

# DMP NEWSLETTER

Division of Material Physics

## Summer 2008

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### Dates to Remember

**Sept. 7, 2008 (Friday)**

Deadline for submitting invited speaker suggestions for DMP Focus Topics

**Nov. 21, 2008, (Friday)**

APS Abstract deadline submitted via the [web](#)

**March 16-20, 2009** (with tutorials, etc., March 15):  
APS March Meeting in Pittsburgh, PA

### A Note from the Chair

Welcome to the 2008 Summer Newsletter of the Division of Materials Physics.

**March Meeting.** The organizers of the DMP Focus Topics for the upcoming March meeting (March 16-20, 2009) in Pittsburgh have been chosen and are listed in this newsletter. Now is the time to input your suggestions for invited speakers. Your input should go directly to the Focus Topic organizers who are preparing invited speaker nominations for their topic. DMP also sponsors a few select symposia, and these suggestions should go directly to [Ramamoorthy Ramesh](#), 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.

**Outreach.** Although there is a general feeling and certainly a lot of talk about the importance of Materials Physics and science in general, this may change in a very short notice. There are several ways in which we individually can contribute to improve the perception of science and Material Physics; participating in some form of outreach activities and/or writing to the legislature. The APS has a series of outreach activities, which can be accessed by contacting [Rebecca Thompson-Flagg](#) and at the following web sites:

- [PhysicsCentral](#)
- [PhysicsQuest](#)
- [Color Me Physics](#)
- [Adopt-a-Physicist](#)

An additional way, is to contact elected official and candidates for political office to argue the importance of science and materials physics in particular. In an election year this may be a very fruitful activity. A useful web site, sponsored by many interested professional societies, in which these types of issues are discussed and which encourages personal participation is:

[Scientists and Engineers for America.](#)

There are many arguments that can be made justifying that these types of activities are not very productive. While I have no proof that any of this works, I can assure you that it will make you feel like you are doing something useful.

**Useful Information.** The following documents addressing general scientific issues related to Materials Physics maybe of general interest to you:

1. **CMMP 2010: [An Assessment of and Outlook for Condensed-Matter and Materials Physics](#)**
2. **Directing Matter and Energy: [Five Challenges for Science and the Imagination](#)**
3. **Condensed-Matter and Materials Physics: [The Science of the World Around Us](#)**

**Input Requested** I would appreciate receiving your general and/or specific comments regarding the DMP activities and in what form we can improve these. More specifically, I would appreciate receiving information in very brief format regarding:

a) **Public Speakers in Materials Physics** including title of possible talks, geographic area, email contact

b) **Movies in Material Physics**, web site

c) **Audio visuals**, web site

I am trying to put together a repository of information useful to Materials Physicists, which hopefully would be made available through the DMP web page. Of course, your contribution to this is crucial and will not be possible without it.

**International Members.** As we all know Materials Physics is a truly international research activity. Because of this it would be desirable to have a stronger participation in our activities from the international members. Thus I would like to encourage international members to volunteer for DMP activities by writing directly to me (ischuller@ucsd.edu) and request all DMP committees to encourage the participation of qualified non US Materials Physicists in our activities.

**Acknowledgements.** The DMP thanks 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 David Vanderbilt who served as Chair and all that is associated with this, Ted Einstein who has served as the Secretary/ Treasurer which is a major job and David Cahill and Steven Louie, who have finished their term as Members at Large.

Ivan K. Schuller,  
DMP Chair

## **Nominations for DMP Officers and Executive Committee Members**

A DMP election will be held late in 2008 to elect a Vice-Chair, a Division Councilor, and a 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, [Jeff Lynn](#). 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](#)) by October 1, 2008.

## **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 2009 APS March Meeting (Pittsburgh, PA, March 16-20, 2009). 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 these Focus Topics. The deadline for submitting such suggestions is September 7, 2008. Suggestions can be made by emailing the suggestion directly to the appropriate focus topic organizers who are listed after the Focus Topic descriptive paragraphs. Please also send a copy to [Ramamoorthy Ramesh](#), the main DMP organizer of Focus Topics.

