

NEWSLETTER

Division of Materials Physics

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Summer 2007

Dates to Remember

Friday August 31, 2007: Deadline for submitting invited speaker suggestions for DMP Focus Topics

Tuesday November 27, 2007, 5:00 pm EST: APS Abstract deadline submitted via the web at http://abstracts.aps.org

Monday March 10 to Friday March 14, 2008 (with tutorials, etc., on March 9): APS March Meeting in New Orleans, LA

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 2008 APS March Meeting (New Orleans, LA, March 10-14, 2008). 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.

DMP members are encouraged to make suggestions for invited speakers for Focus Topics. The deadline for submitting suggestions is August 31, 2007. Suggestions can be made by emailing the suggestion directly to the appropriate focus topic organizers who are listed after the Focus Topic descriptive paragraphs. Also, please send a copy to Ivan Schuller (ischuller@ucsd.edu), the main DMP organizer of Focus Topics.

Your suggestions should provide the following information:

- 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.
- A brief justification of the nomination (880 character limit, including spaces).

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 be posted at this location, too.

Nominations for DMP Officers and Executive Committee Members

A DMP election will be held in late 2007 to select a Vice Chair, a Secretary-Treasurer, and two new At-Large Members of the Executive Committee. Suggestions for nominees may be sent by 1 September 2007 to DMP Nominating Committee Chair David Vanderbilt (dhv@physics.rutgers.edu). In addition, DMP bylaws provide that the slate determined by the Nominating Committee can be augmented with additional names by a petition process. Such a petition, expressing the wishes of at least 5% of the DMP membership, must be received by DMP Secretary-Treasurer Ted Einstein (dmpsectr@physics.umd. edu) by 1 October 2007.

A Note from the Chair

It a pleasure to welcome you to the current newsletter of the Division of Materials Physics. The organizers for the Focus Topics for the upcoming March meeting in New Orleans have been chosen and are listed in this newsletter, and this is the time to input your suggestions for invited speakers; your input should go directly to the FT organizers who are preparing invited speaker nominations for their topic. DMP also sponsors a few select symposia, and these suggestions should go directly to Ivan Schuller, the DMP Program Chair this year. This is your meeting, so please make the effort to contribute to its organization and help identify the best and most deserving invited speakers in your area of expertise.

In more general terms, this is a particularly exciting time for our area of research because of the strong and increasing support of the Federal Government. The President's American Competitiveness Initiative (ACI), which grew out of the National Academy Report entitled "Rising Above the Gathering Storm" requested by Congress, has strong bipartisan support. However, Congress did not pass a budget before the election, and then the new Congress decided to postpone any real budget decisions by enacting a year-long continuing resolution. Nevertheless, the strong support of the ACI allowed it to be one of a very few exceptions, and it was enacted this year despite the continuing resolution, a truly phenomenal political result. The ACI calls for doubling the budget, in real terms, over the next several years. The ACI funding has been implemented to a large extent this year, and Congressional support looks quite promising for the coming budget cycle. The Materials Physics community owes a debt of gratitude to the scientists who made the case and to the politicians who heard the plea and acted. This success also highlights the positive effects of contacting your congressional representatives, such as the congressional letter writing campaign organized at the March meeting. Contacting your congressional representatives really helps! And it's just as important now to continue these efforts, to maintain the momentum that has been developed. Speaking of momentum, there are some noteworthy items and trends contained in the National Academies decadal report just released on the current state of the materials research enterprise and future directions of the field: CMMP 2010: An Assessment of and Outlook for Condensed-Matter and Materials Physics.

Finally, I would like to take this opportunity to thank the members of the 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 Art Hebard and Julia Hsu, who have stepped down as Members at Large. And a special thanks to Lynn Boatner, who has completed four years of leadership as Vice-Chair, Chair-Elect, Chair, and Past-Chair of the Division of Materials Physics. Thanks. Looking forward to seeing you in New Orleans.

Jeff Lynn, Chair

List of DMP-Sponsored or Co-Sponsored Focus Topics and Sorting Categories for the 2008 APS March Meeting

The co-sponsoring units are indicated in between parentheses.

