

DMP NEWSLETTER

Division of Materials Physics

A Division of The American Physical Society • www.aps.org/units/dmp

Summer 2004

Call For Invited Speaker Suggestions

The Division of Materials Physics **Focused Topic Program** for the 2005 APS March Meeting (Los Angeles, California; March 21-25, 2005) is given below.

The DMP Focused Topics generally consist of a number of sessions per topic with typically one invited speaker per session. The remainder of the session consists of contributed presentations.

Suggestions for invited speakers for a given DMP Focus Topic may be made by the deadline date of August 31, 2004 by using the web-based form on the APS website at: <http://www.aps.org/units/dmp/invited.cfm>

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DATES TO REMEMBER:

August 31, 2004 (Tuesday)
Deadline Date for
Submitting Suggestions for
DMP Invited Speakers

Dec. 1, 2004 (Wednesday)
APS Abstract deadline
submitted via the web at
<http://abstracts.aps.org>

March 21-25, 2005
APS March Meeting in
Los Angeles, California

List of DMP-Sponsored or Co-Sponsored Topics and Sorting Categories for the 2005 APS March Meeting

- 1.8.1 Metallic Glasses (DMP)
- 2.9.1 Wide Band Gap Semiconductors (DMP)
- 3.9.3 Lattice Dielectric Properties of Complex Oxides and Semiconductor-Oxide Interfaces (DMP/FIAP)
- 4.14.4 Organic Electronics, Photonics and Magnetics (DMP/DPOLY)
- 6.11.1 Theory and Simulation of Magnetism and Spin Dependent Properties (DCOMP/DMP/GMAG)
- 6.11.2 Magnetic Nanoparticles, Nanostructures and Heterostructures (DMP/GMAG)
- 6.11.3 Phase Complexity and Enhanced Functionality in Magnetic Oxides (DMP/GMAG)
- 6.11.4 Spin Transport and Magnetization Dynamics in Metal-Based Systems (GMAG/DMP)
- 6.11.5 Spin-Dependent Phenomena in Semiconductors (DMP/GMAG)
- 7.9.1 Simulation and Theory of Complex Materials (DCOMP/DMP)
- 7.9.2 Nanotubes and Nanowires: Devices and Applications (DMP)
- 7.9.3 Light Emission from Silicon (FIAP/DMP)
- 7.9.4 Novel and Complex Oxides (DMP/FIAP)
- 7.9.5 Carbon Nanotubes and Related Nanomaterials (DMP)
- 7.9.6 Computational Nanoscience (DAMOP/DCOMP/DMP)
- 7.9.7 Theory of Nanotubes and Carbon Based Nanostructures (DCOMP/DMP)
- 9.9.1 Intrinsic Inhomogeneity in Multiferroic Materials (DMP)
- 12.9.1 Friction, Fracture and Deformation (DMP/GSMP) (same as 12.10.1)
- 13.9.2 Optical Properties of Nanostructures and Nanophotonics (DMP)
- 13.9.3 Materials for Molecular Electronics (DMP)
- 13.9.4 Materials and Device Physics: Issues for Quantum Computing (DMP)
- 14.9.2 Morphology and Composition Evolution in Thin Films and Surfaces (DMP)
- 14.9.3 Fundamental Challenges in Transport Properties of Nanostructures (DMP)
- 19.9.1 Earth and Planetary Materials (DCOMP/DMP)
- 19.9.2 Simulations of Matter at Extreme Conditions (DCOMP/DMP)

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Call for Invited Speaker Suggestions, Continued...

Alternatively, suggestions for invited speakers may be made directly by contacting the appropriate session organizers who are listed after the Focus Session descriptive paragraphs given below. The web-based form for invited speaker nominations will contain fields for:

- The nominator's name, affiliation, phone number and e-mail address.
- The suggested speaker's name, affiliation, address, phone number, fax, and e-mail.

- The title of the suggested talk and a brief justification of the nomination (880 character limit).