Your suggestions should provide the following information: 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).

The web-based nomination form contains fields for all of these items. If you use the web-based form, your invited speaker nomination will be sent automatically to the appropriate Focus Topic organizers when you push the "submit" button at the end of the process. However, it is advisable to send an email to the first-listed organizer asking for confirmation that the nomination has been received.

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, too.

## List of DMP-Sponsored or Co-Sponsored Focus Topics and Sorting Categories for the 2009 APS March Meeting

The co-sponsoring units are indicated in between parenthesis.

### 02.8.2: Dopants and defects in semiconductors (DMP)

[Eugene Haller](#), University of California at Berkeley

[Matthew McCluskey](#), Washington State University

[Michael Stavola](#), Lehigh University

The properties of semiconductors are determined by the presence of impurities and defects. Defects control carrier concentration, mobility, lifetime, and recombination; they are also responsible for processes that involve atomic transport such as migration, diffusion, and precipitation of impurities and host atoms. In dilute III-N-V alloys, impurities even modify the band gap. The control of defects and impurities 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 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 dopants and defects in semiconductors, from the bulk to the nanoscale, is the subject of this focus session. The electronic, structural, optical, magnetic and isotopic properties of dopants and defects in elemental and compound semiconductors; SiO<sub>2</sub> and alternative dielectrics; wide band-gap semiconductors such

as diamond, SiC, metal-oxides, and the group-III nitrides; and organic semiconductors are of interest. Abstracts on experimental and theoretical investigations are solicited.

### **03.8.1: Dielectric, Ferroelectric and Piezoelectric Oxides (DMP)**

[Dillon D. Fong](#), Argonne National Laboratory  
[Matthew Dawber](#), Stony Brook University  
[Gustau Catalan](#), University of Cambridge

This topic will focus on fundamental advances in the growth, characterization, and experimental as well as theoretical understanding of dielectric, ferroelectric, piezoelectric, and multiferroic oxides in bulk, thin-film, superlattice, and nanostructured forms. Contributions on functional oxides of all structural types are encouraged. Areas of interest include the physics of structural and ferroelectric phase transitions, domain structure and dynamics, lattice dielectric properties, the impact of disorder on cooperative behavior, progress in theoretical approaches to ferroelectricity, multiferroicity, and relaxor behavior, as well as understanding of oxide synthesis and growth mechanisms. A major thrust will be to explore how bulk dielectric, ferroelectric, and piezoelectric properties 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.

### **04.14.5: Organic Electronics, Photonics & Magnetism (DMP/DPOLY)**

[Vitaly Podzorov](#), Rutgers University  
[Antoine Kahn](#), Princeton University

Organic small-molecule and polymer materials are actively studied for their interesting electronic, photonic and magnetic properties. This focus topic covers the recent developments in this field. Contributions are solicited on the following studies of organic semiconductors and related devices: charge carrier transport, optical properties (e.g., spectroscopy, physics of excitons, nonlinear optics, lasing, photonic bandgap materials), issues related to energetics of organic-organic and organic-inorganic interfaces, magneto-transport phenomena (e.g., magnetoresistance, spin dependent phenomena, magneto-optics). Studies of device physics of organic field-effect transistors, photovoltaic cells, lasers, spin valves, and sensors will be presented. Both theoretical and experimental studies are welcome.

### **05.17.1: Iron Pnictides and Other Novel Superconductors (DMP)**

[Igor Mazin](#), Naval Research Laboratory  
[Ian Fisher](#), Stanford University

The discovery of superconductivity in Fe pnictides has again demonstrated the potential of non-cuprate superconductors both in terms of high critical temperatures, currents and field, and in terms of fundamentally new superconducting states. Considerable progress has been made in recent months to understand both the normal and superconducting states of these materials and their parent compounds. This focused session will cover both theory and experiment on these and other non-cuprate unconventional superconductors, including, but not limited to, noncentrosymmetric superconductors, CeCoIn<sub>5</sub> and related materials, superconducting skutterudites, organics and intercalated graphites, etc.

