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Dates to Remember

Sept. 6, 2011 (Tuesday) Deadline for submitting invited speaker suggestions for DMP Focus Topics. DMP online nomination: http://ultron.aps.org/forms/aps.cgi?ID=201101 **September 16, 2011** Deadline for nominations for DMP Officers and Executive Committee Members

November 11, 2011 (Friday) Abstract deadline for the 2012 APS March Meeting. Submission is via the web at http://abstracts.aps.org Note that there has been major updating of the sorting categories from previous years.

February 1, 2012 DMP Deadline for APS Fellowship Nomination **February 27 - March 2, 2012** (with tutorials, etc., February 26): APS March Meeting in Boston, Massachusetts

A Note from the Chair

It is a pleasure to extend a welcome from the Executive Committee of the Division of Materials Physics. This Summer Newsletter contains important information for the upcoming March Meeting in Boston (February 27 - March 2, 2012).

This year, the DMP Executive Committee has been working with the Executive Committee of the Division of Condensed Matter Physics and other APS Units to systematically revisit and update numerous sorting categories for the March Meeting. These updates are aimed toward better sorting of abstracts, and will further improve the organization of what is already a spectacular contributed program of talks. We will naturally welcome feedback and advice for further improvements in years to come, since the field is dynamic and constantly evolving.

As in previous years, DMP is organizing interdisciplinary Focus Topics for the March Meeting that will cover many different facets of materials physics. The process is being coordinated by Chair Elect, Darrell Schlom, and all the members of the Executive Committee helped to select the topics and to invite the organizers. The Focus Topics are a major contribution of DMP to the March Meeting, and we encourage you to review the topics, suggest invited speakers to the organizers, and plan to submit contributed aspects to the topics that overlap with your interests. Your input of invited speaker suggestions is particularly important to the success of the meeting, and we hope you will be able to offer your advice to the organizers of the various topics.

Student presenters are invited to apply for an Iris Ovshinsky Student Travel Award, available to students whose abstracts are placed in DMP-sponsored contributed sessions. Information is included below

While the deadline is not immediate, we also encourage all members to plan nominations for APS Fellowship. Nominating a deserving colleague is a great way to acknowledge their contributions. While the deadline is February 1, 2012, starting early is always a good idea, and detailed instructions are available on the DMP website.

Finally, I would like to take this opportunity to thank the members of the DMP Executive Committee who have recently completed their service, for the generous donation of their time and expertise in carrying out the work of DMP. These are Daniel Dessau and Julie Borchers, who have stepped down as Members at Large. And a special thanks to Ramamoorthy Ramesh, who has completed four years of leadership as Vice-Chair, Chair-Elect, Chair, and Past-Chair of the Division of Materials Physics.

Looking forward to seeing you in Boston!

Peter Schiffer, DMP Chair

The American Physical Society - Division of Materials Physics Iris Ovshinsky Student Travel Awards

The Iris Ovshinsky Student Travel Awards have been established to assist the career of student researchers. The Awards are named after Iris Ovshinsky who had a very strong interest and commitment to scientific education. The awards have been endowed by the Ovshinsky family, their colleagues at Energy Conversion Devices (ECD) companies and all their numerous friends from many social, intellectual and business relationships.

We anticipate that there will be eight \$500 awards each year to enable students to participate in the APS March Meeting sessions, which are sponsored by the Division of Materials Physics. The selection committee will consist of the following officers of the Division of Materials Physics: Secretary/Treasurer, Vice Chair and Past Chair.

Students interested in being considered for an award must apply online at https://www.cems.umn.edu/orgs/ovshinksy-award/

The **Iris Ovshinsky Student Travel Awards** for the 2011 March Meeting were presented to: Evgeniya Akatyeva (U. of Minnesota), Wen-Pin Hsieh (UIUC), Irfan (U. of Rochester), Bharat Jalan (UCSB), Xiaoting Jia (MIT), John Lyons (UCSB), Guang Sheng (Penn State), Joel Varley (UCSB), Jairo Velasco (UC Riverside), Pu Yu (UC Berkeley)

Pictures taken at the 2011 March Meeting Awards Reception



2011 Ovshinsky Student Travel Award winners together with the DMP officers: Peter Schiffer, Ramamoorthy Ramesh, Chris Palmstrøm, Darrell Schlom and Robert Nemanich



2011 APS-DMP Fellows Awards Recipients together with Chris Palmstrøm (Secretary/Treasurer) and Robert Nemanich (Chair)

Nominations for DMP Officers and Executive Committee Members

A DMP election will be held late in 2011 to elect a Vice-Chair, and two new at-large Executive Committee Members. The Nominating Committee shall nominate at least two candidates for the ballot for each office. Suggestions for candidates for these offices can be made to the Chair of the Nominating Committee, Robert Nemanich (Robert.Nemanich@asu.edu). In addition, candidates can be nominated directly to be placed on the ballot, by petition of five percent of the membership of the Division. Such petitions must be received by the Secretary-Treasurer (Chris Palmstrøm cpalmstrom@ece.ucsb.edu) by September 16, 2011.

Call for Invited Speaker Suggestions

With this issue of the Newsletter, the Division of Materials Physics announces the program of DMP Focus Topics for the 2012 APS March Meeting (Boston, MA, February 27 - March 2, 2012). A Focus Topic generally consists of a series of sessions, each of which is typically seeded with one invited talk, the remainder of the session being composed of contributed presentations.

September 6, 2011 is the deadline to submit suggestions for DMP Focus Topic invited speakers for the 2012 March Meeting.

