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Dear Colleagues,

2011 was a great year for *Journal of Physics: Condensed Matter* (JPCM), with the journal’s impact strengthening in the community and our ever-increasing readership enjoying high-quality science. In January, I took over as Editor-in-Chief from David Ferry who has steered this journal through some significant changes. I hope that throughout, and after, my tenure as Editor-in-Chief the journal will remain a place that the condensed matter community chooses to publish exciting research.

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Direct graphene growth on MgO: origin of the band gap
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2011 J. Phys.: Condens. Matter 23 072204

A 2.5 monolayer (ML) thick graphene film grown by chemical vapor deposition of thermally dissociated C₂H₄ on MgO(111), displays a significant band gap. The apparent six-fold low energy electron diffraction (LEED) pattern actually consists of two three-fold patterns with different ‘A’ and ‘B’ site diffraction intensities. Similar effects are observed for the LEED patterns of a 1 ML carbon film derived from annealing adventitious carbon on MgO(111), and for a 1.5 ML thick graphene film grown by sputter deposition on the 1 ML film. The LEED data indicate different electron densities at the A and B sites of the graphene lattice, suggesting that the observed band gap results from lifting the graphene HOMO/LUMO degeneracy at the Dirac point. The data also indicate that disparities in A site/B site LEED intensities decrease with increasing carbon overlayer thickness, suggesting that the graphene band gap size decreases with increasing number of graphene layers on MgO(111).

Plasmon electron–hole resonance in epitaxial graphene
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2011 J. Phys.: Condens. Matter 23 012001

The quasiparticle dynamics of the sheet plasmons in epitaxially grown graphene layers on SiC(0001) has been studied systematically as a function of temperature, intrinsic defects, influence of multilayers and carrier density using electron energy loss spectroscopy with high energy and momentum resolution. The opening of an inter-band decay channel appears as an anomalous kink in the plasmon dispersion which we describe as a resonance effect in the formation of electron–hole pairs. Due to the inevitable strong coupling of plasmons with single particle excitations in reduced dimensions, such signatures are generally expected.
Photonic heat transfer across an interface: thermal boundary resistance

B N J Persson¹,², A I Volokitin²,³ and H Ueba¹

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2011 J. Phys.: Condens. Matter 23 045009

We present a general theory of phononic heat transfer between two solids (or a solid and a fluid) in contact at a flat interface. We present simple analytical results which can be used to estimate the heat transfer coefficient (the inverse of which is usually called the ‘thermal boundary resistance’ or ‘Kapitza resistance’). We present numerical results for the heat transfer across solid–solid and solid–liquid He contacts, and between a membrane (graphene) and a solid substrate (amorphous SiO₂). The latter system involves the heat transfer between weakly coupled systems, and the calculated value of the heat transfer coefficient is in good agreement with the value deduced from experimental data.

Atomistic simulation of a graphene-nanoribbon–metal interconnect

A Smolyanitsky and V K Tewary

Materials Reliability Division, National Institute of Standards and Technology, Boulder, CO 80305, USA

2011 J. Phys.: Condens. Matter 23 355006

We report a molecular statics simulation of the physical processes responsible for binding and lattice distortions in a nanoscale electrical interconnect with realistic boundary conditions. The interconnect consists of a graphene ribbon interfaced with the (111) crystallographic surfaces (over 11000 atoms overall) of two nickel electrodes. We quantify the graphene lattice distortions by mapping strains, as well as out-of-plane atomic displacements on a grid, throughout the simulated interconnect. The results suggest strongly localized graphene lattice distortions at the edges and strains that do not exceed 0.5% elsewhere. Such strains are not expected to affect the electrical properties of the graphene nanoribbon interconnect.

A density functional theory study of Mn nanowires on the Si(001) surface

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The structure of experimentally observed Mn nanolines on the Si(001) surface is investigated using density functional theory (DFT) and the DFT + U method. A candidate line structure consisting of a two-atom sub-unit is proposed, based on total energy and appearance in simulated scanning tunnelling microscopy images. The electronic and magnetic properties of this structure are investigated. The atoms in the line are strongly antiferromagnetically coupled with individual Mn atoms having moments of 4 µB. The atoms in the sub-unit are seen to move further apart by 0.57 Å upon forcing ferromagnetic alignment.
Nanobubbles and micropancakes: gaseous domains on immersed substrates

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Topical Review

Surface nanobubbles and micropancakes are two recent discoveries in interfacial physics. They are nanoscopic gaseous domains that form at the solid/liquid interface. The fundamental interest focuses on the fact that they are surprisingly stable to dissolution, lasting for at least 10–11 orders of magnitude longer than the classical expectation. So far, many articles have been published that describe various different nucleation methods and 'ideal' systems and experimental techniques for nanobubble research, and we are now at the stage where we can begin to investigate the fundamental questions in detail. In this topical review, we summarize the current state of research in the field and give an overview of the partial answers that have been proposed or that can be inferred to date. We relate nanobubbles and micropancakes, and we try to build a framework within which nucleation may be understood. We also discuss evidence for and against different aspects of nanobubble stability, as well as suggesting what still needs to be done to obtain a full understanding.

Liquids, soft matter and biological physics

Structure and flow of droplets on solid surfaces

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2011 J. Phys.: Condens. Matter 23 184111

Special issue on nano- and microfluidics

The structure and flow of droplets on solid surfaces is investigated with imaging and scattering techniques and compared to simulations. To access nanostructures at the liquid–solid interface advanced scattering techniques such as grazing incidence small-angle x-ray scattering (GISAXS) with micrometer-sized beams, GISAXS and in situ imaging ellipsometry and GISAXS tomography are used. Using gold nanoparticle suspensions, structures observed in the wetting area due to deposition are probed in situ during the drying of the droplets. After drying, nanostructures in the wetting area and inside the dried droplets are monitored. In addition to drying, a macroscopic movement of droplets is caused by body forces acting on an inclined substrate. The complexity of the solid surfaces is increased from simple silicon substrates to binary polymer brushes, which undergo a switching due to the liquid in the droplet. Nanostructures introduced in the polymer brush due to the movement of droplets are observed.