### **5.17.2: Hybrid Magnetic-Superconducting Systems (DMP/GMAG)**

[Jose Martin](#), Universidad de Oviedo – CINN  
[Charles Reichhardt](#), Los Alamos National Laboratory  
[Jacobo Santamaria](#), Universidad Complutense de Madrid

The focus topic will highlight experimental, theoretical and computational work on hybrid superconducting/magnetic structures. The main subjects will include: vortex motion control and imprinting of the ferromagnetic response on superconducting films with arrays of magnetic nanostructures such as dots and nanowires; proximity effects, Andreev reflections, spatial modulation of the order parameter, non-collinear magnetization effects, and spin injection in both conventional and complex oxide superconducting/ferromagnetic multilayers and heterostructures; and pi-phases, proximity and triplet states in hybrid Josephson junctions. Also, superconducting-magnetic nanocomposites, reentrant superconductors and novel hybrid devices will be considered.

#### **6.14.1: Theory and Simulation of Magnetism and Spin-Dependent Properties (DCOMP/DMP/GMAG)**

[Kirill Belashenko](#), University of Nebraska  
[Aldo Romero](#), CINVESTAV – Unidad Queretaro  
[Dieter Suess](#), Vienna University of Technology

This focus topic centers on recent advances in the theory and numerical simulations of static and dynamical spin-dependent properties of magnetic materials and structures. This is a broad topic including, in particular, basic theory of magnetism, spin-dependent transport, magnetic phase transitions, magnetic hysteresis, spin waves, spin relaxation, spin transfer torques, exchange bias, interlayer magnetic coupling, novel concepts in magnetic recording, dynamics of domain walls and other topological defects. Particular interest is in low-dimensional magnetic systems and nanostructures such as interfaces, multilayers, thin films, nanowires, nanodots, and molecular magnets. Approaches include first-principles techniques, multiscale modeling, many-body theory, effective spin Hamiltonians, Monte Carlo simulations, Langevin dynamics, micromagnetic modeling, and combinations of these techniques. We especially encourage contributions showing benefits of cross-pollination between analytical and numerical approaches for explaining and predicting specific experimental results and materials or systems properties.

#### **6.14.2: Magnetic Nanostructures: Materials and Phenomena (DMP/GMAG)**

[Matthias Bode](#), Argonne National Laboratory  
[Yumi Ijiri](#), Oberlin College

This topic focuses on magnetic nanostructures, including 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 investigating these materials for proximity and structural disorder effects, magnetic quantum confinement, interlayer magnetic coupling, exchange spring, exchange bias, magnetic anisotropy, inter-particle interactions, and relaxation dynamics as well as 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 new/improved physical and/or chemical methods, high-resolution characterization methods with site and/or element specificity, and unusual physical phenomena present in these systems.

#### **6.14.3A: Bulk Properties of Complex Oxides (DMP/GMAG)**

[Jaime Fernandez-Baca](#), Oak Ridge National Laboratory  
[Karin Rabe](#), Rutgers University

Transition metal oxides exhibit a wide range of novel phenomena, which originate from the complexity induced by competing interactions and the presence of multiple ground states. Associated with this complexity is a tendency for short range order such as the formation of stripes, ladders, checkerboards, 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 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 (experiment, theory and simulation) of bulk complex oxides, including multiferroics, manganites, nickelates, cobaltites, and ruthenates.