DMP is sponsoring or co-sponsoring 33 different Focus Topics for the 2012 March Meeting. DMP members are encouraged to make suggestions for invited speakers for these Focus Topics via the web --> http://ultron.aps.org/forms/aps.cgi?ID=201101
Your nomination will go to the organizers of the Focus Topic you suggest an invited speaker for and will aid the organizers in their selection of invited speakers. A complete listing of DMP-sponsored Focus Topics and their descriptions are given below.

In suggesting speakers please keep in mind that speakers who gave an invited talk at the previous March Meeting are ineligible.

Thank you in advance for your help in making the March Meeting a success.

Finally, note that the contents of this Newsletter will be available electronically on the DMP website at http://www.aps.org/units/dmp. In case of any need for corrections or updates, these will also be posted at this location.

List of DMP-Sponsored or Co-Sponsored Focus Topics and Sorting Categories for the 2012 APS March Meeting

NOTE: New Sorting Categories from Previous Years

01. Polymers and Soft Matter Physics

01.1.8 Organic Electronics and Photonics (DMP/DPOLY) (same as 23.1.2)

Dean M. DeLongchamp, NIST, <u>dean.delongchamp@nist.gov</u> Calvin K. Chan, Sandia National Laboratories, <u>cchan@sandia.gov</u> Richard R. Lunt Michigan State University, <u>rlunt@msu.edu</u>

The electronic, excitonic, and photonic properties of organic materials, including small molecules and polymers, continue to be the subject of active fundamental and applied research. This focus topic covers recent developments in this field. In particular, contributions are solicited from the following areas related to organic semiconductor materials and devices:

- Charge carrier transport and injection
- Exciton dynamics and transport
- Organic-organic and organic-inorganic interfaces
- Optical and optoelectronic properties
- Correlations to primary chemical structure, microstructure, and morphology
- Fundamental progress in device design, processing, and modeling, including work on light-emitting devices, photovoltaic cells, field-effect transistors, switches, and lasers

01.1.9 Polymers for Energy Storage and Conversion (DPOLY/GERA/DMP)

Nitash Balsara, University California, Berkeley, nbalsara1@gmail.com

Advances in development of polymeric materials and polymer based devices for energy applications have generated new knowledge, concepts and strategies for solar energy conversion, generation of light and energy storage. This symposium covers recent developments in this field. Contributions are solicited for research related to the above topics such as utilizing polymer – nanofiller, multijunction, multilayer based energy capture and conversion schemes, polymers as variable band gap materials, polymers in the capacity of light emitting and charge carrier transport materials and for energy storage device such as Lithium ion polymer batteries or block copolymers for ultracapacitors. Advances in physics underlying polymer enabled energy devices such as in solar cells, light emitting diodes, batteries and capacitors and their efficiency and performance is solicited through both theoretical and experimental studies.

04. **Biological Physics**

04.1.10 Structure and Dynamics of Membranes (DBIO/DPOLY/DMP/DCOMP) (same as 01.1.25 and 16.1.17)

Mu-Ping Nieh, University of Connecticut, mu-ping.nieh@ims.uconn.edu

Natural and biomimetic membranes provide a fundamental understanding of membraneassociated proteins, practical application as delivery carriers for pharmaceuticals and diagnostic agents, the coating of biosensors, nano- or micro-reactors etc. The molecules forming biomimetic membranes (such as lipids, surfactants, polymers or their mixtures) generally self-assemble into rich structural phases with interesting dynamics, some of which are not fully understood. In order to optimize their applications, it is essential to fully understand the structure and dynamics of biomimetic membranes. This session will include presentations on structural characterization and dynamic studies of biomimetic membranes (including monolayer or bilayer membranes, substrate-supported membranes, polymerized membranes) and their interaction with membrane-associated biomolecules.

04.1.17 Materials and Functional Structures for Biological Interfaces (DMP/DBIO)

Robert Ros, Arizona State University, Robert.Ros@asu.edu Robert Riehn, North Carolina State University, rriehn@ncsu.edu Hongbo Peng, IBM Research Division, pengho@us.ibm.com

Materials and functional structures (including thin layers, membranes, and pores) for biological interfaces are of interest for many fundamental questions for example in biophysics, biochemistry and cell biology, but also play an important role for many biomedical applications and in biotechnology.

This focus topic addresses recent experimental and theoretical developments in materials for micro- and nanostructured surfaces, biopatterning, supported and unsupported membranes, micro- and nanofluidic systems, and nanopores. These materials and functional structures address applications including 3D cell culture, implants, biosensors, bioanalytics, and DNA sequencing. They enable the study of protein adsorption, cell adhesion, cell mechanics, cell motility, cell membranes, cell receptors, cytoskeleton, chemotaxis, intercellular communication, and cancer progression, as well as the structure and dynamics of biomolecules.

07. **Insulators and Dielectrics**

07.1.1 Dielectric, Ferroelectric, and Piezoelectric Oxides (DMP/DCOMP) (same as 11.1.1 and 16.1.8)

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This topic focuses on dielectric, ferroelectric, and piezoelectric phenomena in oxides, their characterization by a broad range of techniques, and the growth of such materials in bulk, thin-film, superlattice, and nanostructured forms. Experimental results as well as theoretical, modeling/simulation, and materials-design approaches will be discussed. Specific areas of interest include domain structure and dynamics, lattice dielectric properties, impact of disorder on cooperative behavior, physics of phase transitions, and the coupling between ferroelectric, piezoelectric, optical, transport, and multiferroic properties. This topic will in particular discuss how such properties are modified by nanoscale geometries, the effects of strain, surfaces and interfaces, chemical environment, and electrical boundary conditions. Contributions addressing how local properties in interfacial or other nanoscale systems can be harnessed in macroscopic applications will be particularly encouraged. As there is potential overlap with other focus topics in the areas of multiferroics and interfacial effects, the organizers will share information to group abstracts in a consistent fashion. In general, authors in these areas are encouraged to submit their abstracts to this topic if the presented work focuses on ferroelectric or piezoelectric properties.

