Division of Material Physics A Division of the American Physical Society

Summer 2005

In this Issue ...

- Dates to Remember
- Call for Invited Speaker Suggestions
- List of DMP-Sponsored or Co-Sponsored FocusTopics and Sorting Categories for the 2006 APS March Meeting
- DMP 2006 March Meeting Program of Focus Topics and **Call for Abstracts**

July 11, 2005 - Minor update to Focus Topic 6.11.5 July 12, 2005 - Minor updates to Focus Topics 6.11.4 & 6.11.5

Abstract Deadline

All contributed abstracts must be submitted via the official APS web site at http://abstracts.aps.org/ by Wednesday, November 30, 2005. If you intend for your abstract to be part of a Focus Topic, be sure to choose the Sorting Category Code associated with that Focus Topic.

Invited abstracts are due on the same date. Authors of invited abstracts will be instructed where to submit their abstracts in the official APS invitation letter.

Dates to Remember

Aug. 31, 2005 (Wednesday)

• Deadline for submitting invited speaker suggestions for DMP Focus Topics

Nov. 30, 2005 (Wednesday)

• APS Abstract deadline submitted via the web at http://abstracts.aps.org

March 13-17, 2006

• APS March Meeting in Baltimore, Maryland

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 2006 APS March Meeting (Baltimore, MD, March 13-17, 2006). 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 August 31, 2005. Suggestions can be made in either of two ways: (1) by emailing the suggestion directly to the appropriate session organizers who are listed after the Focus Topic descriptive paragraphs, or (2) by using the web-based form on the APS website at http://www.aps.org/units/dmp/invited.cfm.

If you send your suggestion by direct email, please 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 nominationwill 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 <u>http://www.aps.org/units/dmp</u>. In case of any need for corrections or updates, these will also be posted at this location.

List of DMP-Sponsored or Co-Sponsored Focus Topics and Sorting Categories for the 2006 APS March Meeting

2.8.1 Wide Band Gap Semiconductors (DMP)
3.8.1 Dielectric, Ferroelectric, and Piezoelectric Oxides (DMP)
4.15.4 Organic Electronics, Photonics, and Magnetics (DMP/DPOLY)
5.11.1 Magnesium Diboride and Related Compounds (DMP)
6.11.1 Theory and Simulation of Magnetism and Spin-Dependent Properties (DCOMP/DMP/GMAG)
6.11.2 Nanostructured Magnetic Materials (DMP/GMAG)
6.11.3 Complex Multifunctional Oxides (DMP/GMAG)
6.11.4 Spin Transport and Magnetization Dynamics in Metal-Based Systems (GMAG/DMP/FIAP)
6.11.5 Spin-Dependent Phenomena in Semiconductors (DMP/GMAG)
7.8.1 Simulation and Theory of Complex Materials (DCOMP/DMP)
7.8.3 Carbon Nanotubes and Related Materials (DMP)
7.8.4 Computational Nanoscience (DCOMP/DMP)
12.7.1 Friction, Fracture, and Deformation (DMP/GSNP)
13.6.1 Optical Properties of Nanostructures (DMP)
13.6.2 Fundamental Challenges in Transport Properties of Nanostructures (DMP)
13.6.3 Materials Issues for Quantum Computing and Quantum Engineering (DMP)
13.6.4 Thermal, Thermoelectric, and Mass Transport at the Nanoscale (DMP)
13.6.5 Nanoscale Materials Physics of Phase Transitions (DMP)
14.9.1 Morphology and Composition Evolution in Thin Films and Surfaces (DMP)
19.3.1 Earth and Planetary Materials (DMP/DCOMP)
19.3.2 Simulations of Matter at Extreme Conditions (DCOMP/GSCCM/DMP)

DMP 2006 March Meeting Program of Focus Topics and Call for Abstracts

2.8.1 Wide Band Gap Semiconductors (DMP)

Recent advances in the quality of wide band gap semiconductor materials including the nitrides, carbides, and oxides have allowed exploration of fundamental materials parameters, physics, and novel device applications. This session will include topics ranging from characterization, determination and control of fundamental material properties to the implementation of nanostructure designs that introduce new functionality to the wide band gap systems. Areas of interest include, but are not limited to, growth (bulk crystals, heterostructures and nanostructures), polarization effects, ferromagnetism, optical, structural and electrical characterization of materials including local probe techniques, properties of

heterostructures, and device physics. Of particular interest are studies of lower dimensional (1D and 0D) nano-wires and quantum dots. New device designs that exploit the unique properties of the wide band gap materials will also be considered.