Once the web-based nomination form is complete, there is a "submit" button at the bottom of the page. The invited speaker nomination submission will be sent to the appropriate focus topic organizers. If you choose to contact the focus session organizers directly, then please provide all of the information listed above.

ABSTRACT DEADLINE

The abstracts for contributed (and invited) papers are due at the APS by December 1, 2004 — (Please note that this is a Wednesday this year!!)

Contributed abstracts are to be submitted via the web:
<http://abstracts.aps.org/>

Contributors are encouraged to also send a copy of their abstract (conforming to the APS regulations) to the appropriate focus sessions organizers – **but remember that this copy does not replace the official web-based submission to the APS!!**

(Abstracts for invited papers are also due on December 1, 2004 and are to be sent to the special web address that will be provided in the official APS letter of invitation to present an invited paper at the March, 2005 meeting.)

Note that the information in this newsletter will be available in a periodically updated & corrected form on the DMP website at: <http://www.aps.org/units/dmp>

DMP 2005 March Meeting Focus Topic Program Call for Abstracts

1.8.1 Metallic Glasses (DMP)

Complexity is an inherent property of bulk and Al-based amorphous metals; they are multi-component and are suggested to have significant intermediate and short range order. Unlike crystal phases, complete structural information cannot be obtained from experiment, and due to the wide range in relevant time scales it is not possible to simulate glass structures by quenching the liquid at realistic rates. This session seeks contributions describing theoretical, modeling, and experimental studies that confront this complexity and contribute to the basic understanding of glass structure, glass formability and stability, atomic level processes, the glass transition, and physical properties.

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VISA INFORMATION WEBSITE:

The APS has set up a site with useful visa information:

<http://www.aps.org/intaff/visa/index.cfm>
APS March 2005 Meeting attendees who require visas to enter the U.S. should consult this site. The issuance of visas may currently require up to several months; therefore, visa applications should be made well in advance of the March 2005 meeting.

2.9.1 Wide Band Gap Semiconductors (DMP)

Significant progress has been made in controlling carrier doping, interface properties, and band gaps in wide band gap semiconducting materials, including oxides, nitrides, and carbides. Within this session, areas of interest will include studies of carrier doping, ferromagnetism in transition metal doped materials, alloy doping for band gap, lattice spacing, and polarization effects. Structures of interest will include single crystals, thin films, superlattices, heterostructures, quantum dots, and nanowires. Novel devices and dissimilar materials integration will also be considered.

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3.9.3 Lattice Dielectric Properties of Complex Oxides and Semiconductor-Oxide Interfaces (DMP/FIAP)

Exciting new classes of device applications are becoming viable because of advances in ultrathin film growth of epitaxial multifunctional oxides and oxide-semiconductor systems. A thorough understanding of the dielectric coupling of complex oxides on semiconductor substrates, especially in the context of heterostructures and heterointerfaces, will be a prerequisite for future device technology development. Central issues such as the stability of and the electrostatics at the interface already dominate the field and need to be addressed in the broadest perspectives. This session will focus on fundamental experimental and theoretical advances in this area. Special attention will be given to piezoelectric, ferroelectric and multiferroic oxides and their solid solutions, and to high-K dielectrics (including epitaxial single-crystal perovskites as well as transition-metal oxides and silicates) and their interfaces with semiconductors. The main themes will revolve around the structural and electronic properties and their interplay both from an experimental and theoretical point of view. Some of the areas to be covered are: the characterization of the geometrical and electronic structure of dielectric-semiconductor interfaces and the role and importance of interface phases that are system-specific and tunable; the consequences of band alignment, charge accumulation, and defects for the

properties of semiconductor-oxide interfaces; the role of lattice coupling in multifunctional heterostructures and of order parameter coupling in multifunctional single phase systems; understanding of how the lattice dielectric constant varies with crystal structure, composition, and chemical substitution; size effects in ferroelectrics and novel applications of electrostatic boundary conditions, such as electric-field induced structural phase transitions.