07.1.2 Topological Insulators: Synthesis and Characterization (DMP) (NEW)

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Recent theoretical work has nucleated significant interest in materials known as "topological insulators" wherein the combined effects of the spin-orbit interaction and fundamental symmetries can lead to an insulator with a bulk energy gap but with gapless surface (or edge) states. The field is still at a nascent stage where concerted efforts in materials synthesis and characterization will be essential for exploring the full panoply of phenomena predicted by theory. This topic will focus on fundamental advances in the synthesis of candidate topological insulator crystals in various forms including bulk single crystals; exfoliated and epitaxial thin films; epitaxially modulated heterostructures; nanowires and nanoribbons. Of equal interest is the characterization of these samples using structural, electrical, magnetic, optical and other techniques, with particular focus on identifying samples whose properties are dominated by the surface states.

08. Semiconductors

08.1.2 Dopants and Defects in Semiconductors (DMP)

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Impurities and native defects profoundly affect the electronic and optical properties of semiconductor materials. Incorporation of impurities is nearly always a necessary step for tuning the electrical properties in semiconductors. In some cases, as in dilute III-V alloys, impurities even modify the band gap. Defects control carrier concentration, mobility, lifetime, and recombination; they are also responsible for the mass-transport processes involved in migration, diffusion, and precipitation of impurities and host atoms. The control of impurities and defects is the critical factor that enables a semiconductor to be engineered for use in electronic and optoelectronic devices as has been widely recognized

in the remarkable development of Si-based electronics, the current success of GaN-based blue LED and lasers, and the emergence of ZnO for nanoelectronics sensors, and transparent conducting displays. The fundamental understanding, characterization and control of defects and impurities are essential for the development of new devices, such as those based on novel wide-band gap semiconductors, spintronic materials, and low-dimensional structures.

The physics of dopants and defects in semiconductors, from the bulk to the nanoscale, including surfaces and interfaces, is the subject of this focus topic. The electronic, structural, optical, and magnetic properties of impurities and defects in elemental and compound semiconductors, SiO2 and alternative dielectrics, wide band-gap materials such as diamond, SiC, group-III nitrides, and oxide semiconductors are of interest. Abstracts on experimental and theoretical investigations are solicited.

09. Superconductivity

09.1.1 Fe-based Superconductors: Synthesis, Characterization, and Modeling (DMP/DCOMP) (same as 16.1.9)

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Johnpierre Paglione, University of Maryland, <u>paglione@umd.edu</u> John Tranquada, Brookhaven National Laboratory, <u>itran@bnl.gov</u>

This focus topic will concentrate on the synthesis, characterization, and modeling of Febased superconductors and related compounds. The broad goal is the understanding of the relationship between the spectrum of different crystalline, magnetic and electronic structures found to be related to high critical temperatures in this new family of high-temperature superconductors, as well as the potential for new superconducting systems to be discovered. Relevant topics include: (i) the synthesis of new iron-based superconducting materials; (ii) their characterization using a variety of experimental techniques such as neutron scattering, angle resolved photoemission, electron scanning microscopy, and transport and thermodynamic measurements; and (iii) modeling of these materials and computer intensive studies of their properties.

09.1.2 Search for New Superconductors (DMP)

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This topic will focus on fundamental advances in the growth, characterization, and experimental as well as theoretical understanding of new superconducting materials with the exclusion of the recently discovered magnesium diborides, pnictides, and calcoginides. The main goal of this focus topic is to explore non-conventional ideas in superconductivity, and to foster the exchange of information about discoveries that may conceive a change in our understanding of superconductivity. Its purpose is to promote interaction among theorists and experimentalists and seed new directions in superconductivity research, especially in areas cutting across traditional disciplinary

boundaries. Areas of interest include new approaches in the study of superconductivity in complex materials, metamaterials, heterojunctions, and hybrid structures. The focus topic will cover a wide range of novel superconductors such as organics and intercalation compounds. The creation of superconducting nanostructures with atomic scale control using physical and chemical methods is also of interest. The focus topic will specifically include research on understanding of mechanisms for improvements in superconducting materials, engineering superconductors with ab initio methods, empirical approaches in the search for novel superconductors, and theoretical predictions leading past serendipitous discovery to predictive design.

10. Magnetism

10.1.1 Magnetic Nanostructures: Materials and Phenomena (DMP/GMAG) (same as 13.1.2)

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This topic focuses on magnetic nanostructures such as thin films, multilayers, nanoparticles. nanowires. nanocomposites. superlattices. nanorings. hvbrid nanostructures, spin phenomena in nanoscale organics, magnetic point contacts and selfassembled as well as patterned magnetic arrays. The sessions will include methods used to synthesize such nanostructures, the variety of materials used, and the latest, original theoretical and experimental advances. There is a special interest in novel properties that arise at the nanoscale, as well as synthesis and characterization techniques demonstrating nano- or atomic-scale control of properties. Phenomena and properties of interest include: magnetization dynamics, magnetic interactions, magnetic quantum confinement, spin tunneling and spin crossover, proximity and structural disorder effects, strain effects, microwave resonance and microwave assisted reversal, magnetic anisotropy, and thermal and quantum fluctuations.