Organizers:

Michael J. Manfra Bell Laboratories, Lucent Technologies Room 1C-368 600 Mountain Ave. Murray Hill, NJ 07974 Phone: (908) 582-1137 Fax: (908) 582-4868 Email: <u>manfra@lucent.com</u>

Ben V. Shanabrook Head, Electronic Materials Branch Code 6870 Naval Research Laboratory Washington, DC 20375-5000 Phone: (202) 767-3693 Fax: (202) 767-1165 Email: <u>shanabrook@nrl.navy.mil</u>

3.8.1 Dielectric, Ferroelectric, and Piezoelectric Oxides (DMP)

This topic will focus on fundamental advances in the growth, characterization, and theoretical understanding of dielectric, ferroelectric, and piezoelectric oxides in bulk, ultrathin-film, and superlattice form. Functional oxides of all structure types are included, such as perovskites, distorted fluorite high-K dielectrics, ZnO, etc. Topics of interest for bulk materials include structural and ferroelectric phase transitions, lattice dielectric properties, etc. However, a major thrust will be to explore how bulk dielectric, ferroelectric, and piezoelectric properties are modified in thin-film, superlattice, or other nanoscale geometries, as for example in structures grown using atomic-layer controlled techniques (e.g., MBE, PLD, or ALD). In particular, contributions are welcome that explore the effects of strain epitaxy, surfaces, electrical boundary conditions, interfaces, etc.

Organizers:

Eric J. Cockayne MS 8520 Ceramics Div NIST 100 Bureau Dr Gaithersburg, MD 20899 Phone: (301) 975-4347 Fax: (301) 975-5334 Email: cockayne@nist.gov

Darrell G. Schlom Dept of Materials Sci & Engr Penn State Univ 108 MRI Bldg-Rsch Park University Park, PA 16803-6602 Phone: (814) 863-8579 Fax: (814) 863-0618 Email: <u>schlom@ems.psu.edu</u>

Yong Liang Freescale Semiconductor, Inc., AZ34, EL 519 Tempe, Arizona 85284 Phone: (480) 413-7118 Fax: (480) 413-3294 Email: yong.liang@freescale.com

4.15.4 Organic Electronics, Photonics, and Magnetics (DMP/POLY)

Small organic molecules and polymer-based materials enable new classes of electronic, photonic and magnetic devices. This focus session considers the latest developments in the physics of these materials. Contributions are solicited in the areas of organic conductors, semiconductors, and magnetic physics. The broad range of topics include: electronic structure, charge transport, morphology, self-assembly, surfaces and interfaces, optics and non-linear optics, photonic crystals, magnetism and spin transport. Contributions of device physics may include electric and magnetic field effects, FETs, LEDs, photovoltaics, lasers, spin valves, and sensors. Electronic systems ranging from large area down to micro- and nanoscale will be addressed. Both theoretical and experimental papers on organic systems ranging from single or small collections of molecules to polycrystalline thin films and bulk single crystals will be included.