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4.14.4 Organic Electronics, Photonics and Magnetics (DMP/DPOLY)

Organics, both small molecules and polymeric materials, are actively investigated for a wide range of electronic, photonic, magnetic physics and device applications. This focus session considers the latest developments in these fields. Contributions are solicited in the areas of organic conductor, semiconductor, and magnetic physics. The broad range of topics include electronic structure, charge transport, optics and non-linear optics, photonic crystals, magnetism and spin transport studies. Contributions of device physics may include electric and magnetic field effects, FETs, LEDs, photovoltaics, lasers, spin valves, and sensors. Both theoretical and experimental papers will be presented. Studies at the nano- and meso-scale are welcome.

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6.11.2 Magnetic Nanoparticles, Nanostructures and Heterostructures (DMP/GMAG)

This session focuses on emerging magnetic properties at the nanometer-scale. Magnetic nanostructures include films, multilayers, nanocomposites, hybrid structures, wedges, nanowires, magnetic point contacts, nanoparticles, self-organized and ordered nanoparticle arrays, and patterned films. This session will cover experimental and theoretical advances in low-dimensional magnetism, proximity effects, interlayer magnetic coupling, exchange spring, exchange bias, magnetic quantum confinement, magnetic anisotropy, effects of structural disorder, hysteresis modeling, and other magnetic phenomena. Of special interest are the fabrication of nanostructures with atomic-scale control, synthesis and assembly of nanoparticles and arrays, high-resolution characterization methods with site and/or element specificity, novel techniques for the creation of nanoscale magnetic features, and other unusual physical phenomena present in these systems.

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6.11.3 Phase Complexity and Enhanced Functionality in Magnetic Oxides (DMP/GMAG)

Magnetic materials with several strongly-coupled physical degrees of freedom are susceptible to microscopic phase complexity which has been found to be conducive to high-functionality. One important example of the enhanced functionality in response to external magnetic fields is the colossal magnetoresistance effect in manganites which directly correlates with multi-scale phase coexistence. Other examples include large magneto-electric effect, magneto-capacitance effect, and magneto- calorimetric effect in complex materials.

6.11.1 Theory and Simulation of Magnetism and Spin Dependent Properties (DCOMP/DMP/GMAG)

The purpose of this focus topic is to explore recent advances in theory and modeling of magnetic and spin dependent properties of materials. The topic will include methods and materials systems as well as magnetic and spin dependent properties. Of particular concern are magnetic materials in reduced dimension, where surface and interface effects become increasing dominant and influence the spin structure, spin dynamics and spin transport. Thus it is expected that a significant part of this focus topic will be devoted to theoretical and computational issues in connection with magnetic nanosystems such as 2D-multilayers, 1D-wires, 0D-particles, molecules, and impurities; including metals, alloys, magnetic semiconductors, magnetic oxides and magnetic molecules in various environments (isolated structures as well as embedded in the bulk and on surfaces). Properties include magnetic structure, mechanisms of exchange coupling, anisotropy, spin-dynamics, damping mechanisms, domain structure, hysteretic phenomena, phase transitions, magneto-optics, spin transport, spin injection and quantum tunneling. Methods include first-principles density functional theory based methods (LDA, etc) as well as new developments for strongly correlated systems (such as LDA plus dynamical mean field theory), spin models, Monte Carlo and spin dynamics methods, and micromagnetic modeling. Of particular interest are methods for multiscale modeling that bridge length scales and approaches to extend the time scale of simulations.

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Scientific understanding of the interrelationship between phase complexity and macroscopic physical properties is of prime importance for controlling the technological functionality of complex materials, and will be the main focus of the session. Experimental, theoretical and computational investigations in this topic, of both of fundamental and applied nature, will be addressed. Among the main goals is an understanding of the relation between magnetic and electronic properties with other physical phenomena such as magneto-transport, lattice, elastic and magnetic excitations, surface behavior, and electron correlation effects. The similarities between the many different compounds will be emphasized.