#### **6.14.4: Complex Oxide Thin Films (DMP/GMAG)**

[Dimitri Basov](#), University of California, San Diego

[Marc Ulrich](#), Army Research Office

[Maria Varela](#), Oak Ridge National Laboratory

A rich variety of intriguing behaviors has been observed in complex oxides, many of which remain still far from understood. High  $T_c$  superconductivity, ferroelectricity or colossal magnetoresistance are just a few of them. When grown in the form of thin films, heterostructures or nanostructured systems, they often exhibit additional effects resulting from epitaxial strain, reduced dimensionality, charge transfer, proximity effects or phase competition across interfaces. Since all this phenomenology can deeply alter the macroscopic physical properties, their understanding acquires a special relevance. This Focus Topic explores the physical properties of thin complex oxide films and heterostructures, paying special attention to the role of interfaces. It also will focus on the mechanisms by which the macroscopic properties are affected, which may include strain, electronic phase separation, charge transfer or localization, structural defects, etc. These mechanisms have an important role in the interaction between spin, charge, lattice and orbital degrees of freedom in films. This Focus Topic will provide a forum to discuss recent developments in both theoretical and experimental work on these issues, including growth, characterization (by x-ray, neutron or electron scattering, scanning probe microscopy techniques, etc) and physical properties (transport, thermodynamic measurements, magnetometry, etc) of complex oxide films, heterostructures and nanostructured systems.

#### **6.14.5: Spin Transport & Magnetization Dynamics in Metal-Based Systems (GMAG/DMP/FIAP) (same as 6.12.7)**

[Yaroslav Bazaliy](#), University of South Carolina

[Casey Miller](#), University of South Florida

This topic focuses on the experimental and theoretical aspects of spin transport, spin transfer, and magnetization dynamics in metal-based systems; related phenomena in semiconductor systems will be covered in a separate focus topic. Topics of interest include all aspects of spin-dependent transport and scattering in the diffusive, ballistic, tunneling and hot electron regimes. These are spin diffusion, relaxation, and accumulation, spin transport through interfaces, spin injection and detection, mechanisms for magnetic damping (especially in magnetic nanostructures), etc. A major topic is the interplay between spin currents and magnetization dynamics in magnetic nanostructures: spin-transfer, spin pumping and related phenomena. Also included are the studies on spin transport in ferromagnetic-normal metal and ferromagnetic-superconductor systems. Relevant phenomena include giant magnetoresistance (GMR), tunneling magnetoresistance (TMR), spin polarization measurements, spin filtering, current-induced magnetization dynamics: magnetization switching, driven oscillations, motion of magnetic domain walls, vortices and other defects and related processes, studied in time and frequency domains.

#### **6.14.6: Spin Dependent Phenomena in Semiconductors (GMAG/DMP/FIAP)**

[Ian Appelbaum](#), University of Delaware

[Scott Crooker](#), Los Alamos National Laboratory

[Lu Sham](#), University of California, San Diego

The field of spin-dependent phenomena in semiconductors is developing rapidly, with significant advances recently in a widening range of material systems (e.g., silicon, diamond, carbon nanotubes, graphene), in semiconductor nanostructures (e.g., self-assembled and lithographically-defined quantum dots), and in hybrid ferromagnetic/semiconductor device structures. This series of Focus Sessions solicits contributions aimed at understanding spin-dependent processes in magnetic and non-magnetic structures incorporating semiconducting materials. Topics include: (i) growth, characterization, electrical, optical and magnetic properties of (ferro-)magnetic semiconductors and hybrid ferromagnet-semiconductor structures including quantum dots, nanocrystals, and nanowires; (ii) transport and dynamical effects in semiconductors with or without spin-orbit interactions; (iii) electrical and optical spin injection, spin Hall effects, spin interference, spin filtering, spin lifetime effects, spin dependent scattering, and spin torque; (iv) manipulation, detection, and entanglement of electrical and nuclear spins in quantum systems such as dots, impurities and point defects; and (v) spin-dependent devices and device proposals involving ferromagnets and semiconductors.