10.1.2 Emergent Properties in Bulk Complex Oxides (DMP/GMAG) (same as 11.1.2 and 12.1.10)

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Tanusri Saha-Dasgupta, S.N. Bose National Centre, <u>tanusri@bose.res.in</u>
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The emergence of exotic states of matter from the intricate coupling of the electronic and lattice degrees of freedom is a unique feature in strongly correlated electron systems. Included in this class are the complex oxides of 3-, 4-, and 5-d transition metal compounds that exhibit a wide range of novel physical properties stemming from the complex nature of the competing interactions and nearly degenerate multiple ground states. Associated with this complexity is a tendency for new forms of order such as the formation of stripes, ladders, checkerboards, or phase separation, and an enhanced response to external influences. This Focus Topic explores the nature of the various ground states observed in bulk specimens of complex oxides and their competing interactions, the ways in which the spin, lattice, charge and orbital degrees of freedom

respond on a variety of length scales, and how they interact and compete with each other to produce novel phenomena. It provides a forum to discuss recent developments and results covering basic aspects (new materials synthesis, experiment, theory and simulation) of bulk systems. Note there is some overlap in topic with other DMP and GMAG focus sessions on oxides. The organizers of all of the related focus sessions will share information and work together with the March Meeting Program Committee to make an optimal meeting program.

10.1.3 Magnetic Oxide Thin Films and Heterostructures (DMP/GMAG) (same as 11.1.3 and 12.1.11)

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Magnetism in complex oxides has long been a rich field of study in solid state physics as there are strong interactions between spin, charge, lattice, and orbital degrees of freedom. Furthermore, when magnetic oxides are grown as thin films they often exhibit additional effects resulting from epitaxial strain, reduced dimensionality, charge transfer, proximity effects, or phase competition and/or coupling across interfaces. This Focus Topic is dedicated to advances in the understanding of the electronic and magnetic properties of oxide thin films, heterostructures, superlattices, and nanostructures with an emphasis on growth, characterization, theoretical modeling and novel device physics. Specific areas of interest include, but are not limited to, (anti)ferromagnetism, strongly correlated "Mott" thin films, growth of oxide materials, control of their magnetic properties, domain structures, advances in techniques to probe and image different types of magnetic order in complex oxide thin films (including optical and electron-probes and neutron/synchrotronbased techniques), magneto-transport, and recent developments in theoretical prediction and materials-design approaches to magnetic oxide thin films, superlattices, and nanostructures. Note there is some overlap in topic with other DMP and GMAG focus sessions. As a rule of thumb, if magnetism plays a key role in the investigation or the properties observed, then the talk is appropriate for this focus topic. The organizers of all of the related focus sessions will share information and work together with the March Meeting Program Committee to make an optimal meeting program.

10.1.4 Spin Transport and Magnetization Dynamics in Metals-Based Systems (GMAG/DMP/FIAP) (same as 23.12.3)

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Jonathan Sun, IBM Research, <u>jonsun@us.ibm.com</u> Shufeng Zhang, University of Arizona, <u>zhangs@physics.arizona.edu</u>

Spin-related effects in metals and in ferromagnetic heterostructures are generally robust and readily observed at room temperature. Fundamental discoveries such as giant and tunnel magnetoresistance and current-induced spin-transfer torque are moving from discovery to applications rapidly, while fundamental spin-dependent transport physics and novel materials and thin film structures are being actively explored in all-metal junctions and magnetic tunnel junctions for deeper understandings and potentially new

functional materials and devices for applications. This Focus Topic aims to capture new developments in these areas, including experimental and theoretical aspects of spin transport and magnetization dynamics in metal-based systems, such as ultrathin films, lateral nanostructures, perpendicular nanopillars, and tunnel junctions.

In particular, contributions describing new results in the following areas are solicited:

- The interplay between spin currents and magnetization dynamics in magnetic nanostructures; spin-transfer, spin pumping and related phenomena, including current-induced magnetization dynamics in heterostructures and domain wall motion in magnetic wires.
- Theoretical predictions and/or experimental discovery of half-metallic band structures, both in bulk solids and at the surfaces of thin films. Spin transport and magnetization dynamics in magnetic nanostructures (e.g. TMR, CPP-GMR and lateral spin valve structures) based on half-metallic materials.
- Effects of the spin-orbit interaction on steady-state and dynamical properties of nanostructures including: the (inverse) spin and anomalous Hall effects, microscopic mechanisms of magnetization damping, and the effects of interface spin-orbit interaction.
- Magnetic response to electric field (e.g anisotropy, phase transition, exchange bias,...) including: electric field activation in hybrid metals/oxide structures, piezoelectric layer coupled to ferromagnetic films, electrolyte/ferromagnetic systems
- Ultrafast magnetization response to (and reversal by) intense laser pulses; magnetization dynamics at elevated temperatures and thermally assisted magnetization reversal.
- Thermoelectric spin phenomena such as giant-magneto thermopower and Peltier effects, spin-Seebeck effect, spin and anomalous Nernst and Ettingshausen effects (spin caloritronics).
- Thermal gradient and/or RF driven magnetization dynamics in (composite) nanostructures including spin wave excitation, propagation, and detection (magnonics), as well as vortices.
- Interactions between electronic spin-current and magnon propagations in thin film and device structures.