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6.11.4 Spin Transport and Magnetization Dynamics in Metal-Based Systems (GMAG/DMP)

This focus session will focus on experimental and theoretical investigations that elucidate and/or utilize the transport and transfer of spin in metal-based magnetic systems. Studies that emphasize spin phenomena in semiconductor systems will be covered in a separate focus session. Topics of interest include all aspects of spin-dependent transport and scattering, in the diffusive, ballistic, tunneling and hot electron transport regimes as evidenced, for example, in giant magnetoresistance (GMR), tunneling magnetoresistance (TMR), ballistic magnetoresistance, tunneling spectroscopy of spin states, spin filtering and related effects. Also of particular interest are studies of the interplay between non-equilibrium carriers and magnetization dynamics in point contacts, magnetic pillar structures and magnetic nanowires. Additional topics include, but are not limited to, interfacial spin transport, spin injection and detection, spin relaxation time, damping mechanisms in ferromagnets, and spin-current-driven domain wall dynamics, as well as studies in ferromagnetic - normal metal and ferromagnetic - superconductor systems.

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6.11.5 Spin-Dependent Phenomena in Semiconductors (DMP/GMAG)

Recent progress in the understanding of spin-dependent phenomena in semiconductors has resulted from a combination of research on fundamental optical and transport properties as well as innovative materials science and device development. This focus topic addresses spin injection, manipulation, transport, and detection in conventional as well as ferromagnetic semiconductors. Abstracts are solicited in the general areas of 1) spin dynamics and transport in semiconductors, including spin transport in mesoscopic systems, electrical spin injection and detection, optical spin injection and detection, optical and electronic control of spin coherence, effects of spin-orbit coupling, and hyperfine effects; 2) growth, characterization, electronic structure, and electrical and optical control of magnetic properties in ferromagnetic semiconductors; 3) ferromagnet-semiconductor devices, including new approaches to spin injection and detection; and 4) developments in related fields, such as organic semiconductors and quantum computing, that relate to spin-dependent phenomena in semiconductors.

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7.9.1 Simulation and Theory of Complex Materials (DCOMP/DMP)

Advances in computational methods to address materials and condensed matter problems continue to develop in producing exceedingly realistic simulations of physical

phenomena as well as providing predictions and enhancement of various properties for length and time scales that span from the subatomic, to atomic, to mesoscopic and even to the continuum limit. In this focused topic the recent progress in such simulations will be demonstrated for a wide spectrum of applications. Here complex systems signify those systems with spatial complexity, systems with a large number of structural units (atoms or molecules) and/or systems of multidimensional and multi-component character. The computational approaches may include implementation of large scale density functional calculations, model Hamiltonians in many-body theory, simulations based on empirical potentials, as well as Monte Carlo, coarse graining, accelerated dynamics and kinetic theory techniques. Applications of these methods are suitable to simulate the behavior of periodic, disordered and defect-containing systems including metallic, semiconducting, insulating and magnetic states of matter. Abstracts with applications to biological systems and those that directly link computational findings to experimental data are also encouraged.

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7.9.2 Nanotubes and Nanowires: Devices and Applications (DMP)

Nanotubes and nanowires are fabulous one-dimensional materials with diverse properties and enormous potential applications. This focus session is dedicated to recent developments in novel device and application studies based on carbon nanotube and various nanowires. This includes, but is not limited to: (1) applications of nanotubes and nanowires to electronic, spintronic, photonic, mechanical, and sensing devices, (2) self-assembling, manipulation and integration of nanotube and nanowire devices into nanosystems, (3) the theory of nanotube and nanowire device operation and system integration, (4) the physics needed to understand the materials properties of nanotubes and nanowires relevant to device applications. Experimental and theoretical submissions are solicited in the following topical areas: 1) nanoelectronic devices and systems (e.g. transistors, memories and spintronic

devices), 2) nanophotonic devices (e.g. light emitting diodes, photovoltaic cells and lasers), 3) mechanical, electromechanical and field-emission devices (e.g. field-emission tips, mechanical resonators and switches) and 4) chemical and biological sensors (gas sensors, protein and DNA sensors).