Organizers:

Denis Fichou CEA-Saclay SPCSI/DRECAM/DSM 91191 Gif-sur-Yvette France Phone: 33(0)1 69 08 43 74 Fax: 33(0)1 69 08 84 46 Email: <u>fichou@drecam.cea.fr</u>

John A. Rogers Univ of Illinois 1304 W Green St Urbana, IL 61801 Phone: (217) 244-4979 Fax: (217) 294-1190 Email: jrogers@uiuc.edu

David C. Martin University of Michigan 2022 H. H. Dow Building Ann Arbor, MI 48109-2136 Phone: (734) 936-3161 Fax: (508) 256-8352 Email: milty@umich.edu

5.11.1 Magnesium Diboride and Related Compounds (DMP)

The two weakly-coupled bands and superconducting gaps of magnesium diboride result in interesting new physics and phenomena not seen in one-gap superconductors. The possibility of modifying interband and intraband scattering offers special opportunities to develop remarkably high upper critical fields. Low flux creep, composite vortex structures and composite phase textures resulting from the internal Josephson effect add additional interest. Alloying and artificial damage of MgB₂ remains an interesting route to modification of the properties and understanding of the multi-band scattering. Four years after the discovery of superconductivity in magnesium diboride, it is possible to think seriously that industry-standard Nb-based superconductors for both high-field and electronic applications may be under challenge. This session addresses the physics and applications of magnesium diboride and related compounds from both theoretical and experimental viewpoints. Topics include various aspects of two-band superconductivity, electronic structure calculations, studies of phonons and electron-phonon coupling, sp $^{2}/sp^{3}$ bonding and optical phonons, doping and alloying, strain and disorder, flux pinning, wires and tapes, and the Josephson effect and devices. Superconductivity in borides, borocarbides, hole-doped diamond, and related compounds is also of interest, as are papers on multifunctional heterostructures involving magnesium diboride.

Organizers:

David C. Larbalestier 909 ERB University of Wisconsin 1500 Engineering Dr. Madison, WI 53706 Phone: (608) 263-2194 Fax: (608) 263-1087 Email: <u>larbalestier@engr.wisc.edu</u>

Lance D. Cooley Materials Science Department Brookhaven National Lab Bldg. 480 Upton, NY 11973 Phone: (631) 344-5204 Fax: (631) 344-4071 Email: <u>Idcooley@bnl.gov</u>

Paul C. Canfield 59 Physics Iowa State University Ames, IA 50011 Phone: (515) 294-6270 Fax: (515) 294-0689 Email: canfield@ameslab.gov

John M. Rowell Visiting Professor, Arizona State University 102 Exeter Dr. Berkeley Heights, NJ 07922 Phone: (908) 464-6994 Email: jmrberkhts@aol.com

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 (including magnetic x-ray scattering), 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.

Organizers:

Wei Cai Stanford University Durand Building, Room 259 Stanford, CA 94305-4040 Phone: (650) 736-1671 Fax: (650) 723-1778 Email: <u>caiwei@stanford.edu</u>

Bruce Harmon Ames Laboratory and Iowa State University Ames, Iowa 50011 Phone: (515) 294-5772 Email: <u>harmon@ameslab.gov</u>

Renat Sabirianov Department of Physics (UNO) University of Nebraska Omaha, NE 68182-0266 Phone: (402) 554-372 Email: <u>rsabirianov@mail.unomaha.edu</u>

6.11.2 Nanostructured Magnetic Materials (DMP/GMAG)

This session focuses on magnetic materials and phenomena at the nanometer-scale. Magnetic nanostructures include films, multilayers, nanocomposites, hybrid structures, wedges, nanowires, magnetic point contacts, nanoparticles, nanoparticle arrays, and patterned films. 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, effects of structural disorder, hysteresis

modeling, and other magnetic phenomena. Of special interest is 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.

Organizers:

Sara Majetich Physics Department Carnegie Mellon University Pittsburgh, PA 15213-3890 Phone: (412) 268-3105 Fax: (412) 681-0648 Email: sm70@andrew.cmu.edu

E. Dan Dahlberg School of Physics and Astronomy University of Minnesota 116 Church St. S.E. Minneapolis, MN 55455 Phone: (612) 624-3506 Fax: (612) 624-4578 Email: <u>dand@umn.edu</u>