02.8.2

Dopants and Defects in Semiconductors (DMP)

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The properties of semiconductors are determined by the presence of small concentrations of impurities and defects (10¹¹-10¹⁹ cm⁻³). Defects control carrier concentration, mobility, lifetime, and recombination and sometimes act as compensation centers; also they are responsible for processes that involve atomic transport such as migration, diffusion, and precipitation of impurities and host atoms. The control of defects and impurities is the critical factor that enables a semiconductor to be used in electronic and optoelectronic devices as has been widely recognized in the remarkable development of Si-based electronics, the difficulties encountered with II-VI based optoelectronics, and the recent success of the GaN-based blue LED and lasers. The fundamental understanding, characterization and control of defects are proving to be important for the development of novel wide-band gap semiconductors and future solid-state based spintronic devices. The physics of doping and defects in semiconductors is the subject of this focus session. The electronic, structural, optical, magnetic and isotopic properties of dopants and defects in elemental, compound, and wide band-gap semiconductors are of interest. Abstracts on experimental and theoretical investigations are solicited.

03.8.1

Dielectric, Ferroelectric and Piezoelectric Oxides (DMP)

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This topic will focus on fundamental advances in the growth, characterization, and experimental as well as theoretical understanding of dielectric, ferroelectric, pyroelectric, piezoelectric, and multiferroic oxides in bulk, thin-film, superlattice, and nanostructured forms. Contributions on functional oxides of all structure types are encouraged. Areas of interest include the physics of structural and ferroelectric phase transitions, lattice dielectric properties, coupling in multiferroics, the impact of disorder on cooperative behavior, progress in theory approaches to ferroelectricity, multiferroicity, and relaxor behavior, as well as understanding of synthesis and growth mechanisms. A major thrust will be to explore how bulk dielectric, ferroelectric, piezoelectric properties and the coupling of order parameters are modified in thin-film, superlattice, or other nanoscale geometries, for example by the effects of strain, surfaces and interfaces, chemical environment, and electrical boundary conditions.

04.14.4

Organic Electronics, Photonics & Magnetics (DM/DPOLY)

Lynn Loo, Univ. of Texas, lloo@che.utexas.edu **Jim Kushmerick**, NIST, james.kushmerick@nist.gov

The incorporation of organic materials into device architectures has made great strides in recent years. This symposium will explore the fundamental physics which dictate the performance and behavior of organic electronic, photonic and magnetic systems. Specific subtopics include, OFETs, OLEDs, organic photovoltaics as well as organic magnets. Special attention will be given to understanding the organic -inorganic interface.

05.17.1

MgB₂ & Other Novel Superconductors (DMP)

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Warren Pickett, pickett@physics.ucdavis.edu

The discovery of phonon-mediated superconductivity with high critical temperature in MgB₂ offers significant lessons for the search of high temperature BCS superconductors. Since then other non-cuprate superconductors with novel properties also have been discovered. Meanwhile, new physics arising from the multiband effects in MgB, has attracted considerable theoretical and experimental efforts. Some of these effects have important implications for high-magnetic-field and electronic applications. This focus topic will cover both theoretical and experimental results on MgB, and other novel superconductors such as electron-doped (Zr,Hf)NCl, Y,C3, and metals with covalent bonding. The subjects include various aspects of two-band superconductivity such as dependence of the two gaps on disorder and magnetic field, studies of phonons and electron-phonon coupling, vortex dynamics and flux pinning, and the Josephson effect and devices. Theoretical insights and experimental investigations of existing and predicted novel superconductors are important aspects of this focus topic.

05.17.2

Electronic and Vortex Mechanisms for Higher Performing Superconductors (DMP)

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There is a growing recognition that in order to exploit superconductors for energy challenges (especially the Electric Grid of the future) transformational breakthroughs are needed in superconductor performance. Further, the need is far more than just higher Tc materials but rather a comprehensive understanding of vortex matter (both from a phenomenological and microscopic perspective). This includes mechanisms and methods for generating and manipulating vortices, so called 'pinscape engineering,' and a microscopic theory of vortex creep dynamics. Directly coupled to this is a clearer understanding of the electronic mechanisms that give rise to unconventional pairing states and novel magnetic field-temperature phase diagrams. Fortunately, remarkable progress is being made in this area, exploiting nanotechnology to both produce and characterize these pinning landscapes and

the inhomogeneity that appears to be intrinsic in superconductors displaying strong correlation. This focus topic will bring together the leaders who are making these advances and would have as a specific objective of bridging the usually disparate communities that focus on one hand on the epitaxial science for enhancing critical current and on the other hand of exploring fundamental aspects of vortex physics. The recent success of the Department of Energy-Office of Basic Energy Sciences workshop on "Basic Research Needs for Superconductivity" indicates the time is right for bringing these communities together for extended technical discussions.