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7.9.3 Light Emission from Silicon (FIAP/DMP)

Efficient light emission from silicon is still the holy grail of silicon technology. Several recent developments have catapulted silicon light emission into the headlines, promising room temperature lasing in the near future. Several different approaches have been used to increase internal efficiencies to more than 10%. Additional challenges are encountered in the design of laser structures on the basis of Si-light emission. In this focus topic we plan to evaluate progress and discuss the physics of visible and near IR light emission from silicon-based light emitters. The areas of interest are: (1) silicon nanostructures – nano-crystalline (nc) Si, quantum wires, quantum dots; (2) Er-based light emission of silicon-based materials; (3) Efficient intrinsic and impurity-related light emission in silicon; (4) current Si-based LED's and device designs for Si-based lasers

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7.9.4 Novel and Complex Oxides (DMP/FIAP)

Transition metal oxides (TMOs) have been at the forefront of materials physics since the discovery of superconductivity in the cuprates in 1986. In general, TMOs are characterized by physical complexity resulting from the coexistence and competition between different kinds of order involving charge, orbital, lattice, and spin degrees of freedom. The complexity of TMOs is directly responsible for their tunability; the balance between competing phases is subtle and small changes in the composition of a sample or its external environment can produce large changes in its physical properties. An astonishing variety of ground states and new phenomena have been uncovered in recent years. It is both their complexity and tunability that make TMOs attractive for applications. This focus session will focus on novel phenomena and new forms of order in oxides other than the well-studied cuprates and manganites.

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7.9.5 Carbon Nanotubes and Related Nanomaterials (DMP)

Broad interest in the fundamental properties of carbon nanotubes and their exploitation in a wide range of applications continue at an increasing pace, due in large part to their unique chemical, mechanical, thermal, optical and electrical properties. This focused topic concerns recent developments in (1) the fundamental understanding of nanotube properties, including synthesis, processing, purification, electrical, optical, thermal, mechanical, and chemical properties and (2) on potential applications, such as nanosensors, nanopropes, field emitters, display devices, field-effect devices, composite

materials, and high surface area storage media. Experimental and theoretical contributions are solicited in the following areas: 1) synthesis and characterization of carbon nanotubes, nanohorns, and nanotube peapods, 2) optical spectroscopy of carbon nanotubes, 3) electrical transport in carbon nanotubes, 4) thermal and magnetic properties of carbon nanotubes, 5) mechanical properties of nanotubes and their composites, 6) chemical functionalization, properties, and separation techniques 7) electronic properties and devices, 8) gas adsorption and storage, 9) field emission, 10) structure and properties of filled carbon nanotubes, 11) multifunctional nanotube composites and 12) other experimental and theoretical results from quasi-one dimensional systems which relate to carbon nanotubes.

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7.9.6 Computational Nanoscience (DAMOP/DCOMP/DMP)

When the size of the physical systems is reduced to the nanometer scale, many novel physical phenomena emerge. Computational studies can be used to both interpret experimental observations of these phenomena and provide much-needed insight into their underlying physical origin. Recent advances in computational methodologies for studying nanoscale materials have made it possible to reliably predict many physical and chemical properties of nanostructures. This session will provide a comprehensive overview of recent computational work in the field of nanoscale materials. Abstracts are solicited to address all issues related to the physics at the nanoscale. Subjects to be covered include, but are not limited to, classical,

semi-empirical and ab-initio simulations of the growth, structural, mechanical, vibrational, opto-electronic and reactivity properties of nanoscale quantum dots and wires.