#### **6.14.8: Spin Dependent Physics in Organic Materials (GMAG/DMP)**

[Joaquin Fernandez-Rossier](#), Universidad de Alicante

[Andrew Kent](#), New York University

[Jagadeesh Moodera](#), Massachusetts Institute of Technology

This focus topic is on spin transport and dynamics in organic materials including organic semiconductors, graphene, carbon nanotubes and molecular magnets. Research at the intersection of several forefront areas in condensed matter and material physics are of interest: spin electronics, carbon-based materials and molecular magnetism. Organic materials are of particular interest for spin transport and dynamics because weak spin orbit interactions and hyperfine interactions may lead to long spin lifetimes. Phenomena/ materials of interest include, hybrid ferromagnetic/organic structures, spin transport in graphene, Kondo effect, spin qubits in diamond, quantum tunneling and coherence in molecular nanomagnetism, organic magnetoresistance and all related topics.

#### **07.11.1: Carbon Nanotubes & Related Materials (DMP)**

[David Tomanek](#), Michigan State University

[Tony F. Heinz](#), Columbia University

[Annick Loiseau](#), ONERA-CNRS

Interest in the fundamental properties and applications of carbon nanotubes and related allotropes 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 related materials, including characterization, synthesis, processing, purification, chemical, mechanical, thermal, electrical, optical, opto-electronic and magnetic properties, and (ii) in their potential applications as nanosensors, nanoprobe, 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:

1. Synthesis and characterization of pure and doped nanostructures of carbon and boron nitride, including nanotubes, nanohorns, and other graphitic nanostructures;
2. purification, separation and chemical functionalization of these nanostructures;
3. the structure and properties of hybrid systems, including filled and chemically modified carbon nanotubes and nanotube peapods;
4. mechanical and thermal properties of these nanostructures and their composites;

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

The symposium will also 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.

#### **07.11.2: Graphene (DMP)**

[Antonio H. Castro Neto](#), Boston University

[Alessandra Lanzara](#), University of California, Berkeley

[Young-Woo Son](#), Konkuk University

Description: The discovery of graphene in 2004 has stirred a lot of interest in the scientific community followed by an exponential growth in the literature. The excitement behind this discovery has two main driven forces: basic science, and technological implications. Graphene is a condensed matter realization of the Dirac equation with a Fermi-Dirac velocity of order of one hundredth of the velocity of light. This fact has strong implications in many of the physical properties of these systems: the electronic density of states vanishes at the Fermi level, there is very poor screening of the Coulomb interaction, the Dirac fermions interact very strongly with disorder, and Landau's Fermi liquid theory is not applicable. There has been an intense experimental effort in recent years in graphene research. Cutting-edge research techniques such as infrared absorption, and angle resolved photoemission (ARPES), are being used to study this system. The FT will cover the latest developments in graphene research, both experimentally and theoretically.

#### **07.11.5: Computational Nanoscience (DMP/DCOMP)**

[Jeffrey B. Neaton](#), Lawrence Berkeley National Laboratory

[Alexander A. Demkov](#), University of Texas, Austin

When the characteristic dimensions of a physical system are reduced to the nanometer scale, new properties and physical phenomena emerge. Computational studies play an important role in understanding the physical origin of these new properties and phenomena, interpreting experiments, developing structure-function relationships, and enabling rational design. This session will provide an overview of recent applications and methodological developments at the frontier of computational nanoscience for the study of inorganic, organic, and biological nanostructures, and their assemblies and interfaces. Nanoscale phenomena to be covered include, but are not limited to, assembly, growth, and dynamics; structure and morphology; mechanical and vibrational response; and electronic, optical, plasmonic, and transport properties. Studies addressing the impact nanoscale surfaces and hybrid interfaces are strongly encouraged. Contributions covering new methods and algorithms that lead to better predictive capabilities, and that bridge multiple time and/or length scales, are also solicited.

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

[Tom Dickinson](#), Washington State Univ.