05.17.3 Hybrid Magnetic-Superconducting Systems (DMP)

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The focus session will be dedicated to hybrid superconducting/magnetic structures from the theoretical as well as the experimental point of view. The main subjects include superconducting/magnetic multilayers and nanostructures, magnetic proximity effect and Andreev reflection, and exotic magnetic phases in superconductors. Special attention will be paid to non-centrosymmetric superconductors both with singlet and triplet pairing, Fulde-Ferrell-Larkin-Ovchinnikov states, heterojunctions with non-collinear magnetizations, pi-phase junctions, superconducting/magnetic hybrids with spiral magnetic structures, Josephson effects involving half metallic systems, and complex oxide ferromagnet/superconductor multilayers.

06.11.1

Theory & Simulation of Spin Dependent Effects & Properties (DCOMP/DMP/GMAG)

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This focus topic centers on recent advances in the theory and numerical simulations of spin-dependent properties of magnetic materials and structures. Covered phenomena include magnetic hysteresis, spin transport, spin relaxation, spin torque, exchange spring, exchange bias, interlayer magnetic coupling, anomalous Hall effect, and dynamics of topological defects. Particular attention will be paid to magnetic systems with a reduced number of spatial dimensions from 0D molecular magnets and nanodots to 1D nanowires and 2D thin films and interfaces. Approaches include material-specific ab-initio techniques (LDA and beyond) as well as a combination of these methods with multi-scale modeling, atomic-scale effective spin Hamiltonians, Monte-Carlo simulations, Langevin dynamics, and micromagnetic modeling. We especially encourage contributions showing the benefits of cross-pollination between analytical and numerical approaches for explaining and predicting specific experimental results and materials or systems properties.

06.11.2

Magnetic Nanostructures: Materials and Phenomena (DMP/GMAG)

Dan Ralph, Cornell Univ., ralph@ccmr.cornell.edu **Sergei Urazhdin**, West Virginia Univ., sergei.urazhdin@mail.wvu.edu

This topic focuses on magnetic materials and phenomena at the nanometer-scale. Magnetic nanostructures include thin films, multilayers, nanoparticles, nanowires, nanorings, nanocomposites,

core-shell structures, hybrid structures, magnetic point contacts and self-assembled as well as patterned magnetic arrays. This session will cover both experimental and theoretical advances in low dimensional magnetism, proximity effects, interlayer magnetic coupling, exchange spring, exchange bias, magnetic quantum confinement, magnetic anisotropy, glassy dynamics, memory effect and other relaxation phenomena, inter-particle interactions, effects of structural disorder, modeling of hysteresis, thermal and quantum fluctuations, and other nanoscale magnetic phenomena. Of special interest is the fabrication of nanostructures with atomic-scale control using physical and chemical methods, self and directed assembly of nanostructure 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.

06.11.3 Complex Oxides (DMP/GMAG)

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Transition metal oxides exhibit a wide range of intriguing phenomena which originate from the complexity induced by the close competition of multiple interactions and the presence of various ground states with incompatible order. Associated with this complexity is a tendency for short range order such as the formation of stripes, ladders, checkerboards, dimers, or phase separation, and an enhanced response to external fields that gives rise to giant and colossal effects with potential for applications. This Focus Topic explores the nature of the various ground states observed in these complex oxides and the interactions responsible, the ways in which the spin, charge, orbital, and strain degrees of freedom respond on a variety of length scales, how they interact and compete with each other to produce the unusal phenomena in the bulk and film, and how they change near surfaces and interfaces and in particular near interfaces between two such systems with competing groundstates, where novel phenomena may occur. It provides a forum to discus recent developments and results covering basic and applied aspects from synthesis and fabrication to experiment, theory and simulation of bulk, films, and artificial superlattices of complex oxides, including multiferroics, manganites, nickelates, cobaltites, ruthenates, and their interfaces.