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7.9.7 Theory of Nanotubes and Carbon Based Nanostructures (DCOMP/DMP)

Within the few years since their discovery, carbon nanotubes have emerged as pioneering materials of the flourishing research field of nanotechnology. This field experienced a rapid expansion with the recently realized ability to create new complex carbon-based nanostructures. Some of these are obtained by functionalizing nanotubes or filling them with nanostructures such as fullerenes, others are very different carbon-based nanostructures such as schwarzites or diamondoids. All of these systems exhibit an ever expanding range of intriguing physical phenomena. Unlike in other emerging areas of nanotechnology, the research effort in carbon nanostructures has been driven by theoretical predictions of unexpected properties such as their conductance depending crucially on their chirality, their high mechanical rigidity and toughness, their unusual high thermal conductivity. Other fundamental predictions, such as realization of one-dimensional magnets or the statistics of the electron gas related to that of a Luttinger

liquid, have not yet been confirmed definitely by experiments. This focus topic is designed to provide an updated and comprehensive overview of the recent theoretical work in the field of nanotubes and carbon based nanostructures. Theoretical abstracts are solicited to address all issues related to nanotubular materials, their composites, and other carbon based nanostructures including nanocrystalline diamond, fullerenes, metallofullerenes and nanotube peapods. Subjects to be covered include: growth, structural, mechanical, electronic, transport, optical and field emission properties, electronic excitations and correlation effects, phenomenology, device development, functionalization, and energy storage.

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9.9.1 Intrinsic Inhomogeneity in Multiferroic Materials (DMP)

Static and dynamic fluctuations arise over a wide range of length scales in chemically homogeneous single crystal bulk and thin film samples of transition metal oxides with strong electron correlation. Modern experimental techniques are currently revealing the nature of these fluctuations, and hitherto unknown forms of order over nano-scale to mesoscopic distances. Moreover, there is growing interest in multiple order parameter oxides. For example, there are multiferroic materials that display coupled ferromagnetic and ferroelectric order parameters within a single phase. The purpose of this focused session is to exploit the collective expertise across a range of related oxide materials systems in order to achieve an overview that describes the nature, enhancement, coupling and texture of single and multiple order parameters.

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12.9.1 Friction, Fracture and Deformation (DMP/GSMP) (same as 12.10.1)

This session will explore recent developments in the areas of friction, fracture, and deformation in materials; research areas that have recently drawn renewed interest within the physics community. This session covers all length scales from the nanometer to tectonic scales. Topics of interest include tribochemistry, nano-scale mechanics, dislocation patterns, grain boundary and interface effects, fracture initiation, crack propagation, tribology of smooth and rough surfaces including fractal interfaces. The session welcomes experimental, computational, and analytical studies of atomistic, mesoscopic, statistical, and multi-scale aspects of deformation, friction, and fracture instabilities in various classes of solids, including granular, crystalline, amorphous, micro-fabricated and nano-structured solid systems of metallic, silicon-based, ceramic, glassy, or polymeric type.

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13.9.2 Optical Properties of Nanostructures and Nanophotonics (DMP)

The confinement of electromagnetic radiation and its interaction with nanostructured materials is an important area of research driven by technological and scientific challenges. In the technology arena, nanophotonics may enable high optical data storage densities or high bandwidth data transmission capacities in all-optical telecommunications networks, as well as nanoscale lithography of semiconductor devices. There is also a strong fundamental scientific interest in the unique optical physics that can be driven by the electromagnetic near-fields surrounding nanostructures. Areas of interest are broad, with ramifications in fields ranging from condensed matter physics to biological nanostructures. Specific examples would be collective near-field interactions in plasmonic devices for the transport of energy or new biochemical sensor materials utilizing large enhancements for single molecule sensitivity. In this focus session, we invite a broad range of contributions dealing with advances in the generation, characterization, and theory of nanooptical materials. General areas of interest include but are not limited to: colloidal nanoparticles, quantum dots and quantum wells; plasmonic materials and devices; hybrid nanoparticle heterostructures; self-assembled nanostructures; lithographic structures and waveguides; nano-phosphors; optoelectronic nanomaterials; functional nanomaterials and nanostructured devices for optical storage, information processing and other optical applications; photonic band-gap materials and metamaterials (left-handed materials).

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13.9.3 Materials for Molecular Electronics (DMP)

This focus session will address the use of materials for molecular electronics, ranging from single molecules to single

crystals of molecular conductors (e.g. pentacene). The session will examine theory, experiment, and device applications of physical phenomena in these material systems. Of particular interest are linear and nonlinear charge transport, trapping mechanisms, field effect devices and the effects of morphology, extending from single molecules to polycrystalline structures to single crystals.