[Richard Haglund](#), Vanderbilt Univ.

[Leonid V. Zhigilei](#), Univ. of Virginia

This session focuses on materials physics issues involved in laser-materials interactions including those relevant to laser-driven techniques for material removal, modification, processing, and deposition. Also, we consider laser-based diagnostic 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 ultrafast time-resolved techniques including x-ray and electron diffraction; nonlinear response of materials at high intensity; 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.

### **13.6.1: Optical Properties of Nanostructures (DMP)**

[Feng Wang](#), University of California, Berkeley

[Sohrab Ismail-Beigi](#), Yale University

[James Schuck](#), Lawrence Berkeley National Labs

[John Rehr](#), University of Washington

There is currently great interest in optical properties of nanoscale structures, ranging from chemically synthesized nanoparticles, nanorods, nanowires and nanotubes, to nanofabricated graphene devices and plasmonic metamaterials. Many unique optical phenomena emerge on this nanometer scale. The principal aim of the focus topic sessions on 'optical properties of nanostructures' is to bring together colleagues from different disciplines who are active in optical study of nanostructures to advance the understanding of novel optical phenomena in these materials. Theoretical and experimental research on the optical properties of a broad range of nanostructures will be covered in these sessions.

### **13.6.2: Fundamental Challenges in Transport Properties of Nanostructures (DMP)**

[Mark S Hybertsen](#), Brookhaven National Laboratory

[Daniel C Ralph](#), Cornell University

This focus topic will address the fundamental issues that are critical to understand, characterize and control electronic transport in nanostructures, with potential for impact in fields such as advanced information processing, solar energy utilization, or nano-mechanical devices. Contributions are solicited in areas that reflect recent advances in synthesis and assembly, characterization and theory for a variety of nanosystems, including those based on individual quantum dots, nanowires, molecules and self-assembled functional systems. 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 nanostructures.

Separate focus sessions sponsored or cosponsored by DMP will organize presentations on carbon nanotubes, graphene, magnetic nanostructures, photovoltaics, and thermoelectrics.

### **13.6.3: Materials Issues for Quantum Computing & Quantum Engineering (DMP)**

[David P. Pappas](#), NIST

[William D. Oliver](#), MIT Lincoln Laboratory

Key challenges to the realization of a practical condensed-matter quantum computer are the identification and characterization of materials-based decoherence sources, and their mitigation through the development of alternative materials, growth methods, and fabrication techniques. In this Focus Topic, we call for papers

investigating the development, characterization, and/or implementation of materials targeting quantum-coherent solid-state structures, including (but not limited to) quantum dots in Si and GaAs, superconducting flux, phase, and charge qubits, and spin-polarized devices. Particular attention will be given to works which identify, characterize, or eliminate decoherence sources that are intrinsic to the device functionality, e.g., tunnel junctions, and/or those that arise primarily from device engineering, fabrication and processing, e.g., surface, edge, and material defects.

#### **13.6.4: Thermoelectric Materials & Phenomena (FIAP/DMP)**

[A. Shakouri](#), University of California, Santa Cruz

[D.G. Cahill](#), University of Illinois, Urbana Champaign

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[i]. 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  $ZT$ .

#### **14.9.1: Controlled Self-Organization of Functional Thin Film Nanostructures(DMP)**

[Sanjay V. Khare](#), University of Toledo

[Suneel Kodambaka](#), University of California, Los Angeles

[Janice E. Reutt-Robey](#), University of Maryland at College Park

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 depends on fundamental understanding of the evolution of thin-film morphology, electronic structure, and atomic composition. This focus session will highlight recent experimental and theoretical developments associated with the formation and stability of nanostructures, surfaces, thin films, and interfaces, of hard and soft matter. 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)**