6.11.3 Complex multifunctional oxides (DMP/GMAG)

The broad range of functionalities associated with solid oxides results in large part from the complexity of their electronic structures, and the close competition they exhibit between multiple magnetic and electronic phases. These factors can lead to large responses to external stimuli and the occurrence of striking phenomena such as colossal magnetoresistance and giant magnetoelectric or magnetocalorimetric effects. This symposium will explore recent advances in the fundamental physics and potential technological applications of such complex and multifunctional oxide materials. Sessions will focus both on phenomena of current interest, such as colossal magnetoresistance, multiferroic behavior, magnetoelectronic phase separation, and orbital and charge ordering, as well as specific materials classes that are receiving increased attention, including manganites, cobalt oxides (perovskites and the sodium cobaltates), and ruthenates. The interplay between bulk and thin film synthesis, characterization of structural, electronic and physical properties, and theory and simulation, will be emphasized.

Organizers:

Chris Leighton Department of Chemical Engineering and Materials Science University of Minnesota Minneapolis, MN 55455 Phone: (612) 625 4018 Fax: (612) 626 7246 Email: <u>leighton@umn.edu</u>

Nicola A. Spaldin Materials Department University of California Santa Barbara, CA 93106-5050 Phone:(805) 893-7920 Fax: (805) 893-7221 Email: <u>nicola@mrl.ucsb.edu</u>

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

This session will focus on experimental and theoretical investigations that elucidate and/or utilize the transport and transfer of spin 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. 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, spin-current-driven 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 session.

Organizers:

Mark Stiles Stop 8412 NIST 100 Bureau Drive Gaithersburg, MD 20899-8412 Phone: (301) 975-3745 Fax: (301) 926-2746 Email: mark.stiles@nist.gov

John Q. Xiao Department of Physics and Astronomy University of Delaware Newark, DE 19716 Phone: (302) 831-6547 Fax: (302) 831-1637 Email: jqx@udel.edu

Allan MacDonald Physics Department University of Texas Austin, TX 78712 Phone: (512) 232-9113 Fax: (512) 471-9637 Email: macd@physics.utexas.edu

6.11.5 Spin Dependent Phenomena in Semiconductors (DMP/GMAG)

Recent advances in understanding the physics of spin-dependent phenomena in semiconductors have come from the mutual influence of research on fundamental optical and transport properties, materials physics, and devices. This focused session solicits abstracts that explore a fundamental understanding of spin-dependent processes in magnetic and non-magnetic structures incorporating semiconductors. Topics include 1) spin dynamics and transport in nonmagnetic semiconductors, including spin transport in mesoscopic systems, electrical or optical spin injection, manipulation, and detection, optical and electronic control of spin coherence, and hyperfine effects; 2) growth, characterization, electrical, optical and magnetic properties, and control of magnetic properties in ferromagnetic semiconductors and hybrid ferromagnet-semiconductor structures and devices; and 3) developments in related fields, such as organic semiconductors and quantum computing, that relate to spin-dependent phenomena in semiconductors.

Organizers:

Peter E. Schiffer Department of Physics Penn State University 104 Davey Lab, Box 135 University Park, PA 16802 Phone: (814) 865-5982 Fax: (814) 865-3604 Email: schiffer@phys.psu.edu

Michael E. Flatté Department of Physics and Astronomy University of Iowa Iowa City, IA 52242 Phone: (319) 335-0201 Fax: (319) 353-1115 Email: <u>michael_flatte@mailaps.org</u>

Allan MacDonald University of Texas Austin, TX 78712 Phone: (512) 232-9113 Fax: (512) 471-9637 Email: macd@physics.utexas.edu

7.8.1 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.

Organizers:

Jeff Grossman Center for Integrated Nanomechanical Systems Berkeley Nanosciences and Nanoengineering Institute University of California Berkeley, CA 94720-1726 Phone: (510) 642-8358 Fax: (510) 642-9879 Email: jgrossman@berkeley.edu

Alberto G. Franceschetti National Renewable Energy Laboratory 1617 Cole Boulevard Golden, CO 80401 Phone: (303) 384-6645 Fax: (303) 384-6432 Email: <u>alberto_franceschetti@nrel.gov</u>

7.8.3 Carbon Nanotubes and Related Materials (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 focus 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, nanoprobes, 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 doped and pure carbon nanotubes and nanohorns, 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, and nanotube peapods 11) multifunctional nanotube composites and 12) other experimental and theoretical results from quasi-one dimensional systems which relate to carbon nanotubes.