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13.9.4 Materials and Device Physics: Issues for Quantum Computing (DMP)

The area of quantum computing has emerged in the past decade from a theoretical curiosity to a significant sub-field of many physics departments and other research institutions. The time seems ripe for a more concerted effort to explore materials and device issues for potential hardware realizations of important quantum computing and quantum information science applications. This focus session is aimed toward this goal: to define the current state-of-the-art of quantum computing strategies and hardware devices, to define new device concepts and materials issues associated with them, and to determine the limitations of current proposed quantum computing devices and strategies. Abstracts in any of these areas are encouraged. For further information please contact one of the co-organizers listed below.

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14.9.2 Morphology and Composition Evolution in Thin Films and Surfaces (DMP)

Exploiting growth and kinetic instabilities to form surface nanostructures and patterns has emerged as a key element in strategies for nanoscale fabrication. The success of this approach depends on understanding the evolution of thin-film morphology, electronic structure and composition. This focus session will highlight recent experimental and theoretical developments associated with the formation and stability of nanostructures, surfaces, thin films and interfaces.

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14.9.3 Fundamental Challenges in Transport Properties of Nanostructures (DMP)

This focus topic will address the issues which are critical to our understanding, characterization and control of transport phenomena in nanostructures including molecular devices, carbon nanotubes, semiconductor nanowires, quantum dots, single-electron devices and other novel structures. The contributions are solicited in the following areas: 1) fabrication of

nanostructures including synthesis, self assembly and other bottom-up approaches, novel lithographic and other top-down techniques, and integration with contacts; 2) structural characterization of materials and interfaces at the nanoscale relevant for understanding and controlling transport properties; 3) theoretical advances in modeling structural and transport properties of nanoscale systems; 4) experimental and theoretical studies of transport properties of nanoscale structures and devices.

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19.9.1 Earth and Planetary Materials (DCOMP/DMP)

This focus session on Earth and Planetary Materials will highlight new experimental, computational and theoretical approaches toward understanding a variety of materials in the interiors of Earth-like and Jovian planets. The main interest lies in the exploration of ices, fluids, minerals as well as more complex and imperfect planetary materials over an enormous range of thermodynamics conditions. Recent advances in theoretical and experimental techniques have led to breakthroughs in our understanding of the physical and chemical properties of Earth materials that were deemed inconceivable only a few years ago. For example, recent progress in laser-based spectroscopy, the second- and third-generation synchrotron sources, neutron scattering, high pressure-temperature instrumentation and high-end computing power has fundamentally altered how we quantify Earth materials and their interaction with the local environment. Of particular importance is that we now have *in situ* methods that make possible the determination of the properties and behavior of Earth materials under conditions ranging from extreme deep-earth temperatures and pressures to ambient conditions. The goal of the Earth and Planetary Materials session will be to explore research in this area, the technological edge that makes it possible, and the science that inspires it.

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19.9.2 Simulations of Matter at Extreme Conditions (DCOMP/DMP)

Such varied phenomena as the atmosphere of a white dwarf star, the interior of an extra solar planet, an atomic cluster subjected to an intense radiation field, shock compression phenomena, or a cell membrane under strain, all represent basic materials under extreme conditions. Despite their diversity, a close correlation exists among the methods employed in the description of these media. This focus session concerns recent advances in theoretical and computational studies and methodologies applied to metallic, organic/inorganic, and biological materials as well as liquids, plasmas, and atomic/molecular clusters exposed to high pressures, temperature extremes, external fields, or interactive environments. Contributed and invited presentations will include such diverse computational approaches as atomistic (quantum, semi-classical, and classical), mesoscopic (grain-scale), continuum, and multi-scale. Representative scientific areas of interest are: 1) deformation and fracture, 2) equation of state, 3) phase transitions, 4) chemical events, 5) shocked energetic materials, 6) unusual behavior, 7) intense field interactions, 8) biological systems and 9) environmental effects.

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