06.11.4+ 16.12.10

Spin Transport & Magnetization Dynamics in Metal Based Systems (GMAG/DMP/FIAP)

Eric Fullerton, Univ. of California-San Diego, efullerton@ucsd.edu **M. Tsoi**, Univ. of Texas, tsoi@physics.utexas.edu

This topic will focus on experimental and theoretical investigations of the transport and transfer of spin, as well as magnetization dynamics, in metal-based magnetic systems. 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), tunneling spectroscopy of spin states, spin filtering and related effects. Furthermore, a main focus will be magnetization dynamics in confined geometries investigated both in the time and frequency domain. Also of particular interest are studies of the interplay between spin currents and magnetization dynamics in magnetic nanostructures. Additional topics include, but are not limited to, spin-charge-separation in transport processes including spin-diffu-

sion and spin-relaxation, interfacial spin transport, spin injection and detection, mechanisms for magnetic damping, especially in magnetic nanostructures, spin-current-driven magnetization and domain wall dynamics, and studies in ferromagnetic — normal metal and ferromagnetic — superconductor systems. Studies that emphasize spin phenomena in semiconductor systems will be covered in a separate focus topic.

06.11.5

Spin Dependent Phenomena in Semiconductors (GMAG/DMP/FIAP)

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Since the discovery of ferromagnetism in GaMnAs and very long spin lifetimes in semiconductors and semiconducting nanostructures, there has been growing interest in exploring the spin dependent properties of a variety of semiconductors, particularly after the successes of metallic spintronic heterostructures for magnetic storage. This series of sessions solicits contributions focused on ferromagnetism in semiconducting materials, novel effects in semiconductors either because of large spinorbit interactions or the lack of such interaction, spin injection, spin Hall effect, spin interference, spin filtering, spin lifetime effects, spin dependent scattering, spin torque and domain structure and motion. Also solicited are memory and logic device based structures. We expect that there will be multiple sessions spanning the meeting.

07.11.1

Carbon Nanotubes & Related Materials (DMP)

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Interest in the fundamental properties and applications of carbon allotropes, including carbon nanotubes, graphene, and patterned graphene, continues to grow. The reason for this interest lies in the unique combination of chemical, mechanical, thermal, optical, opto-electronic, spectroscopic, electrical and magnetic properties of these systems.

This focus topic addresses recent developments in (i) the fundamental understanding of nanotubes and graphene, including characterization, synthesis, processing, purification, chemical, mechanical, thermal, electrical, optical, opto-electronic and magnetic properties, and (ii) in their potential applications as nanosensors, nanoprobes, field emitters, displays, field-effect transistors, composite materials, high surface-area storage media, superconducting and magnetic devices, and others.

Experimental and theoretical contributions are solicited in the following areas:

- synthesis and characterization of pure and doped nanostructures of carbon and boron nitride, including nanotubes, nanohorns, and graphene;
- 2) purification, separation and chemical functionalization of these nanostructures;
- the structure and properties of hybrid systems, including filled carbon nanotubes, nanotube peapods, and chemically modified graphene;
- 4) mechanical and thermal properties of these nanostructures and their composites;

- 6) electrical and magnetic properties of these systems; and
- their spectroscopic (angle resolved photoemission and scanning tunneling microscopy), optical (Raman scattering), structural (atomic force microscopy), opto-electronic, mesoscopic, and transport properties.

Also, the symposium will cover the broad range of unique applications of these nanosystems, including their use for:

- 7) gas adsorption and storage;
- 8) multifunctional nanotube composites;
- 9) chemical and bio-sensing applications;
- 10) field emission; and
- 11) a new generation of magnetic and electronic devices.

