of the recent theory of electrostatic interactions of a braid of two free-ended DNA molecules. Our model reproduces the known features of DNA supercoiling in an environment of low ionic strength. Our results also give the first plausible explanation for the occurrence of tightly interwound molecules observed in cryo-electron microscopy and atomic force microscopy in a high ionic strength environment. We suggest several new experiments to test the predictions of this theory.
Quantum critical phase and Lifshitz transition in an extended periodic Anderson model

M S Laad, S Koley and A Taraphder

2012 J. Phys.: Condens. Matter 24 232201

We study the quantum phase transition in f-electron systems as a quantum Lifshitz transition driven by selective-Mott localization in a realistic extended Anderson lattice model. Using dynamical mean-field theory (DMFT), we find that a quantum critical phase with anomalous $\omega/T$ scaling separates a heavy Landau–Fermi liquid from ordered phase(s). This non-Fermi liquid state arises from a lattice orthogonality catastrophe originating from orbital-selective Mott localization. Fermi surface reconstruction occurs via the interplay between and penetration of the Green function zeros to the poles, leading to violation of Luttinger's theorem in the strange metal. We show how this naturally leads to scale-invariant responses in transport. Thus, our work represents a specific DMFT realization of the hidden-FL and FL* theories, and holds promise for the study of ‘strange’ metal phases in quantum matter.

Strain dependence of polarization and piezoelectric response in epitaxial BiFeO$_3$ thin films


2012 J. Phys.: Condens. Matter 24 162202

Epitaxial strain has recently emerged as a powerful means to engineer the properties of ferroelectric thin films, for instance to enhance the ferroelectric Curie temperature ($T_C$) in BaTiO$_3$. However, in multiferroic BiFeO$_3$ thin films an unanticipated strain-driven decrease of $T_C$ was reported and ascribed to the peculiar competition between polar and antiferrodistortive instabilities. Here, we report a systematic characterization of the room-temperature ferroelectric and piezoelectric properties for strain levels ranging between $-2.5\%$ and $+1\%$. We find that polarization and the piezoelectric coefficient increase by about $20\%$ and $250\%$, respectively, in this strain range. These trends are well reproduced by first-principles-based techniques.
New insights into electron spin dynamics in the presence of correlated noise

S Spezia, D Persano Adorno, N Pizzolato and B Spagnolo

2012 J. Phys.: Condens. Matter 24 052204

The changes in the spin depolarization length in zinc-blende semiconductors when an external component of correlated noise is added to a static driving electric field are analyzed for different values of field strength, noise amplitude and correlation time. Our results show that, for electric field amplitudes lower than the Gunn field, the dephasing length shortens with increasing noise intensity. Moreover, a nonmonotonic behavior of spin depolarization length with the noise correlation time is found, characterized by a maximum variation for values of noise correlation time comparable with the dephasing time. Instead, in high field conditions, we find that, critically depending on the noise correlation time, external fluctuations can positively affect the relaxation length. The influence of the inclusion of the electron–electron scattering mechanism is also shown and discussed.

Vibrational spectrum of solid picene (C_{22}H_{14})


2012 J. Phys.: Condens. Matter 24 252203

Recently, Mitsuhashi et al observed superconductivity with a transition temperature up to 18 K in potassium doped picene (C_{22}H_{14}), a polycyclic aromatic hydrocarbon compound (Mitsuhashi et al 2010 Nature 464 76). Theoretical analysis indicates the importance of electron–phonon coupling in the superconducting mechanisms of these systems, with different emphasis on inter- and intra-molecular vibrations, depending on the approximations used. Here we present a combined experimental and ab initio study of the Raman and infrared spectrum of undoped solid picene, which allows us to unambiguously assign the vibrational modes. This combined study enables the identification of the modes which couple strongly to electrons and hence can play an important role in the superconducting properties of the doped samples.
Topical reviews

Topical reviews in JPCM provide an up-to-date authoritative overview on a wide variety of topics. Some highlights of 2012 are listed here.