Organizers:

Vasili Perebeinos IBM Research Division T.J. Watson Research Center P.O. Box 218 Yorktown Heights, NY 10598 Phone: (914) 945-3567 Fax: (914) 945-4531 Email: yperebe@us.ibm.com

Tobias Hertel Department of Physics and Astronomy Vanderbilt University 6301 Stevenson Center Lane Nashville, TN 37235 Phone: (615) 322-2864 Fax: (615) 343-7263 Email: <u>tobias.hertel@vanderbilt.edu</u>

Junichiro Kono ECE Department, MS 366 PO Box 1892 Rice University Houston, TX 77251-1892 Phone: (713) 348-2209 Fax: (713) 348-5686 Email: <u>kono@rice.edu</u>

7.8.4 Computational Nanoscience (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 interpret experimental observations of these phenomena, provide much-needed insight into their underlying physical origin, and thus 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 a comprehensive overview of recent computational work in the field of nanoscale materials with particular emphasis on techniques that allow 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 reactivity properties of nanofeatured structures and materials and the interplay between functionality and local structural environment.

Organizers:

Lin-Wang Wang Mail Stop 50F Lawrence Berkeley National Laboratory 1 Cyclotron Road Berkeley, CA 94720 Phone: (510) 486-5571 Fax: (510) 486-5812 Email: <u>lwwang@lbl.gov</u>

Marco Buongiorno Nardelli Center for High Performance Simulation and Department of Physics North Carolina State University Raleigh. NC 27695-7518 and CCS-CSM - Oak Ridge National Laboratory Oak Ridge, TN 37831 Phone: (919) 513-0514 Fax: (919) 5134804 Email: mbnardelli@ncsu.edu

12.7.1 Friction, Fracture and Deformation (DMP/GSNP)

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 nanoscale to tectonic scales. Topics of interest include tribochemistry, nanoscale mechanics including AFM indentation phenomena, dislocation patterns, grain boundary and interface effects, fracture initiation, crack propagation, the tribology of smooth and rough surfaces including fractal interfaces, and material deformation under applied stress including cutting. The session welcomes experimental, computational, and analytical studies of atomistic, mesoscopic, continuum, statistical, and multiscale 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.

Organizers:

H. G. E. Hentschel Math. & Sci. Ctr., Phys. Dept. Emory University 400 Dowman Drive Atlanta, GA 30322 Phone: (404) 727-0764 Fax: (404) 727-0873 Email: phshgeh@physics.emory.edu

Yue Qi MC 480-106-224 GM Research and Development Center 30500 Mound Rd Warren, MI 48090-9055 Phone: (586) 947-0751 Fax: (586) 986-8697 Email: yue.gi@gm.com

Udo D. Schwarz Department of Mechanical Engineering Yale University P.O. Box 208284 New Haven, CT 06520 Phone: (203) 432-7525 Fax: (203) 432-6775 Email: udo.schwarz@yale.edu

13.6.1 Optical Properties of Nanostructures (DMP)

This focused session will be devoted to techniques to predict and understand the optical, photoemission, x-ray absorption, and other spectroscopic properties of materials at the nanoscale. The emphasis will be on current topics and applications. Contributions from both theory and experiment are encouraged. Topics of interest will include, but are not limited to: (1) optical and dielectric (including nonlinear response) properties of semiconductors, insulators and oxides; (2) electron and x-ray spectroscopies via x-ray absorption, emission, and scattering; applications to metals, surfaces, and complex systems; (3) electronic excitations in confined systems, e.g., polymers, clusters, nanocrystals, quantum dots, and nanostructured materials.