07.11.3

Computational Nanoscience (DMP/DCOMP)

Eric Schwegler, Lawrence Livermore National Labs, schwegler@llnl.gov **Serdar Ogut**, Univ. of Illinois, ogut@uic.edu

Jim Chelikowsky, Univ. of Texas, jrc@ices.utexas.edu

When the size of a physical system is reduced to the nanometer scale, many novel physical phenomena emerge. Computational studies can be used to interpret experimental observations of these phenomena, provide much-needed insight into their underlying physical origin, and thus enable the design nanomaterials with desired properties. Recent advances in computational methodologies for studying nanoscale materials have made it possible to reliably predict many physical and chemical properties of nanostructures that span multiple time and length scales. This session will provide an overview of recent computational work in the field of nanoscale materials with particular emphasis on techniques that allow for an efficient multi-scale integration from the micro- to the nanoscale. Subjects to be covered include, but are not limited to, computational studies of the growth, structural, mechanical, vibrational, electronic, opto-electronic and catalytic properties of nanoscale structures and materials and the interplay between functionality and local structural environment.

07.11.4

Probing and Modifying Materials with Lasers: Fundamentals and Applications (DMP)

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This session focuses on materials physics issues involved in laser-materials interactions including those relevant to a variety of laser-driven techniques used for material removal, processing, and deposition. Also, we wish to consider laser based diagnostics techniques that probe transient atomic and molecular dynamics as well as electronic and vibrational phenomena in materials and at surfaces. The session aims to bring together researchers involved in experimental, theoretical, and computational investigations in the general area of laser-materials interactions to facilitate active broad-ranging interdisciplinary discussions. Topics of interest include but not limited to time-resolved x-ray and electron diffraction pump-probe techniques; laser interactions with "soft materials" (molecular and polymer systems and biological tissue); effects of pulse duration, wavelength and pulse repetition frequency; generation of nanoparticles, laser nano-patterning, micro- and nano-fabrication; theory and simulations of laser-materials interactions.

12.7.1

Friction, Fracture & Deformation (DMP/GSNP)

Mark Robbins, Johns Hopkins Univ., mr@pha.jhu.edu Chris Schuh, MIT, schuh@mit.edu

Friction, fracture and plastic deformation represent strongly non-equilibrium responses of solids to mechanical perturbations. Common behavior is observed in a wide range of materials and on length scales ranging from the atomic to the tectonic. This focus topic will explore recent advances in the fundamental and mechanistic understanding of these processes using theory, experiment and computer simulation. Subjects of interest include dislocation plasticity, grain boundary and interface effects, indentation, nanoscale mechanics, friction of smooth or fractal surfaces, tribochemistry, crack nucleation and propagation, and earthquake fault structure and dynamics. Materials include metals, polymers and ceramics with local structures ranging from crystalline to amorphous and large-scale structures that are granular, microfabicated or nanostructured.

13.6.1

Optical Properties of Nanostructures (DMP)

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Advances in synthesis and material processing bring us many new nanostructures; each has its own unique optical properties that are usually different from those of the bulk counterpart. The principal aim of this symposium is to bring together colleagues from different disciplines who are interested in the characterization of optical properties of nano-structures and the understanding of the exotic phenomena at a microscopic level. The symposium will cover the theoretical and experimental research on the optical properties of a broad range of nano-structures such as nanotubes, graphene, quantum wires and quantum dots. Also, the symposium will cover the optical properties of artificial nano-structures which can be used to manipulate light at the nanoscale length through the excitation of plasmonic or structural resonances. These structures can realize useful properties such as enhanced local field, resonant transmission, reduced cross-section, enhanced near-field resolution and stronger light-matter interactions; and these exotic properties may have impact in many areas such as optical storage, lithography and sensing.

13.6.2

Fundamental Challenges in Transport Properties of Nanostructures (DMP)

Erik Isaacs, Argonne National Lab., isaacs@anl.gov **Doug NateIson**, Rice Univ., nateIson@rice.edu

This focus topic will address the fundamental issues that are critical to our understanding, characterization and control of electronic transport in electronic, optical, or mechanical nanostructures. Contributions are solicited in areas that reflect recent advances in our ability to synthesize, characterize and calculate the transport properties of individual quantum dots, molecules and self-assembled functional systems. Resolving open questions regarding transport in nanostructures can have a huge impact on a broad range of future technologies, from quantum computation to light harvesting for energy. Specific topics of interest include: fabrication or synthesis of nanostructures

involved with charge transport; nanoscale structural characterization of materials and interfaces related to transport properties; advances in the theoretical treatment of electronic transport at the nanoscale; and experimental studies of charge transport in electronic, optical, or mechanical nanostructures.