Histone-based self-assembly into DNA-wrapped meso-clusters

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2011 J. Phys.: Condens. Matter 23 072206

IOP Fast Track Communications
Yielding in dense suspensions: cage, bond, and rotational confinements

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2011 J. Phys.: Condens. Matter 23 035102

The effect of weak particle anisotropy on the onset of fluidity in dense suspensions of glasses of repulsive, weakly attractive and strongly attractive spherical and dumbbell shaped particles is explored. Yield stresses are found to scale with volume fraction showing a divergence at random close packing for all systems. However the onsets of yielding in suspensions of spherical and dumbbell shaped particles are shown to display qualitatively different behaviors.Suspensions of hard spheres exhibit a single yield stress (strain) while suspensions of spheres experiencing short range attractions in dense gels display two yielding events. Double yielding occurs when attractions between particles are only a few kT and the suspensions are sufficiently dense. For dumbbell suspensions, single yielding is observed for hard dumbbell glasses in a region where the glasses are expected to be plastic while double yielding is observed when the particles are expected to have localized centers of mass and localized orientations. Double yielding is also observed for dense dumbbell suspensions that experience attractions while only single yielding events are observed in strongly attractive gels for both dumbbells and spheres. These results are discussed in the light of recent theories and simulations of mechanisms of localization in suspensions of spherical and weakly anisotropic particles.

Loop formation of microtubules during gliding at high density

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2011 J. Phys.: Condens. Matter 23 374104

Special section on cooperative dynamics

The microtubule cytoskeleton, including the associated proteins, forms a complex network essential to multiple cellular processes. Microtubule-associated motor proteins, such as kinesin-1, travel on microtubules to transport membrane bound vesicles across the crowded cell. Other motors, such as cytoplastic dynein and kinesin-5, are used to organize the cytoskeleton during mitosis. In order to understand the self-organization processes of motors on microtubules, we performed filament gliding assays with kinesin-1 motors bound to the cover glass with a high density of microtubules on the surface. To observe microtubule organization, 3% of the microtubules were fluorescently labeled to serve as tracers. We find that microtubules in these assays are not confined to two dimensions and can cross one other. This causes microtubules to align locally with a relatively short correlation length. At high density, this local alignment is enough to create ‘intersections’ of perpendicularly oriented groups of microtubules. These intersections create vortices that cause microtubules to form loops. We characterize the radius of curvature and time duration of the loops. These different behaviors give insight into how crowded conditions, such as those in the cell, might affect motor behavior and cytoskeleton organization.
The origin of the attraction between like charged hydrophobic and hydrophilic walls confining a near-critical binary aqueous mixture with ions

Faezeh Pousaneh and Alina Ciach

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The effect of ionic solute on a near-critical binary aqueous mixture confined between charged walls with different adsorption preferences is considered within a simple density functional theory. For the near-critical system containing small amounts of ions, a Landau-type functional is derived on the basis of the assumption that the correlation, \( \xi \), and the Debye screening length, \( k^{-1} \), are both much larger than the molecular size. The corresponding approximate Euler–Lagrange equations are solved analytically for ions insoluble in the organic solvent. A nontrivial concentration profile of the solvent is found near the charged hydrophobic wall as a result of the competition between the short-range attraction of the organic solvent and the electrostatic attraction of the hydrated ions. An excess of water may be present near the hydrophobic surface for some range of the surface charge \( \xi k \). As a result, the effective potential between the hydrophilic and the hydrophobic surface can be repulsive far from the critical point, then attractive and again repulsive when the critical temperature is approached, in agreement with a recent experiment (Nellen et al. 2011 Soft Matter 7 5360).

Model system consisting of water, organic liquid (for example lutidine) and ions between negatively charged hydrophilic (dark, blue) and hydrophobic (light, red) walls.

Electronic properties of corrugated graphene: the Heisenberg principle and wormhole geometry in the solid state

Victor Atanasov and Avadh Saxena

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2 Theoretical Division and Center for Nonlinear Studies, Los Alamos National Laboratory, Los Alamos, NM 87545, USA

2011 J. Phys.: Condens. Matter 23 175301

Adopting a purely two-dimensional relativistic equation for graphene’s carriers contradicts the Heisenberg uncertainty principle since it requires setting the off-the-surface coordinate of a three-dimensional wavefunction to zero. Here we present a theoretical framework for describing graphene’s massless relativistic carriers in accordance with this most fundamental of all quantum principles. A gradual confining procedure is used to restrict the dynamics onto a surface and normal to the surface parts, and in the process the embedding of this surface into the three-dimensional world is accounted for. As a result an invariant geometric potential arises in the surface part which scales linearly with the mean curvature and shifts the Fermi energy of the material proportional to bending. Strain induced modification of the electronic properties or ‘straintronics’ is clearly an important field of study in graphene. This opens an avenue to producing electronic devices: micro- and nano-electromechanical systems (MEMS and NEMS), where the electronic properties are controlled by geometric means and no additional alteration of graphene is necessary. The appearance of this geometric potential also provides us with clues as to how quantum dynamics looks in the curved space–time of general relativity. In this context we explore a two-dimensional cross-section of the wormhole geometry, realized with graphene as a solid state thought experiment.

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Melting of graphene: from two to one dimension

K V Zakharchenko, Annalisa Fasolino, J H Los and M I Katsnelson

Radboud University of Nijmegen, Institute for Molecules and Materials, Heyendaalseweg 135, 6525 AJ Nijmegen, The Netherlands


IOP Fast Track Communications

The high temperature behaviour of graphene is studied by atomistic simulations based on an accurate interatomic potential for carbon. We find that clustering of Stone–Wales defects and formation of octagons are the first steps in the process of melting which proceeds via the formation of carbon chains. The molten state forms a three-dimensional network of entangled chains rather than a simple liquid. The melting temperature estimated from the two-dimensional Lindemann criterion and from extrapolation of our simulation for different heating rates is about 4900 K.