10.1.5 Spin Dependent Phenomena in Semiconductors (GMAG/DMP/FIAP) (same as 08.1.1 and 23.1.4)

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The field of spin-dependent phenomena in semiconductors shows rapid and significant advances and challenges in a widening range of new effects, new materials systems (e.g., heterostructures, oxides, silicon, diamond, graphene and organics), and new structures (e.g., self-assembled and lithographically defined semiconductor quantum structures, wires and carbon nanotubes, hybrid ferromagnetic/semiconductor structures). This focus topic solicits contributions aimed at understanding spin-dependent processes in magnetic and non-magnetic structures incorporating semiconducting materials. Topics include: (i) electrical and optical spin injection, spin Hall effects, spin-dependent topological effects, spin interference, spin filtering, spin lifetime effects, spin dependent scattering, and spin

torque; (ii) growth, characterization, electrical, optical and magnetic properties of (ferro-)magnetic semiconductors, nanocomposite and hybrid ferromagnet/semiconductor structures including quantum dots, nanocrystals, and nanowires; (iii) spin-dependent transport and dynamical effects in semiconductors with or without spin-orbit interactions; (iv) manipulation, detection, and entanglement of electrical and nuclear spins in quantum systems such as dots, impurities and point defects; (v) high temperature ferromagnetism in semiconductors and semiconductor oxides; and (vi) spin-dependent devices and device proposals involving ferromagnets and semiconductors.

10.1.6 Frustrated magnetism (DMP/GMAG)

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Oleg Tchernyshyov, Johns Hopkins University, olegt@jhu.edu

Simple antiferromagnets on bipartite lattices have well-understood ground states, elementary excitations, thermodynamic phases and phase transitions. At the forefront of current research are frustrated magnets where competing interactions suppress magnetic order and may lead to qualitatively new behavior. Frustrated magnets are expected to have unusual, quantum-disordered ground states and fractionalized excitations akin to those found in one-dimensional antiferromagnets. They are also sensitive to nominally small perturbations and interact in a non-trivial way with orbital and lattice degrees of freedom.

This Focus Topic solicits abstracts for presentations that explore both theoretical and experimental aspects of the field. The themes to be represented are united by geometrical frustration: valence-bond solids and other exotic magnetic orders, spin ice, quantum spin liquids, order from disorder, magnetoelastic coupling, and novel field-induced behavior. Also of interest are the effects of strongly fluctuating spins on properties beyond magnetism including transport, thermal transport and ferroelectricity.

Please note that Low-dimensional and Molecular Magnetism is now a separate focus topic (06.1.8).

10.1.7 Spin-Dependent Physics in Carbon-Based Materials (GMAG/DMP)

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This focus topic is on spin transport, spin dynamics and exchange in carbon-based materials, including organic and molecular solids, all-carbon systems, organic radical systems, and π -conjugated organic/polymeric systems. These issues are of great current interest because of breakthrough results in the field of 'organic spintronics'. Research at the intersection of several forefront areas in condensed matter and material physics will be covered: spin injection at the inorganic to organic interface, the degree of spin polarization attainable by organic based solids, spin coherence and relaxation, hyperfine interaction between the electronic spin and nuclear magnetic moments, and magnetic exchange and magnetic ordering. Phenomena and materials of interest include hybrid ferromagnetic/organic structures, spin transport in graphene and carbon nanotubes, spin

qubits in diamond, quantum tunneling of the magnetic moment, and triplet states, as well as magnetic field effects (such as organic magnetoresistance), singlet/triplet issues and spin resonance in organic semiconductors.

10.1.8 Low-Dimensional and Molecular Magnetism (GMAG/DMP) (NEW)

Enrique del Barco, University of Central Florida, <u>delbarco@physics.ucf.edu</u> Jürgen Schnack, Bielefeld University, <u>jschnack@uni-bielefeld.de</u> Vivien Zapf, Los Alamos National Laboratory, <u>vzapf@lanl.gov</u>

The control and manipulation of spin and charge degrees of freedom in nanoscale systems has become a major challenge during the last decades, triggered by exciting applications in emerging technologies such as quantum computation and spintronics among others. For this goal to be accomplished, a complete understanding of the quantum behavior of interacting electronic and even nuclear spins in solid state systems is necessary. For conventional three dimensional magnetic materials a robust framework for describing the low temperature structures, phase transitions, and excitations exists. However, when fluctuations are enhanced by low dimensionality, qualitatively new behavior can emerge. Low dimensional magnetic systems have become prototype systems in this direction. For example, the synthetic flexibility of molecule-based magnets allows the magnetic quantum response of the system to be engineered. This Focus Topic solicits abstracts that explore inorganic and organic molecule-based as well as solid state systems, and both theoretical and experimental aspects of the field. Topics of interest include: magnetism in zero, one, and two dimensions (e.g. quantum dots, single molecule magnets, spin chains, lattices), order by disorder, the role of magnetoelastic, spin-orbit and superexchange couplings, quantum critical low dimensional spin systems, topological excitations, quantum tunneling of magnetization, coherence phenomena and novel field-induced behavior.

12. Complex Structured Materials, Including Graphene

12.1.1 Graphene: Growth, Mechanical Exfoliation, and Properties (DMP) (NEW)

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Graphene, a single atomic layer of carbon that is crystallized in the honeycomb configuration, continues to attract strong interest within the scientific community because of its unique mechanical, thermal, and electronic properties. A number of approaches have been developed to synthesize single- and few-layer films of graphene on suitable substrates. These include mechanical exfoliation from graphite, Si sublimation and subsequent graphene formation on SiC substrates, graphene formation on metal surfaces by chemical vapor deposition, and graphene formation by ion implantation. This graphene focus topic will cover (i) graphene growth on substrates, (ii) modeling the growth processes to deduce the underlying growth mechanisms, (iii) characterization and modeling of the structural, electronic, and optical properties of the synthesized graphene, (iv) methods for separating and transferring graphene from their underlying substrates, and (v) methods for mechanical exfoliation of graphene from graphite.