Nano-plasmonic antennas in the near infrared regime

N Berkovitch, P Ginzburg and M Orenstein

2012 J. Phys.: Condens. Matter 24 073202

Two-dimensional phonon transport in graphene

Denis L Nika and Alexander A Balandin

2012 J. Phys.: Condens. Matter 24 233203

1D graphene-like silicon systems: silicene nano-ribbons

Paola De Padova, Paolo Perfetti, Bruno Olivieri, Claudio Quaresima, Carlo Ottaviani and Guy Le Lay

2012 J. Phys.: Condens. Matter 24 223001

Electric field control of magnetism in multiferroic heterostructures

C A F Vaz

2012 J. Phys.: Condens. Matter 24 333201

Calculation of dispersion energies

John F Dobson and Tim Gould

2012 J. Phys.: Condens. Matter 24 073201

Protein aggregation and misfolding: good or evil?

Annalisa Pastore and Pierandrea Temussi

2012 J. Phys.: Condens. Matter 24 244101
# Editorial board

**Editor-in-Chief**  
Jason S Gardner  
*NIST, Gaithersburg, USA and Indiana University, USA*

<table>
<thead>
<tr>
<th>Deputy Editors</th>
<th>Liquids, Soft Matter and Biological Physics Section Editor</th>
</tr>
</thead>
</table>
| John E Inglesfield  
*Cardiff University, UK* | Roberto Piazza  
*Politecnico di Milano, Italy* |
| Hideaki Kasai  
*Osaka University, Japan* | |

<table>
<thead>
<tr>
<th>Executive Board</th>
<th></th>
</tr>
</thead>
</table>
| Jon P Bird  
*University at Buffalo, The State University of New York, USA* | Mikhail Katsnelson  
*Radboud University Nijmegen, The Netherlands* |
| Marek Cieplak  
*Polish Academy of Science, Warsaw, Poland* | Talat S Rahman  
*University of Central Florida, Orlando, USA* |
| Peter A Dowben  
*University of Nebraska at Lincoln, USA* | Jeroen van den Brink  
*IFW Dresden, Germany* |

<table>
<thead>
<tr>
<th>Advisory Board</th>
<th></th>
</tr>
</thead>
</table>
| David Bowler  
*University College London, UK* | Renbao Liu  
*Chinese University of Hong Kong, Hong Kong* |
| Gustau Catalan  
*ICREA and CN2, Barcelona, Spain* | David Logan  
*University of Oxford, UK* |
| Pengcheng Dai  
*University of Tennessee, USA and Oak Ridge National Laboratory, USA* | Adam Micolich  
*University of New South Wales, Australia* |
| Robert A de Groot  
*Radboud University, Nijmegen, The Netherlands* | Joel Moore  
*University of California, Berkeley, USA* |
| Sudesh Kumar Dhar  
*Tata Institute of Fundamental Research, India* | Nuno M R Peres  
*Universidade do Minho, Portugal* |
| Rembert Duine  
*Universiteit Utrecht, The Netherlands* | Antonio Pires  
*Universidade Federal de Minas Gerais, Brazil* |
| James Greer  
*Tyndall National Institute, Ireland* | Thomas Pruschke  
*Goettingen University, Germany* |
| John M Gregg  
*Queen’s University Belfast, UK* | Filip Ronning  
*Los Alamos National Laboratory, USA* |
| Shuji Hasegawa  
*Tokyo University, Japan* | Kenji Sakurai  
*National Institute for Materials Science, Tsukuba, Japan* |
| Peter Holdsworth  
*École Normale Supérieure de Lyon* | Zdzislawa Szotek  
*Science and Technology Facilities Council, UK* |
| G Michael Kalvius  
*Technische Universität München, Germany* | Shin-ichi Uchida  
*University of Tokyo, Japan* |
| Akio Kimura  
*University of Hiroshima, Japan* | Yoshiaki Uesu  
*Waseda University, Japan* |
| Aristide Lemaître  
*CNRS–Laboratoire de Photonique et de Nanostructures, France* | Yayu Wang  
*Tsinghua University, China* |
Liquids, Soft Matter and Biological Physics Board