Graphene as a non-magnetic spin current lens

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In spintronics, the ability to transport magnetic information often depends on the existence of a spin current traveling between two different magnetic objects acting as the source and probe. A large fraction of this information never reaches the probe and is lost because the spin current tends to travel omnidirectionally. We propose that a curved boundary between a gated and a non-gated region within graphene acts as an ideal lens for spin currents despite being entirely of non-magnetic nature. We show as a proof of concept that such lenses can be utilized to redirect the spin current that travels away from a source onto a focus region where a magnetic probe is located, saving a considerable fraction of the magnetic information that would be otherwise lost.

Thermal transport by phonons in zigzag graphene nanoribbons with structural defects

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The thermal transport properties by phonons in zigzag graphene nanoribbons with structural defects are investigated by using nonequilibrium phonon Green’s function formalism. We find that the combined effect of the edge and local defect plays an important role in determining the thermal transport properties. In the limit $T \to 0$, the thermal conductance approaches the universal quantum value $3\kappa_0 (\kappa_0 = \pi^2 k_B^2 T/3h)$ even when structural defects are present in graphene nanoribbons. The thermal transport shows a noticeable transformation from quantum to classical features with increasing temperature in the system. A suggestion to tune the thermal conductance by modulating structural defects and the ribbon width in graphene nanoribbons is presented.

Schematic diagram representing an infinitely large graphene sheet under the effect of a gate voltage that acts only in a limited region of space (represented by the grey area). The gated region has a boundary with a curvature defined by the radius $R$ that lies at a distance $L$ from the magnetic atoms. The section delimited by the two horizontal dotted lines is the unit cell used in representing the system with lateral periodic boundary conditions.
Electronic properties of graphene nanostructures
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In this review, recent developments in the fabrication and understanding of the electronic properties of graphene nanostructures are discussed. After a brief overview of the structure of graphene and the two-dimensional transport properties, the focus is put on graphene constrictions, quantum dots and double quantum dots. For constrictions with a width below 100 nm, the current through the constriction is strongly suppressed for a certain back gate voltage range, related to the so-called transport gap. This transport gap is due to the formation of localized puddles in the constriction, and its size depends strongly on the constriction width. Such constrictions can be used to confine charge carriers in quantum dots, leading to Coulomb blockade effects.

Correlated conformation and charge transport in multiwall carbon nanotube-conducting polymer nanocomposites
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The strikingly different charge transport behaviours in nanocomposites of multiwall carbon nanotubes (MWNTs) and conducting polymer polyethylenedioxythiophene–polystyrene-sulfonic-acid (PEDOT–PSS) at low temperatures are explained by probing their conformational properties using small-angle x-ray scattering (SAXS). The SAXS studies indicate the assembly of elongated PEDOT–PSS globules on the walls of nanotubes, coating them partially, thereby limiting the interaction between the nanotubes in the polymer matrix. This results in a charge transport governed mainly by small polarons in the conducting polymer despite the presence of metallic MWNTs. At $T > 4$ K, hopping of the charge carriers following one-dimensional variable range hopping is evident which also gives rise to a positive magnetoresistance (MR) with an enhanced localization length ($\sim 5$ nm) due to the presence of MWNTs. However, at $T < 4$ K, the observation of an unconventional positive temperature coefficient of resistivity is attributed to small polaron tunnelling. The exceptionally large negative MR observed in this temperature regime is conjectured to be due to the presence of quasi-1D MWNTs that can aid in lowering the tunnelling barrier across the nanotube–polymer boundary resulting in large delocalization.

Solid structure and lattice dynamics
Phonons in graphene with point defects
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The phonon density of states (DOS) of graphene with different types of point defects (carbon isotopes, substitution atoms, vacancies) is considered. Using a solvable model which is based on the harmonic approximation and the assumption that the elastic forces act only between nearest neighboring ions we calculate corrections to the graphene DOS dependent on the type and concentration of defects. In particular the correction due to isotopic dimers is determined. It is shown that a relatively small concentration of defects may lead to significant and specific changes in the DOS, especially at low frequencies, near the Van Hove points and in the vicinity of the K points of the Brillouin zone. In some cases defects generate one or several narrow gaps near the critical points of the phonon DOS as well as resonance states in the Brillouin zone regular points. All types of defects are characterized by the appearance of one or more additional Van Hove peaks near the (Dirac) K points and their singular contribution may be comparable with the effect of electron–phonon interaction. Besides, for low frequencies and near the critical points the relative change in density of states may be many times higher than the concentration of defects.
Probing the continuous radio frequency spectrum of water relaxation using a carbon nanotube

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First-principles study on thermodynamic properties and phase transitions in TiS2

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Structural and vibrational properties of TiS2 with the CdI2 structure have been studied to high pressures from density functional calculations with the local density approximation (LDA). The calculated axial compressibility of the CdI2-type phase agrees well with experimental data and is typical of layered transition-metal dichalcogenides. The obtained phonon dispersions show a good correspondence with available experiments. A phonon anomaly is revealed at 0 GPa, but is much reduced at 20 GPa. The thermodynamic properties of this phase were also calculated at high pressures and high temperatures using the quasi-harmonic approximation. Our LDA study on the pressure-induced phase transition sequence predicts that the CdI2-type TiS2, the phase stable at ambient conditions, should transform to the cotunnite phase at 15.1 GPa, then to a tetragonal phase (I4/mmm) at 45.0 GPa. The tetragonal phase remains stable to at least 500 GPa. The existence of the tetragonal phase at high pressures is consistent with our previous findings in NiS2 (Yu and Ross 2010 J. Phys.: Condens. Matter 22 235401). The cotunnite phase, although only stable in a narrow pressure range between 15.1 and 45.0 GPa, displays the formation of a compact S network between 100 and 200 GPa, which is evidenced by a kink in the variation of unit cell lengths with pressure. The electron density analysis in cotunnite shows that valence electrons are delocalized from Ti atoms and concentrated near the S network.