12.1.2 Graphene: Structure, Stacking, and Interactions (DMP) (NEW)

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The study of graphene, a single atomic plane of graphite, remains a rapidly growing field of research. This topic will focus on the materials physics of graphene produced by mechanical or chemical means, including single layer, bilayer, trilayer, and higher multilayer graphenes as well as structurally or chemically modified graphenes. We invite experimental and theoretical contributions in the following areas:

- The physics of structurally or chemically modified graphenes, including the effect of defects, edges, adatoms, adsorbates, and strain on graphene's material properties.
- The physics of epitaxial graphenes, including the properties of multilayer graphene films.
- Interactions of exfoliated or chemically grown graphenes with different substrates and the environment.

12.1.3 Graphene Devices: Function, Fabrication, and Characterization (DMP) (NEW)

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The unique properties of graphene have led to great excitement about its potential device applications. However, numerous open questions surround the challenges and promise of creating such devices at a practical level. This Focus Topic relates to experimental and theoretical studies of devices based on single- and multi-layered graphene. The devices considered include (but are not limited to) electronic, optical, mechanical, thermal, and chemical graphene devices. We invite contributions on topics including: (i) the fabrication, measurements, and modeling of graphene devices, (ii) proposals for or tests of devices that exploit the unique properties of graphene, and (iii) materials, environmental, or other issues that enable or limit graphene devices.

12.1.4 Carbon Nanotubes and Related Materials: Synthesis, Properties, and Applications (DMP)

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Interest in the fundamental properties and applications of carbon nanotubes and related materials continues to grow. The reason for this interest lies in the unique combination of electrical, chemical, mechanical, thermal, optical, spectroscopic and magnetic properties of these systems.

This focus topic addresses recent developments in: (i) the fundamental understanding of nanotubes and related materials, including synthesis, characterization, processing, purification, chemical, mechanical, thermal, electrical, optical, and magnetic properties, and (ii) in their potential applications for interconnects, transistors, thermal management, composites, super-capacitors, nanosensors, nanoprobes, field emitters, storage media, and magnetic devices.

Experimental and theoretical contributions are solicited in the following areas:

- 1. Synthesis and characterization of nanotubes, nanohorns, and related nanostructures;
- 2. Control or optimization of growth, including chirality control and in-situ studies;
- 3. Purification, separation, chemical functionalization, alignment/assembly;
- 4. Structure and properties of hybrid systems, including filled and chemically modified carbon nanotubes and nanotube peapods;
- 5. Mechanical and thermal properties of these nanostructures and their composites;
- 6. Electrical and magnetic properties of these systems;
- 7. Mesoscopic, structural, optical, opto-electronic and transport properties as well as their spectroscopic characterization.

The focus topic will also cover the broad applications of these nanosystems, including:

- 8. Electronic devices including interconnects, supercapacitors, transistors, memory;
- 9. Thermal management applications;
- 10. Multifunctional nanotube composites;
- 11. Chemical and bio-sensing applications;
- 12. Field emission; and
- 13. New generations of magnetic and electronic devices.

12.1.5 Van der Waals Bonding in Advanced Materials (DMP)

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Van der Waals bonds occur in all materials and are particularly important in regions with low electron concentration. Van der Waals forces impact material structure and behavior, both when they dominate the binding, and when they compete with other binding mechanisms like covalent or ionic binding. This focus topic will focus on the materials physics of van der Waal interactions, highlighting recent advances in theory and application that lead toward a deeper understanding and more quantitative description. Experimental work that details a van der Waals nature in cohesion or function and theoretical treatments of specific materials problems are featured to stimulate further experiment-theory exchange and calibration.

This focus topic is dedicated to the memory of David C. Langreth, for his inspiring research on van der Waals bonding and for his legacy of experiment-theory exchanges in materials physics.

Contributions are invited from all areas of material physics and especially on the following topics:

• Molecular crystals and thin films, with advances in 3-D molecular architecture

- Nanoporous materials such as zeolites and metal-organic frameworks (MOF's) for hydrogen storage and carbon sequestration
- Layered materials and atomistics of intercalation and exfoliation
- Low dimensional structures, including molecules physisorbed or weakly adsorbed on surfaces, self-assembled functional monolayers and molecular interfaces
- Supramolecular organizations, including biomimetic assemblies and chiral structures

12.1.6 Computational Design of New Materials (DMP/DCOMP) (same as 16.1.10)

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Advances in theoretical understanding, algorithms and computational power are enabling computational tools to play an increasing role in materials discovery, development and optimization. This focus topic will cover recent applications and methodological developments at the frontier of computational materials design, ranging from quantum-level prediction to macro-scale property optimization. Of particular interest is computational and theoretical work that features a strong connection to experiment. Topics include (but are not be limited to) first-principles materials design, algorithms to search the structure-composition design space, and theory/methodological innovations that improve the scope, accuracy and efficiency of computational materials design.

12.1.7 Multiscale Modeling (DCOMP/DMP) (same as 16.1.5)

Timothy C. Germann, Los Alamos National Laboratory, tcg@lanl.gov

The emphasis of this session will be on methods and strategies to bridge spatial and temporal scales in condensed matter and materials systems. A key aim of multiscale modeling is to augment models of large scale systems by applying selected information from smaller scale models. Contributions are invited that demonstrate, for example, methods of coarse-graining from one physical scale to another, adaptive refinement strategies to increase local fidelity on demand, as well as dynamic bridging methods that pass data and parameters from smaller to larger scales. Challenges of the field include propagating the effects of fluctuations and disorder from smaller to larger scales, and quantifying the robustness of predictions. Applications to materials undergoing deformation processes, including structural transformations, materials subjected to radiation fields, as well as those coupling functional properties, such as multiferroics, are welcome. An understanding of the needs and challenges in exploring materials behavior in extreme and/or nonequilibrium conditions involving shock, intense radiation or very high magnetic and electric fields, are especially encouraged.