Patricia Bassereau *Institut Curie*—Section de Recherche, France
Matthias Fuchs *Universität Konstanz, Germany*
Steve Granick *University of Illinois at Urbana-Champaign, USA*
Ludger Harnau *Max-Planck-Institut für Intelligente Systeme, Germany*
Gerhard Kahl *Vienna Technical University, Austria*
Walter Kob *University of Montpellier 2, France*
Alexei A Kornyshev *Imperial College, London, UK*
Raffaele Mezzenga *Eidgenössische Technische Hochschule Zürich, Switzerland*
B Montgomery Pettitt *University of Houston, USA*
Felix Ritort *Universitat de Barcelona, Spain*
Paulo Teixeira *ISEL and Universidade de Lisboa, Portugal*
Veronique Trappe *University of Fribourg, Switzerland*
Claire Wilhelm *Université Paris Diderot, France*
Hiroshi Yokoyama *Kent State University, USA*

Surface, Interface and Atomic-Scale Science Board

Jesper Andersen *Lund University, Sweden*
Scott Chambers *Pacific Northwest National Laboratory, USA*
Pedro L De Andres *Consejo Superior de Investigaciones Científicas, Spain*
Katsuyuki Fukutani *University of Tokyo, Japan*
Thomas Greber *Zurich University, Switzerland*
Roberto Gunnela *Università di Camerino, Italy*
Markus Heyde *Fritz Haber Institut der Max Planck Gesellschaft, Germany*
Natalia Martsinovich *University of Warwick, UK*
J Enrique Ortega *Universidad del Pais Vasco, Spain*
Gianfranco Pacchioni *Università degli Studi di Milano Bicocca, Italy*
Steven Schofield *University College London, UK*
Susan Sinnott *University of Florida, USA*
Christoph Tegenkamp *Universität Hannover, Germany*
Yuanbo Zhang *Fudan University, China*
Contact us

For all enquiries regarding Journal of Physics: Condensed Matter or for further information about the journal please contact:

IOP Publishing
Temple Circus, Temple Way
Bristol BS1 6HG, UK

Tel +44 (0) 117 929 7481  fax + 44 (0) 117 929 4318
E-mail jpcm@iop.org  web iopscience.org/jpcm

JOURNAL TEAM

Our dedicated Journal of Physics: Condensed Matter team at IOP Publishing is here to ensure the peer-review and production processes run as smoothly as possible for our authors.

Publishing Editor
Caroline Andrew

Publishing Administrator
Rosalind Barret

Production Editor
Nicola Cutts

Publishing Editor
Anna Demming

Production Editor
Anna Gardiner

Publishing Administrator
Kayleigh Parsons

Publishing Editor
Philip Semple

Publisher
Lucy Smith

Senior Marketing Executive
Emma Watkins
# Reasons to submit to Journal of Physics: Condensed Matter

## 1. Readership
By submitting to *Journal of Physics: Condensed Matter*, you will benefit from the opportunity to have your work read by influential physicists worldwide. In 2012 alone, articles published in JPCM received over **1.4 million downloads**.

## 2. Fair and fast publication
Your work will be read and reviewed by our team of referees, guided by our active Editorial Board. Once received, the average time for an article to be published is just **95 days**. For fast track communication that figure is even lower, at just **46 days**.

## 3. Recognition and promotion
The JPCM team are dedicated to promoting research and researchers around the world. Articles published in the journal are available for free for the first 30 days after publication, so the research can be seen by anyone in the world. Articles are also promoted using a variety of marketing techniques, including distributing collections at conferences worldwide.

[More information at iopscience.org/jpcm](http://iopscience.org/jpcm)
We would like to thank all of our authors, referees, board members and supporters across the world for their vital contribution to the work and progress of Journal of Physics: Condensed Matter.