[Yue Qi](#), General Motors R&D Center

[Eduardo Saiz](#), Lawrence Berkeley National Lab

The macroscopic behavior of many materials and devices follows from the structure and composition of the interfaces present. This is especially true of nanostructured materials whether conceived for inorganic devices or biomaterials. In effect, both processing and macroscopic properties are essentially controlled by the detailed structure and composition of the interfaces, even if they comprise a small fraction of the total material. Interfaces, including both grain boundaries and heterophase interfaces, have drawn much interest within the physics community. Understanding the quantitative relationships among interface composition, structure and bonding, and macroscopic properties is a prerequisite in the development of materials with new functionalities. The emergence of new generations of experimental and computational methods has resulted in a tremendous progress in the area during the last few years. Numerous novel interface-controlled phenomena have been discovered in superhard materials, ferroelectric superlattices, nanocomposites etc. As a result, a key concept has emerged: interface engineering for the design of new materials and structures with unique properties.

Topics of interest include: heteroepitaxial film growth, structural, mechanical, electrical, thermal and electronic properties of interfaces, including grain boundaries and heterophase interfaces, interfacial transport phenomena, adhesion, wetting and spreading, role of interfaces in material processing in particular nanocomposites and nanostructured materials and interfacial engineering to manipulate macroscopic response. This session welcomes experimental, computational, and analytical studies of all properties of solid-solid and liquid-solid interfaces at various length and time scales. This focus session will highlight innovative concepts of engineering interfaces for new materials and recent theoretical and experimental advances in the understanding and characterization of interfaces. Submissions emphasizing the interplay between observation (experiment) and modeling (theory) are especially encouraged.

#### **16.12.5: Hydrogen Storage: Materials, Measurements & Modeling (FIAP/DMP)**

[Channing Ahn](#), California Institute of Technology

[Jason Allan Graetz](#), Brookhaven National Laboratory

Numerous basic challenges still beset hydrogen storage technologies. Thermodynamic limitations associated with high sorption or formation enthalpies confront strategies whether they are based on traditional metal, complex, chemical or physisorbent materials. For systems that do appear to offer possibilities based on thermochemical data, predicted reaction pathways during hydrogenation/dehydrogenation cycling are not necessarily observed. Also challenging are the kinetic barriers associated with solid-state diffusion in so-called hydride "destabilization" systems, where atomic mobility at temperatures  $< 200$  °C is required. While the use of schemes such as hydride incorporation into scaffolds has been shown to improve kinetic behavior and reversibility, presumably by reducing diffusion distances, transport mechanisms are poorly understood. In this focus session, we encourage contributions that address empirical and computational data that are pertinent to the outstanding issues that relate directly to hydride phase formation and stability.

#### **16.12.6 & 16.12.12: Materials for photovoltaic and photocatalysis (DMP/FIAP)**

[Wladek Walukiewicz](#), Lawrence Berkeley National Labs

[Franz Himpfel](#), University of Wisconsin

[Jeffrey Urban](#), Lawrence Berkeley National Labs

The search for new sources of clean energy is rapidly becoming one of the most pressing technological challenges that we are facing today. One promising avenue is the development of materials with the ability to convert solar irradiation into electrical energy (photovoltaics) or chemical energy (solar fuels). Building upon knowledge gained from studies on bulk solids, enormous progress has been made in developing new, tailored materials via nanostructuring, self-assembly and bio-mimetic methods. Such materials are the key for making renewable energy, such as solar energy conversion, competitive with traditional, "dirty" energy sources. These new types of engineered materials present an avenue to produce devices with efficiencies and properties not found in traditional bulk solids. However, initial investigations into these newly emerging designer materials

has highlighted the need for more direct research into the fundamentals of how charge excitation and transport is impacted by semiconductor interfaces with other semiconductors, metals, gases, and liquids. This Focused Topic session aims at bringing together experts from a variety of disciplines spanning physics, materials science, chemical engineering, and surface science in order to identify the key questions in solar energy conversion, to develop strategies for attacking them, and to report on initial progress and emerging themes in this space.