The TiS2 cotunnite phase at 200 GPa calculated by the LDA: valence electron density (left), and electron localization function (right).

We have obtained the continuous radio frequency spectrum of water molecule relaxation using carbon nanotubes (CNT) as a high-speed nanoprobe. Three sets of characteristic time scales are clearly identified. Two sets are attributed to the electric-field-driven polarization of water molecules bound to CNTs and the collective relaxation of water layers in the vicinity of CNTs, respectively. The third set is appreciable only in air, and can be related to triplet oxygen relaxation.

(a) VGS – VDS characteristics obtained from our CNT field-effect transistor (shown in the inset) in air (solid lines) and in vacuum (dotted lines). VGS was fixed at 1, 3 and 5 V. (b) Schematic of the coplanar waveguide, on top of which a single CNT bridges Au electrodes. (c) Schematic of the real-time measurement circuit.

The TiS2 cotunnite phase at 200 GPa calculated by the LDA: valence electron density (left), and electron localization function (right).
Transport of massless Dirac fermions in graphene monolayers is analysed in the presence of a combination of singular magnetic barriers and applied electrostatic potential. Extending a recently proposed (Ghosh and Sharma 2009 J. Phys.: Condens. Matter 21 292204) analogy between the transmission of light through a medium with modulated refractive index and electron transmission in graphene through singular magnetic barriers to the present case, we find the addition of a scalar potential profoundly changes the transmission. We calculate the quantum version of the Goos–Hänchen shift that the electron wave suffers upon being totally reflected by such barriers. The combined electric and magnetic barriers substantially modify the band structure near the Dirac point. This affects transport near the Dirac point significantly and has important consequences for graphene-based electronics. These intersections create vortices that cause microtubules to form loops. We characterize the radius of curvature and time duration of the loops. These different behaviors give insight into how crowded conditions, such as those in the cell, might affect motor behavior and cytoskeleton organization.

Spin–orbit splitting in graphene on metallic substrates

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Substrate-induced spin–orbit splitting in graphene on Ni, Au and Ag(111) is examined on the basis of density-functional theory. The Rashba splitting of $\pi$ bands along the $M$ direction of the graphene surface Brillouin zone in graphene on Ni(111) is found to be very small (a few millielectronvolts), consistent with the experimental report of Rader I M. Instead, very strong Rashba splitting (near 100 meV) can be obtained for graphene with a certain stretch distortion on a Au substrate. It can be ascribed to the effective match in energy between the C 2p and Au 5d bands, obtained from the analysis of densities of states. The net charge transfer between the graphene and the substrates just affects the spin–orbit effect indirectly. The small spin–orbit splitting induced by the Ag substrates indicates that heavy metals do not always produce large SO splitting. Our findings provide important insights that are useful for understanding the metal-induced Rashba effect in graphene.
Zigzag graphene nanoribbons: bandgap and midgap state modulation

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We study zigzag graphene nanoribbons with periodic edge roughness and report significant band gap opening. Interestingly, such nanoribbons have a near-midgap state with a small band width. We extensively study the electronic structure and the electric-field modulation of the conduction/valence bands and the near-midgap state. We summarize the important electronic-structure features like the band gap, the band width and the effective mass. We show that by applying an external electric field in the width direction, the band width of the near-midgap state varies linearly due to the edge localization, whereas the band gap remains almost constant. Additionally, the effective mass of these states can switch polarity from negative (hole-like) to positive (carrier-like) at the \( \Gamma \)-point with the field modulation.

Electronic structure of passivated zigzag graphene nanoribbons with periodic edge roughness.

Effect of strain on the thermoelectric properties of silicon: an ab initio study

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On the basis of detailed first-principles calculations the anisotropic thermoelectric transport properties of biaxially strained silicon were studied with the focus on a possible enhancement of the power factor. Electron as well as hole doping was examined in a broad doping and temperature range. In the low temperature and low doping regime an enhancement of the power factor was obtained for compressive and tensile strain in the electron-doped case, and for compressive strain in the hole-doped case. In the thermoelectrically more important high temperature and high doping regime a slight enhancement of the power factor was only found for the hole-doped case under small biaxial tensile strain. The results are discussed in terms of band structure effects. An analytical model is presented to understand the fact that the thermopower decreases if degenerate bands are energetically lifted due to a strain-induced redistribution of states.

Electronic structure of passivated zigzag graphene nanoribbons with periodic edge roughness.

Fermi surfaces of electron-doped silicon under compressive strain (left), no strain (middle) and tensile strain (right).

Ab initio random structure searching

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Topical Review

It is essential to know the arrangement of the atoms in a material in order to compute and understand its properties. Searching for stable structures of materials using first-principles electronic structure methods, such as density-functional-theory (DFT), is a rapidly growing field. Here we describe our simple, elegant and powerful approach to searching for structures with DFT, which we call ab initio random structure searching (AIRSS). Applications to discovering the structures of solids, point defects, surfaces, and clusters are reviewed. New results for iron clusters on graphene, silicon clusters, polymeric nitrogen, hydrogen-rich lithium hydrides, and boron are presented.

Left: a structure built by placing carbon atoms randomly within a small sub-box, subject to symmetry constraints. Right: relaxation of this structure within DFT gave the well-known C60 ‘buckyball’.
Electronic structure and Jahn–Teller effect in GaN:Mn and ZnS:Cr

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We present an ab initio and analytical study of the Jahn–Teller effect in two diluted magnetic semiconductors with d³⁰ impurities, namely Mn-doped GaN and Cr-doped ZnS. We show that the correct insulating electronic structure may be obtained by a proper treatment of the strong electron correlation in the 3d shell in combination with the Jahn–Teller distortion which breaks the local symmetry. Using the LSDA + U approach, we treat the zinc-blende and the wurtzite crystal structures of GaN:Mn, as well as zinc-blende ZnS:Cr.