13.6.3

Materials Issues for Quantum Computing & Quantum Engineering (DMP)

Mike Lilly, Sandia National Lab., mplilly@sandia.gov

Quantum computing requires extreme control of two-level quantum systems where it is important to have both long coherence times and the ability to act on the quantum states. While there are many different qubit implementations currently being studied, solid state systems are particularly attractive due the flexibility allowed by a wide range of nanolithography techniques. The price, however, is the strong interaction between the qubit and the material system. In this Focus Session, we will explore issues related fabrication and measurement of solid state qubits. The impact of inherent material properties such as coupling to nuclear spin and bandstructure effects will be discussed. In addition, more generic material quality issues such as oxides limitations, charge traps, and various impurity states will be considered. One goal of the focus session is to bring researchers together and identify where material improvements in one system can benefit other systems.

13.6.4

Thermoelectric Materials & Phenomena (FIAP/DMP)

A. Majumdar, Univ. of California-Berkeley, majumdar@berkeley.edu

About 90 percent of the world's power (approximately 10 TW) is generated by heat engines that convert heat to mechanical motion, which can then be converted to electricity when necessary. Such heat engines typically operate at 30-40 percent efficiency, such that ~ 15 TW of heat is lost to the environment. If even a fraction of this low-grade thermal waste can be converted to electricity in a cost-effective manner, the potential impact on energy could be enormous, amounting to massive savings of fuel and reductions in carbon dioxide emissions. Thermoelectric energy converters can directly convert low-grade heat to electricity using semiconducting materials via the Peltier effect. The performance depends on the thermoelectric figure of merit (ZT) of a material, which is defined as $ZT = S^2T/rk$ where S, r, k, and T are the Seebeck coefficient, electrical resistivity, thermal conductivity and absolute temperature, respectively. To be competitive compared to current engines and refrigerators (efficiency 30-40 percent of Carnot limit), one must develop materials with ZT > 3. Yet, over the last 50 years, the ZT of materials has increased only marginally, from about 0.6 to 1, resulting in performance less than 10 percent of Carnot limit! While there is no fundamental upper limit to ZT, progress has been extremely hard to come by, mainly due to the coupling between S, r, and k – changing one alters the others. It has been shown recently that nanostructuring allows one to either use quantum confinement of carriers or spectrally-dependent scattering of phonons to manipulate S, r, and k in ways that can increase ZT beyond the bulk values. The underlying reasons for this increase are, however, not yet fully understood. The goal of this session is to bring together scientists and engineers focused on quantum and classical transport and coupling of charge and heat in thermoelectric materials in order to increase ZT.

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14.9.1

Controlled Self-Organization of Functional Thin Film Nanostructures (DMP)

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John Wendelken, Oak Ridge National Labs., wendelkenjf@ornl.gov

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

Theoretical and experimental studies of phenomena such as diffusion and surface kinetics, templated and self-assembly, interactions between adsorbed species, phase transitions at surfaces, as well as prediction/characterization of nanostructures with novel properties will be emphasized. Particular emphasis will be placed on tailoring functional (i.e., mechanical, electrical, optical and magnetic) properties of thin-film nanostructures. Novel hybrid nanostructures with potential relevance to biology, catalysis, and energy research will be addressed.

14.9.3

Engineering Interfaces for New Materials: Modeling and Experiments (DMP)

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Interfaces, including both grain boundaries and heterophase interfaces, appear in almost all material applications. The macroscopic behavior of many materials and devices follow from the structure, composition, and bonding of the interfaces. This focus topic will highlight innovative concepts of engineering interfaces for materials with new functionalities and recent theoretical and experimental advances in the understandings of interfaces. It will cover recent developments in the areas of: heteroepitaxial film growth, structural, mechanical, thermal and electronic properties of interfaces, transport phenomena at interfaces, wetting, role of interfaces in material processing, and nano-structured materials with novel physical properties. We welcome experimental, computational, and analytical studies of all properties of solid-solid and liquid-solid interfaces at various length and time scales.