Organizers:

James R. Chelikowsky ACES Bldg. Rm 4.102 Inst. Comp. Eng. & Sci. (C0200) 1 University Station Austin, TX 78712 Phone: (512) 471-3312 Email: jrc@ices.utexas.edu

John Rehr Department of Physics University of Washington P.O. Box 351560 Seattle, WA 98195-1560 Phone: (206) 543-8593 Fax: (206) 685-0635 Email: jjr@phys.washington.edu

Steven G. Louie University of California Physics Department #7300 Berkeley, CA 94720-7300 Phone: (510) 642-1709 Fax: (510) 643-9473 Email: sglouie@uclink.berkeley.edu

13.6.2 Fundamental Challenges in Transport Properties of Nanostructures (DMP)

This focus topic will address issues which are critical to the understanding, characterization and control of electrical transport phenomena in nanostructures including single-molecule devices, self-assembled monolayers, point contacts, semiconductor nanowires, quantum dots, and other novel structures. Contributions are solicited in the following areas: 1) controlled fabrication of nanoscale devices including synthesis, self assembly and other bottom-up approaches, novel lithographic and other top-down techniques, and integration with contacts; 2) experimental studies of structural properties and electrical transport characteristics of nanoscale structures and devices; and 3) theoretical advances in modeling structural properties and electrical transport characteristics are organized more specifically on: (1) carbon nanotubes; (2) organic electronics, photonics, and magnetics; and (3) thermal, thermoelectric, and mass transport at the nanoscale.

Organizers:

Mark S. Hybertsen Applied Physics and Applied Math Columbia University 500 W. 120th St. New York, NY 10027 Phone: (212) 854-8420 Fax: (212) 854-1909 Email: msh2102@columbia.edu

Daniel C. Ralph Department of Physics Cornell University Clark Hall Ithaca, NY 14853 Phone: (607) 255-9644 Fax: (607) 255-6428 Email: <u>ralph@ccmr.cornell.edu</u>

Mark C. Hersam Materials Science and Engineering Northwestern University 2220 Campus Drive Evanston, IL 60208-3108 Phone: (847) 491-2696 Fax: (847) 491-7820 Email: <u>m-hersam@northwestern.edu</u>

13.6.3 Materials Issues for Quantum Computing and Quantum Engineering (DMP)

Many experiments aimed at engineering the quantum behavior of objects have important underlying materials issues. These arise in wide ranging systems such as qubits based on Josephson junctions, quantum dots, spins in semiconductors and quantum behavior of small mechanical resonators, to name just a few. This focus session is aimed at materials issues in quantum computing and quantum engineering, discussing what has been learned about how materials properties influence the coherent quantum behavior of such systems, views on what is possible, and new ideas for obtaining and studying controlled quantum behavior of materials-based qubits. Abstracts in any of these areas are encouraged. For further information please contact one of the co-organizers listed below.

Organizers:

James N. Eckstein Department of Physics University of Illinois 1110 West Green Street Urbana, IL 61801 Phone: (217) 244-7709 Fax: (217) 244-2278 Email: <u>eckstein@uiuc.edu</u>

Keith Schwab Laboratory for Physical Sciences National Security Agency 8050 Green Mead Drive College Park, MD 20740 Phone: (301) 935-6542 Fax: (301) 935-6723 Email: schwab@lps.umd.edu

13.6.4 Thermal, Thermoelectric, and Mass Transport at the Nanoscale (DMP)

The influential role of quantum effects and correlations in nanoscale structures often leads to unexpected and fundamentally interesting behavior. The ability to harness such effects for device applications, however, depends crucially on the thermal and mechanical stability of the constituent nanostructures. In particular, for materials with characteristic dimensions below the electron and phonon mean free paths, thermal and electrical transport may differ dramatically from bulk semi-classical behavior, and the interplay between electrons and phonons will significantly impact device properties and performance. This focus topic centers on fundamental questions related to understanding and controlling thermal, electrical, thermoelectrical, and mass transport in nanostructures. We encourage submission of abstracts in the areas of synthesis, fabrication, characterization, and theory of nanostructures in the context of novel thermal, thermoelectric, and mechanical properties. Nanoscale phenomena of interest include phonon dynamics, thermal conductance, thermoelectric power, specific heat; mass transport, diffusion, and nanofluidics; and local heating, nanoscale friction, dissipation, and elasticity. Relevant systems include nanostructured interfaces and superlattices; embedded nanostructures and nanocomposites; biological and organic complexes; quantum dots, nanowires and nanotubes, organic self-assembled monolayers, and single molecule devices. We encourage experimental, theoretical, and computational contributions, in particular those reporting on interdisciplinary and collaborative research efforts.