We show that the trigonal distortion due to the wurtzite structure is less important than the Jahn–Teller deformation. This observation allows us to construct a simplified phenomenological ligand field theory (trigonal influence is neglected) which completes the ab initio part. Our work corrects previous studies and the obtained energy gain due to the Jahn–Teller effect (from both the LSDA + U calculation and the ligand field theory) is in good agreement with the experimental data. The same is true for the complete set of crystal field parameters obtained from the phenomenological model which agrees well with previous optical measurements.

Synthesis of cubic SrCoO₃ single crystal and its anisotropic magnetic and transport properties

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A large-size single crystal of nearly stoichiometric SrCoO₃ was prepared with a two-step method combining the floating-zone technique and subsequent high oxygen pressure treatment. SrCoO₃ crystallizes in a cubic perovskite structure with space group Pm3m, and displays an itinerant ferromagnetic behavior with the Curie temperature of 305 K. The easy magnetization axis is found to be along the [111] direction, and the saturation moment is 2.5 μB/F.u., in accord with the picture of the intermediate spin state. The resistivity at low temperatures (T) is proportional to T⁵, indicative of the possible effect of orbital fluctuation in the intermediate spin ferromagnetic metallic state. Unusual anisotropic magnetoresistance is also observed and its possible origin is discussed.
Eliashberg theory of excitonic insulating transition in graphene

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A sufficiently strong Coulomb interaction may open an excitonic fermion gap and thus drive a semimetal–insulator transition in graphene. In this paper, we study the Eliashberg theory of excitonic transition by coupling the fermion gap equation self-consistently to the equation of the vacuum polarization function. Including the fermion gap into the polarization function increases the effective strength of the Coulomb interaction because it reduces the screening effects due to the collective particle–hole excitations. Although this procedure does not change the critical point, it leads to a significant enhancement of the dynamical fermion gap in the excitonic insulating phase. The validity of the Eliashberg theory is justified by showing that the vertex corrections are suppressed at the large N limit.

Effects of electronic correlation on x-ray absorption and dichroic spectra at L₂,₃ edge

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We present a new theoretical approach to describe x-ray absorption and magnetic circular dichroism spectra in the presence of electron–electron correlation. Our approach provides an unified picture to include correlations in both charged and neutral excitations, namely in direct/inversion photoemission where electrons are removed/added, and photoabsorption where electrons are promoted from core levels to empty states. We apply this approach to the prototypical case of the L₂,₃ edge of 3d transition metals and we show that the inclusion of many-body effects in the core level excitations is essential to reproduce, together with satellite structures in core level photoemission, the observed asymmetric lineshapes in x-ray absorption and dichroic spectra.
Theory of high-$T_c$ superconductivity: transition temperature

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It is demonstrated that the transition temperature ($T_c$) of high-$T_c$ superconductors is determined by their layered crystal structure, bond lengths, valency properties of the ions, and Coulomb coupling between electronic bands in adjacent, spatially separated layers. Analysis of 31 high-$T_c$ materials (cuprates, ruthenates, ruthenocuprates, iron pnictides, organics) yields the universal relationship for optimal compounds, $k_B T_c0 = \beta/\zeta$, where $\zeta$ is the distance between interacting electronic layers, $\beta$ is a universal constant and $T_c0$ is the optimal transition temperature (determined to within an uncertainty of $\pm 1.4$ K by this relationship). Non-optimum compounds, in which sample degradation is evident, e.g. by broadened superconducting transitions and diminished Meissner fractions, typically exhibit reduced $T_c < T_c0$. It is shown that $T_c0$ may be obtained from an average of the Coulomb interaction forces between the two layers.

Electronic structure of optimally doped pnictide Ba$_{0.6}$K$_{0.4}$Fe$_2$As$_2$: a comprehensive angle-resolved photoemission spectroscopy investigation

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The electronic structure of the Fe-based superconductor Ba$_{0.6}$K$_{0.4}$Fe$_2$As$_2$ is studied by means of angle-resolved photoemission. We identify dispersive bands crossing the Fermi level forming hole-like (electron-like) Fermi surfaces (FSs) around $\Gamma$ (M) with nearly nested FS pockets connected by the antiferromagnetic wavevector. Compared to band structure calculation findings, the overall bandwidth is reduced by a factor of 2 and the low energy dispersions display even stronger mass renormalization. Using an effective tight binding model, we fitted the band structure and the FSs to obtain band parameters reliable for theoretical modeling and calculation of physical quantities.
Temperature-dependent local structure of NdFeAsO$_{1-x}$F$_x$ system using arsenic K-edge extended x-ray absorption fine structure

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Local structure of NdFeAsO$_{1-x}$F$_x$ ($x = 0.0, 0.05, 0.15$ and $0.18$) high temperature iron-pnictide superconductor system is studied using arsenic K-edge extended x-ray absorption fine structure (EXAFS) measurements as a function of temperature. Fe–As bond length shows only a weak temperature and F-substitution dependence, consistent with the strong covalent nature of this bond. The temperature dependence of the mean square relative displacements of the Fe–As bond length are well described by the correlated Einstein model for all the samples, but with different Einstein temperatures for the superconducting and non-superconducting samples. The results indicate distinct local Fe–As lattice dynamics in the superconducting and non-superconducting iron-pnictide systems.