13. Superlattices, Nanostructures, and other Artificially Structured Materials

13.1.1 Nanostructures and Metamaterials: Growth, Structure, and Characterization (DMP)

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Shaping materials on the sub-wavelength scale allows for an unprecedented control of light. This includes nanostructures on a molecular level such as, e.g., graphene as well as lithographically defined plasmonic and metamaterial structures. Optical properties on the nanoscale shall include insights from experimental and/or theoretical research and from research by any of the spectroscopic, scattering, or time-resolved methods spanning from the visible to the far-infrared spectrum. The principal aim of this focus topic is to bring together colleagues from different disciplines to advance our understanding of novel optical phenomena in nanosystems and composite media.

13.1.4 Electron, Ion, and Exciton Transport in Nanostructures (DMP) (same as 14.1.1)

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A host of transformative device technologies depend for their function on fluxes of charge, mass, energy, or combinations thereof. This focus topic will address fundamental challenges and new opportunities to understand and control electron, ion, and exciton transport in nanostructures, with a particular interest in the influence of interfaces between different materials and phases.

Contributions are solicited in areas that reflect recent advances in the experimental characterization and theory of inorganic nanostructures, including those based on individual quantum dots (0-D), nanowires (1-D), and nanoplatelets (2-D). Specific topics of interest include, but not limited to:

- Experimental and theoretical correlation of nanoscale structure with electronic transport properties.
- Influence of dimensionality on charge carrier scattering and phase transitions.
- Transport through metal-semiconductor interfaces.
- Theoretical and experimental progress towards understanding and exploiting memory effects in resistive and capacitive systems.

Separate focus topics sponsored or cosponsored by DMP will organize presentations on transport in carbon nanotubes, graphene, magnetic nanostructures (spin transport), and molecules. Photovoltaics and thermoelectrics will also be the subject of separate focus topic.

13.1.5 Interfaces in Complex Oxides (DMP) (same as 12.1.9)

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The experimental realization of atomically precise interfaces between complex oxide compounds opens a new window in physics and materials science of complex oxides. providing exciting directions for fundamental and applied research. Complex oxides exhibit a rich variety of physical properties like magnetism, ferroelectricity, and superconductivity. Proximity to an interface modifies these properties and sometimes leads to even more intriguing phenomena due to interface-mediated interplay between electronic states. Recent experimental and theoretical studies have shown that the strong coupling between orbital, spin, and structural degrees of freedom that exist in complex oxides can be further exploited at atomically sharp interfaces to obtain novel functional behaviors, potentially useful for technologically important applications. This focus topic aims at bringing together experimental and theoretical researchers working on all aspects of interface-related behavior in complex oxide materials. This includes the growth and characterization of oxide heterostructures, development and application of new interfacerelated measurement techniques, experiment and theory related to interface-induced changes in physical properties and new or modified interface-mediated aggregate responses and collective states. Especially welcome are abstracts focusing on the search for new interface-related phenomena and the use of oxide interfaces as a test-bed for rational design of materials with desirable electronic, magnetic, and transport properties.

There is some overlap in topic with other focus topics related to complex oxide materials; as a rule of thumb, if the interface plays a key role in the investigation or the properties observed, then the talk is appropriate for this focus topic.

14. Surfaces, Interfaces and Thin Films

14.1.2 Surfaces and Interfaces in Nonoxide Nanostructures: Growth, Structure, and Characterization (DMP) (same as 13.1.6)

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Progress in nanoscience depends on the fundamental understanding of the evolution of atomic structure, composition, morphology, and electronic properties at surfaces and interfaces. The ability to understand and control the thermodynamics and kinetics of surface processes will enable the creation of new structures and the discovery of new phenomena. This focus topic will highlight recent experimental and theoretical developments associated broadly with the formation and stability of nanostructured surfaces, thin films, and interfaces of non-oxide materials. Particular emphasis will be placed on their growth kinetics, thermal, chemical, and mechanical stabilities, and their role in energy harvesting and storage applications.

16. General Theory/Computational Physics

16.1.6 Simulations of Matter at Extreme Conditions (DCOMP/DMP/GSCCM)

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The behavior of matter under extreme conditions of high pressures, high temperatures, high strains, and high strain rates is a scientific issue of fundamental importance. Geophysical processes in the core of the Earth and other planets, matter withstanding hypervelocity impacts of comets, shock wave compression of materials, detonation of explosives, high pressure and high temperature synthesis of novel materials, failure of materials reaching their intrinsic limit of performance, etc., all require an understanding of the fundamental mechanisms of materials response at the atomic, microstructural, and continuum levels. Recent developments in the experimental realization of such extreme conditions in the laboratory, advances in ultrafast and ultra-high spatial resolution characterization, extensive efforts to extend simulations to experimental time and length scales by utilizing both the enormous increases in computational power and new simulation methods, all promise new scientific discoveries and important technological breakthroughs. This focus session, consisting of several invited and contributed talks, will assess recent experimental and computational efforts towards exploring the fundamental properties of matter at extreme conditions, including (1) high-pressure and high temperature synthesis and characterization of novel materials; (2) high strain rate phenomena occurring upon ultrafast energy deposition; (3) properties of matter in the warm dense regime; (4) ultrafast laser-matter interactions; (5) static high pressure and shock-induced materials behavior, including plasticity, phase transitions, and chemical reactions; (6) static and dynamic properties of energetic materials, including detonation phenomena, (7) new experimental capabilities in ultrafast and ultra-high spatial resolution characterization; and (8) new computational methods including development of interatomic potentials and multi-scale simulations.