16.12.5

Hydrogen Storage; Materials, Measurements & Modeling (FIAP/DMP)

Hui Wu, National Institute of Standards and Technology, hui.wu@nist.gov **Karl Johnson**, Univ. of Pittsburgh, karlj@pitt.edu

Developing safe and reliable hydrogen storage technologies that meet performance and cost requirements is critical to the realization of the future hydrogen economy. Method to store hydrogen at low pressures and near room temperature are inherently more efficient than high-pressure or liquid storage technologies in principle. The challenge is to develop materials that have high gravimetric and volumetric hydrogen densities at moderate temperature and pressure conditions. The cur-

rent focus on materials-based hydrogen storage includes adsorption in high surface area adsorbents such as metal organic frameworks and various carbon-based materials, absorption in complex metal hydrides, chemical hydrogen storage in chemical hydrides such as light metal borohydrides, and other, more novel approaches.

Many challenges still exist in achieving acceptable densities, kinetics, and reversibility, despite substantial progress in developing new hydrogen storage materials. This focus topic will bring researchers together to discuss current developments in novel hydrogen storage materials, accurate measurement techniques, and advances in modeling and theory.

16.12.6

Materials & Application for Solar Energy (DMP/FIAP)

Antonio Martí Vega, Instituto de Energía Solar-ETSIT, amarti@etsit.upm.es (FIAP)

D. Ginley, National Renewable Energy Labs, david_ginley@nrel.gov

Research on suitable absorber materials for efficient solar energy conversion and their effective application to photovoltaic devices, constitutes a key element in the reduction of the cost of solar energy production to competitive prices. This is especially true as the balance of systems cost drop with scale-up. This session will cover the latest advances in this area including topics such as: advances in high efficiency solar cell devices (multi-junction solar cells, crystalline silicon, etc.) and the development of low cost large area devices (thin films, organics, dyes, etc.). In addition to commercial or near-commercial approaches, the session will cover relevant novel concepts including (nanostructures, multiple carrier generation, intermediate band solar cells, etc.).

16.12.12

Photocatalysis and Photovoltaic: Excitation, Trapping, and Transport of Charge Carriers at Surfaces and Interfaces (DMP)

Ulrike Diebold, Tulane Univ., diebold@tulane.edu

Annabella Selloni, Princeton Univ., aselloni@princeton.edu

Matthias Batzill, Univ. of South Florida, mbatzill@cas.usf.edu

Development of renewable energy sources, and in particular solar energy, are necessary to sustain the global economic growth and to minimize impact of these human activities on the environment. In recent years, this realization has resulted in increased federal funding and research for developing new approaches to harvest sun-light more efficiently. In addition to 'classical' semiconductor photovoltaic devices new concepts and materials are being investigated that enable conversion of light into electrical or chemical energy. In order to increase the efficiency of solar energy conversion devices the material's properties need to be tuned to increase light absorption, minimize the trapping of charge carriers in the material and subsequent recombination of excitons, and maximize the charge carrier separation and transport. In addition, for feasible devices the materials have to be long-lived under operation conditions that require chemical and photo stability of the material. These requirements ask for a better understanding of defect-structures, interface properties, quantum confinement effects, electronic structures, photo-excitation mechanisms, etc. in potential materials for these applications. Fundamental issues such as hot charge carrier injections and multiple charge carrier formation by single photons are also of interest to advance energy conversion. This focus session is intended to bring together research expertise that describes advances made in the photosensitization of materials and outlines the challenges that need to be addressed to make these novel materials feasible for solar energy conversion devices.

19.3.1

Earth & Planetary Materials (DMP/DCOMP)

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Recent discoveries in Earth materials research have highlighted the important synergy between experimental and computational mineral physics approaches to solving problems and understanding processes in the Earth's deep interior. Examples include the discovery of a new phase of magnesium orthosilicate at pressures in the vicinity of the core-mantle boundary [depths of 2900 km] and high-spin to low-spin transitions in iron-bearing minerals at pressures within the lower mantle [660 to 2900 km]. This focus topic will illustrate new work on these topics as well as other scientific and technological advances in the exploration of the behavior of Earth materials using both experimental and computational techniques.

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