Local structural investigation of SmFeAsO$_{1-x}$F$_x$ high temperature superconductors

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A strong revitalization of the field of high temperature superconductivity (HTSC) has been induced recently by the discovery of $T_c$ around 26 K in F-doped LaFeAsO iron pnictides. Starting from this discovery, a huge amount of experimental data have been accumulated. This important corpus of results will allow the development of suitable theoretical models aimed at describing the basic electronic structure properties and nature of superconducting states in these fascinating new systems. A close correlation between structural features and physical properties of the normal and superconducting states has already been demonstrated in the current literature. Advanced theoretical models are also based on the close correlation with structural properties and in particular with the Fe–As tetrahedral array. As for other complex materials, a deeper understanding of their structure–properties correlation requires a full knowledge of the atomic arrangement within the structure. Here we report an investigation of the local structure in the SmFeAsO$_{1-x}$F$_x$ system carried out by means of x-ray total scattering measurements and pair distribution function (PDF) analysis. The results presented indicate that the local structure of these HTSC significantly differs from the average structure determined by means of traditional diffraction techniques, in particular the distribution of Fe–As bond lengths. In addition, a model for describing the observed discrepancies is presented.

Some forthcoming 2012 JPCM special issues:

- Domain wall dynamics in nanostructures
- Non-contact AFM
- Molecular switches at surfaces
- Liquid-solid interfaces
- Van der Waals interactions
- Ultrathin layers of graphene, h-BN and other honeycomb structures
Schrödinger particles on potential and size of the crystalline grains and an increased crystallization temperature. During the crystallization of the amorphous phase, resulting in a reduction in crystalline phase, though it is still possible in the amorphous phase. These results support the suggestion that N segregates at the grain boundaries contrast, insertion of N in the atomic form is very energetically costly in the both the crystalline and amorphous phases at a moderate energy cost. In addition, the path of the centre of mass of the wavepacket does not have to penetrate the barrier during the scattering process. Trembling motion of the charged particle in graphene is observed in the absence of an external magnetic field and can be enhanced by a substrate-induced mass term.

We investigated the structural, electronic and vibrational properties of amorphous and cubic Ge$_2$Sb$_2$Te$_5$ doped with N at 4.2 at.% by means of large scale ab initio simulations. Nitrogen can be incorporated in molecular form in both the crystalline and amorphous phases at a moderate energy cost. In contrast, insertion of N in the atomic form is very energetically costly in the crystalline phase, though it is still possible in the amorphous phase. These results support the suggestion that N segregates at the grain boundaries during the crystallization of the amorphous phase, resulting in a reduction in size of the crystalline grains and an increased crystallization temperature.

Representative relaxed configurations of N in interstitial sites.

Using first-principles calculations we have studied the electronic and structural properties of cation vacancies and their complexes with hydrogen impurities in SnO$_2$, In$_2$O$_3$ and β-Ga$_2$O$_3$. We find that cation vacancies have high formation energies in SnO$_2$ and In$_2$O$_3$ even in the most favorable conditions. Their formation energies are significantly lower in β-Ga$_2$O$_3$. Cation vacancies, which are compensating acceptors, strongly interact with H impurities resulting in complexes with low formation energies and large binding energies, stable up to temperatures over 730 °C. Our results indicate that hydrogen has beneficial effects on the conductivity of transparent conducting oxides: it increases the carrier concentration by acting as a donor in the form of isolated interstitials, and by passivating compensating acceptors such as cation vacancies; in addition, it potentially enhances carrier mobility by reducing the charge of negatively charged scattering centers. We have also computed vibrational frequencies associated with the isolated and complexed hydrogen, to aid in the microscopic identification of centers observed by vibrational spectroscopy.

We investigate the dynamics of a charged particle moving in a graphene layer and in a two-dimensional electron gas, where it obeys the Dirac and Schrödinger equations, respectively. The charge carriers are described as Gaussian wavepackets. The dynamics of the wavepackets is studied numerically by solving both quantum-mechanical and relativistic equations of motion. The scattering of such wavepackets by step-like magnetic and potential barriers is analysed for different values of wavepacket energy and width. We find: (1) that the average position of the wavepacket does not coincide with the classical trajectory, and (2) that, for slanted incidence, the path of the centre of mass of the wavepacket does not have to penetrate the barrier during the scattering process. Trembling motion of the charged particle in graphene is observed in the absence of an external magnetic field and can be enhanced by a substrate-induced mass term.
Dielectrics and ferroelectrics


electronic and local structures of BiFeO₃ films

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The electronic structure of BiFeO₃ (BFO), BiFeO₃–PbTiO₃ solid solution (BFO–PT), and Mn-doped BFO–PT (BFM–PT) films fabricated by chemical solution deposition was investigated by x-ray absorption fine structure (XAFS). The BiFeO₃ shows a large leakage current owing to the mixed valance state of Fe²⁺ and Fe³⁺. The BFO film has a blunt absorption edge jump indicating the charge fluctuated state of the iron ions. The BFO–PT and BFM–PT films have sharp absorption edges, and the absorption energy of these films shifted to opposite energy. The valence fluctuation of the iron ions was closely connected with the leakage current properties. The charge fluctuated BFO film showed a leaky feature, and the charge unfluctuated BFO–PT and BFM–PT films had improved leakage current properties. The valence fluctuation of the iron ions can be controlled by Mn substitution and by making solid solutions.

Nanoscale polarization switching mechanisms in multiferroic BiFeO₃ thin films

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Ferroelectric switching in BiFeO₃ multiferroic thin films was studied by piezoresponse force microscopy, as a function of the tip voltage and sweep direction, for samples with two different intrinsic domain structures. In all films, the switched polarization direction follows the in-plane and out-of-plane components of the highly inhomogeneous electric field applied by the microscope tip. In films with ‘bubble-like’ intrinsic domains, we observed in-plane switching assisted by out-of-plane switching for lower voltage values, and independent in-plane and out-of-plane switching for higher voltages, in both cases allowing full control of the ferroelectric polarization depending on the tip voltage polarity and sweep direction. In films with ‘stripe-like’ intrinsic domains, independent in-plane and out-of-plane switching was observed, but unswitched stripe domains prevented full control of the ferroelectric polarization over large areas. We correlate the observed switching behavior with the field-driven onset of a highly distorted tetragonal phase predicted by ab initio calculations, which leads to a very high in-plane susceptibility during the return to the non-distorted monoclinic phase when the field is decreased. Depending on the specific strain and disorder present in the sample, the transition towards the highly distorted phase may be asymmetrized, and easier to reach when an electric field opposite to the out-of-plane polarization direction is applied.