16.1.7 Non-Adiabatic Dynamics in Irradiated Materials (DCOMP/DMP)

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Jose Alfredo Caro, Los Alamos National Laboratory, <u>caro@lanl.gov</u>

The effects of irradiation on condensed matter are important to varied applications, from the nuclear industry to space technology and cancer therapy. Computer simulations of such irradiation have been constrained to tractable limits as the adiabatic limit (slow projectiles, energy transferred to nuclear motion), or the opposite, in which the energy is transferred to the electron subsystem only. Following the recent success in the first-principles calculation of the electronic stopping power of ions at intermediate velocities in varied solids – based on time-evolving TD-DFT – the moment is ripe for advancing the first-principles computation of nonadiabatic irradiation processes in materials and soft matter. The main aim of this symposium is to put together experts in new developments in electron-ion coupled dynamics, and experts in radiation effects to explore the potential of electronic structure based theoretical/computational approaches to understand irradiation of materials under extreme conditions.

19. Instrumentation and Measurements

19.1.6 Imaging and Modifying Materials at the Limits of Space and Time Resolution (DMP/GIMS)

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This focus topic covers the rapidly evolving field of material modification and imaging/probing with high spatial and temporal resolution. The ability to achieve high spatial resolution in material modification often relies on fast and highly localized energy deposition and, unavoidably, creates the conditions of strong thermodynamic, electronic, and/or mechanical nonequilibrium. The development of advanced imaging techniques capable for providing time-resolved information on the ultrafast structural and phase transformations is critical for gaining fundamental understanding of the material behavior far from the equilibrium and optimization of the conditions in the nanoscale material processing applications. The focus topic aims to bring together researchers involved in experimental, theoretical, and computational investigations in the general area of high-resolution material modification and imaging and to facilitate active broad-ranging interdisciplinary discussions.

Topics of interest include but not limited to:

- material response to intense optical excitation, ion/cluster bombardment, severe mechanical deformation induced by mechanical impact
- photo/shock-induced phase transformations, generation of new metastable phases/structures (bulk, nano, surfaces)
- transient modification of material properties by electronic excitation
- mechanisms of mass and heat transfer under non-equilibrium conditions
- double/multiple laser pulse experiments with variable delay, pulse-shaping techniques
- laser processing below the diffraction limit, nano-patterning, micro- and nano-fabrication
- computer modeling and theoretical analysis of transient material behavior far from equilibrium
- time-resolved experimental imaging of ultrafast processes, including optical pump-probe, x-ray and electron diffraction techniques, emerging techniques for femtosecond diffractive imaging using e.g. free-electron lasers or fast electron beams
- imaging/probing of laser ablation and ablation plume expansion
- time/spatially-resolved imaging of phase transformations, fracture, shock formation, mechanical spallation
- imaging transient molecular dynamics in biological systems using free-electron X-ray lasers, and modeling of subsequent damage processes

23. Applications

23.1.5 Physics of Energy Storage Materials (DMP/GERA/FIAP/DCOMP) (same as 16.1.11 and 22.1.3)

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Energy storage is a cross-cutting topic that impacts applications ranging from transportation and portable electronics to large-scale (grid-based) storage for intermittent, renewable power sources. As the properties of energy storage devices depend critically upon the active materials from which they are constituted, improvements in capacity and power density hinge upon achieving a comprehensive understanding of the underlying materials physics and chemistry. Towards this goal, this Focus Topic will broadly cover the physics of energy storage materials. Specific topics of interest include, but are not limited to: advanced lithium-ion and metal-air batteries; hydrogen storage; supercapacitors; catalytic phenomena in energy storage; thermal storage materials; nanostructured materials; intercalation and insertion compounds; ionic and electronic conductive polymers; novel synthesis methods; recent advances in real-time or in situ characterization techniques; and computational approaches ranging from ab initio calculations to mesoscale and continuum modeling. Of particular interest are studies which elucidate performance-limiting phenomena or which describe novel compounds or synthetic approaches aimed at overcoming these limitations.

23.1.8 Thermoelectric Materials for Power Generation and Cooling (DMP/GERA/FIAP) (same as 13.1.7 and 22.1.1)

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A large portion of the power produced worldwide is lost as heat to the environment. In a typical combustion engine, for instance, only 25% of the fuel chemical energy is used for mobility and accessories. If even a modest fraction of the lost thermal energy can be converted to electricity, the potential impact on energy efficiency could be enormous, leading to improved fuel economy and reduced carbon dioxide emissions. Thermoelectric devices convert heat to electricity directly via the Seebeck effect. Alternatively, under electrical excitation these devices can provide heating and cooling via the Peltier effect. Thermoelectric technology is all solid-state, robust, and have a high power density. From a materials perspective the efficiency of the energy converter depends on the thermoelectric figure of merit (ZT) of the materials comprising it, which is defined as ZT $= \sigma S2 T/k$ where S, σ , k, and T are the Seebeck coefficient, electrical conductivity, thermal conductivity, and absolute temperature, respectively. Although there is no fundamental upper limit to ZT, commercially available materials rarely exceed ZT=1 resulting in performance less than 10 percent of the Carnot limit. The goal of this focus topic is to bring together scientists working on both bulk and nanostructured thermoelectric materials to examine the current approaches for increasing ZT towards improved energy efficiency.

Topics will range from fundamental to applied physics and will include:

- 1. Strategies to understand and control thermal conductivity reduction in thermoelectric materials
- 2. Methods to improve thermoelectric power factor (S2 σ) beyond optimally-doped bulk materials
- 3. Phenomena that influence thermoelectric performance at low temperatures
- 4. Techniques and methods to measure and predict thermoelectric properties