Special section on semiconducting oxides

We assess the thermodynamic doping limits of GaN and ZnO on the basis of point defect calculations performed using the embedded cluster approach and employing a hybrid non-local density functional for the quantum mechanical region. Within this approach we have calculated a staggered (type-II) valence band alignment between the two materials, with the N 2p states contributing to the lower ionization potential of GaN. With respect to the stability of free electron and hole carriers, redox reactions resulting in charge compensation by ionic defects are found to be largely endothermic (unfavourable) for electrons and exothermic (favourable) for holes, which is consistent with the efficacy of electron conduction in these materials. Approaches for overcoming these fundamental thermodynamic limits are discussed.

Nanoscale polarization switching mechanisms in multiferroic BiFeO₃ thin films

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Multiferroic magnetoelectric fluorides: why are there so many magnetic ferroelectrics?

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Topical Review

We review work on multiferroic magnetic fluorides with an aim to correct the popular opinion that magnetic ferroelectrics are rare in nature. After a qualitative summary describing the main families of magnetic fluorides that are piezoelectric and probably ferroelectric, we discuss in detail the most popular recent groups, namely the K3Fe5F15 and Pb5Cr3F19 families.

Evidence of orbital excitations in CaCu3Ti4O12 probed by Raman spectroscopy

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Raman scattering studies on CaCu3Ti4O12 and SrCu3Ti4O12 compounds provide evidence of the physics underlying the giant dielectric effect in the CaCu3Ti4O12 compound. The temperature, polarization, and photon energy dependence of a broad Raman mode observed at high wavenumbers below ~130 K indicates its origin from orbital excitations. The orbital order disorder transition observed around 100 K may be responsible for the conductivity changes required in the internal barrier layer capacitance model, hitherto used to explain the huge dielectric constant above 100 K in these compounds.

The giant anomalous Hall effect in the ferromagnet Fe3Sn2—a frustrated kagome metal

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The kagome-bilayer material Fe3Sn2 has recently been shown to be an example of a rare class of magnet—a frustrated ferromagnetic metal. While the magnetism of Fe3Sn2 appears to be relatively simple at high temperature, with localized moments parallel to the c-axis (Tc = 640 K), upon cooling the competing exchange interactions and spin frustration become apparent as they cause the moments to become non-collinear and to rotate towards the kagome plane, forming firstly a canted ferromagnetic structure and then a re-entrant spin glass (Tf ~ 80 K). In this work we show that Fe3Sn2 possesses an unusual anomalous Hall effect. The saturated Hall resistivity of Fe3Sn2 is 3.2 µΩ cm at 300 K, almost 20 times higher than that of typical itinerant ferromagnets such as Fe and Ni. The anomalous Hall coefficient RH is 6.7 × 10−9 Ω cm G−1 at 300 K, which is three orders of magnitude larger than that of pure Fe, and obeys an unconventional scaling with the longitudinal resistivity, RH ∝ ρxx1.5. Such a relationship cannot be explained by either the conventional skew or side-jump mechanisms, indicating that the anomalous Hall effect in Fe3Sn2 has an extraordinary origin that is presumed to be related to the underlying frustration of the magnetism. These findings demonstrate that frustrated ferromagnets, whether based on bulk materials or on artificial nanoscale structures, can provide new routes to room temperature spin-dependent electron transport properties suited to application in spintronics.

Temperature dependence of the Raman spectrum of CaCu3Ti4O12 (a) and SrCu3Ti4O12 (b) in the parallel polarization (PP) geometry, using the 488 nm laser line.
Magneto-structural properties and magnetic anisotropy of small transition-metal clusters: a first-principles study

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2011 J. Phys.: Condens. Matter 23 136001

Ab initio density-functional calculations including spin–orbit coupling (SOC) have been performed for Ni and Pd clusters with three to six atoms and for 13-atom clusters of Ni, Pd, and Pt, extending earlier calculations for Pt clusters with up to six atoms (2011 J. Chem. Phys. 134 034107). The geometric and magnetic structures have been optimized for different orientations of the magnetization with respect to the crystallographic axes of the cluster. The magnetic anisotropy energies (MAE) and the anisotropies of spin and orbital moments have been determined. Particular attention has been paid to the correlation between the geometric and magnetic structures. The magnetic point group symmetry of the clusters varies with the direction of the magnetization. Even for a 3d metal such as Ni, the change in the magnetic symmetry leads to small geometric distortions of the cluster structure, which are even more pronounced for the 4d metal Pd. For a 5d metal the SOC is strong enough to change the energetic ordering of the structural isomers. SOC leads to a mixing of the spin states corresponding to the low-energy spin isomers identified in the scalar-relativistic calculations. Spin moments are isotropic only for Ni clusters, but anisotropic for Pd and Pt clusters, orbital moments are anisotropic for the clusters of all three elements. The magnetic anisotropy energies have been calculated. The comparison between MAE and orbital anisotropy invalidates a perturbation analysis of magnetic anisotropy for these small clusters.

Absence of long-range magnetic ordering in the pyrochlore compound Er2Sn2O7

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IOP Fast Track Communications

The low temperature behaviour of powder Er2Sn2O7 samples has been studied by magnetic susceptibility, heat capacity, and neutron scattering experiments. We report here the absence of magnetic ordering down to 100 mK. Anomalies in the heat capacity can be accounted for through an analysis of the crystal field spectrum observed by inelastic neutron scattering spectroscopy. These new measurements on Er2Sn2O7 suggest a new lower bound for the frustration index of \( f = |\Theta_{\text{CW}}|/T_N = 14/0.1 = 140 \), placing this compound into a highly frustrated regime.

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Magnetic order in orbital models of the iron pnictides

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2011 J. Phys.: Condens. Matter 23 246001

We examine the appearance of the experimentally observed stripe spin-density-wave magnetic order in five different orbital models of the iron pnictide parent compounds. A restricted mean-field ansatz is used to determine the magnetic phase diagram of each model. Using the random phase approximation, we then check this phase diagram by evaluating the static spin susceptibility in the paramagnetic state close to the mean-field phase boundaries. The momenta for which the susceptibility is peaked indicate in an unbiased way the actual ordering vector of the nearby mean-field state. The dominant orbitally resolved contributions to the spin susceptibility are also examined to determine the origin of the magnetic instability. We find that the observed stripe magnetic order is possible in four of the models, but it is extremely sensitive to the degree of nesting between the electron and hole Fermi pockets. In the more realistic five-orbital models, this order competes with a strong-coupling incommensurate state which appears to be controlled by details of the realistic five-orbital models, this order competes with a strong-coupling magnetic instability. We find that the observed stripe magnetic order is possible in four of the models, but it is extremely sensitive to the degree of nesting between the electron and hole Fermi pockets. In the more realistic five-orbital models, this order competes with a strong-coupling incommensurate state which appears to be controlled by details of the realistic electronic structure below the Fermi energy. We conclude by discussing the implications of our work for the origin of the magnetic order in the pnictides.

Exchange bias effect in alloys and compounds

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Topical Review

The phenomenology of exchange bias effects observed in structurally single-phase alloys and compounds but composed of a variety of coexisting magnetic phases such as ferromagnetic, antiferromagnetic, ferrimagnetic, spin-glass, cluster-glass and disordered magnetic states are reviewed. The investigations on exchange bias effects are discussed in diverse types of alloys and compounds where qualitative and quantitative aspects of magnetism are focused based on macroscopic experimental tools such as magnetization and magnetoresistance measurements. Here, we focus on improvement of fundamental issues of the exchange bias effects rather than on their technological importance.
Journal of Physics: Condensed Matter presents LabTalk, a dedicated section of short news items written by our authors about their latest papers.

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2011 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 2011 special issue programme.

**Strongly correlated electron systems**

**Guest Editors:** Filip Ronning and Cristian Batista  
*2011 J. Phys.: Condens. Matter 23* issue 9

Strongly correlated electrons is an exciting and diverse field in condensed matter physics. This special issue contains a number of contributions on f-electron compounds and also covers recent developments relating to strongly correlated electron systems in d-electron materials, such as Sr$_2$Ru$_2$O$_7$, graphene, and the new Fe-based superconductors.

**Geometrically frustrated magnetism**

**Guest Editor:** Jason S Gardner  
*2011 J. Phys.: Condens. Matter 23* issue 16

Frustrated magnetism is an area that has grown tremendously over the past 20 years. Geometric frustration is a broad phenomenon that results from an intrinsic incompatibility between some fundamental interactions and the underlying lattice geometry based on triangles and tetrahedral. Most studies have centred around the kagomé and pyrochlore based magnets but recent work has looked at other structures including the delafossite, langasites, hyper-kagomé, garnets and Laves phase materials.

**Nano- and microfluidics**

**Guest Editor:** Karin Jacobs  
*2011 J. Phys.: Condens. Matter 23* issue 18

The field of nano- and microfluidics emerged at the end of the 1990s parallel to the demand for smaller and smaller containers and channels for chemical, biochemical and medical applications such as blood and DNA analysis, gene sequencing or proteomics. The articles in this issue have been divided into four subsections: ‘Probing the boundary condition’, ‘Flow over or in special geometries’, ‘Soft objects in fluid flow’ and ‘Manipulating flow’.

**Colloidal suspensions**

**Guest Editors:** Andrei Petukhov, Willem Kegel and Jeroen van Duijneveldt  
*2011 J. Phys.: Condens. Matter 23* issue 19

This issue contains research on a number of themes relating to the topic of colloidal suspensions. These themes are: electrostatics, colloidal rods and platelets, colloid–polymer mixtures and depletion interactions, and colloidal dynamics and crystallization.
Complex dynamics of fluids in disordered and crowded environments

Guest Editors: Daniele Coslovich, Gerhard Kahl and Vincent Krakoviack


The dynamics of fluids under nanoscale confinement has been of great interest both for practical and fundamental reasons. Problems in a wide range of scientific topics, such as polymer and colloidal sciences, rheology, geology, or biophysics, benefit from a profound understanding of the dynamical behaviour of confined fluids. This special section helps shed light on a number of important issues in the field.

Structure and dynamics determined by neutron and x-ray scattering

Guest Editor: Peter Müller-Buschbaum


Neutron and x-ray scattering have emerged as powerful methods for the determination of structure and dynamics. Driven by emerging new, powerful neutron and synchrotron radiation sources, the continuous development of new instrumentation and novel scattering techniques gives rise to exciting possibilities. This special section covers a broad range of different materials from soft to hard condensed matter.

Semiconducting oxides

Guest Editors: Richard Catlow and Aron Walsh

2011 J. Phys.: Condens. Matter 23 issue 33

Semiconducting oxides are amongst the most widely studied and topical materials in contemporary condensed matter science, with interest being driven both by the fundamental challenges posed by their electronic and magnetic structures and properties, and by the wide range of applications, including those in catalysis and electronic devices. This special section aims to highlight recent developments in the physics of these materials, and to show the link between developing fundamental understanding and key application areas of oxide semiconductors.

Vibrations at surfaces

Guest Editor: Talat S Rahman


This special section is dedicated to the phenomenon of vibrations at surfaces—a topic that was indispensable a couple of decades ago, since it was one of the few phenomena capable of revealing the nature of binding at solid surfaces. For clean surfaces, the frequencies of modes with characteristic displacement patterns revealed how surface geometry, as well as the nature of binding between atoms in the surface layers, could be different from that in the bulk solid. Dispersion of the surface phonons provided further measures of interatomic interactions.

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