Organizers:

Jeffrey B. Neaton The Molecular Foundry Lawrence Berkeley National Laboratory Berkeley, CA 94720 Phone: (510) 642-1031 Fax: (510) 642-9345 Email: jbneaton@lbl.gov

Philip Kim Department of Physics Columbia University 538 West 120th Street New York, NY 10027 Phone: (212) 854-0102 Fax: (212) 854-3379 Email: pk2015@columbia.edu

David Tomanek Department of Physics and Astronomy Michigan State University East Lansing, MI 48824-2320 Phone: (517) 355-9702 Fax: (517) 353-4500 Email: tomanek@pa.msu.edu

13.6.5 Nanoscale Materials Physics of Phase Transitions (DMP)

There has been substantial recent progress in the synthesis and characterization of nanoscale materials, as well as in theoretical and computational methods for describing these phase transitions. It is thus now becoming possible to correlate the effects of size, dimensionality and electronic structure with the dynamics and physical properties arising from these phase transitions. This focused topic session aims to bring together theorists and experimentalists working in this area to discuss materials physics questions relating to nanoscale phase transitions. Topics of interest include, but are not limited to relevant experimental, theoretical and computational studies of: 1) model materials: semiconductors, strongly correlated materials, metals and semi-metals; 2) effects of dimensionality: nanoparticles and nanocrystals, nanowires, ultrathin films and surfaces; 3) phase transformations: structure,

dynamics, order-disorder and coherence effects; 4) effects of nanoscale phase transformations on optical, magnetic, conducting and thermal properties. Questions about the suitability of proposed contributions can be addressed to any of the organizers listed below.

Organizers:

Richard Haglund Department of Physics and Astronomy Vanderbilt University 6301 Stevenson Center Nashville TN 37235-1807 Phone: (615) 322-7964 Fax: (615) 343-7263 Email: <u>richard.haglund@vanderbilt.edu</u>

David Singh Condensed Matter Sciences Division Oak Ridge National Laboratory P. O. Box 2008, MS 6032 Oak Ridge TN 38731-6032 Phone: (865) 241-3716 Fax: (865) 574-4143 Email: singhdj@ornl.gov

Eric Mazur Div. of Engineering and Applied Sciences Harvard University Cambridge MA 02138 Phone: (617) 495-8729 Fax: (240) 255-4622 Email: mazur@physics.harvard.edu

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

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 composition. This focus session will highlight recent experimental and theoretical developments associated with the formation and stability of nanostructures, surfaces, thin films, and interfaces. Novel hard/soft hybrid systems with potential biological relevance, such as water and biomolecule interaction with solid surfaces, will also be addressed.

Organizers:

Zhenyu Zhang Condensed Matter Sciences Division Oak Ridge National Laboratory Oak Ridge, TN 37831 Phone: (865) 576-5346 Fax: (865) 574-4143 Email: <u>zhangz@ornl.gov</u>

Shirley Chiang

Department of Physics University of California at Davis Davis, CA 95616-8677 Phone: (530) 752-5989 Fax: (530) 752-4717 Email: chiang@physics.ucdavis.edu

Efthimios Kaxiras Department of Physics Harvard University Cambridge, MA 02138 Phone: (617) 495-7977 Fax: (617) 496-2545 Email: <u>kaxiras@cmt.harvard.edu</u>

19.3.1 Earth and Planetary Materials (DMP/DCOMP)

This focus session on Earth and Planetary Materials will highlight new experimental, computational, and theoretical approaches for understanding a variety of materials existent in planetary environments, from core to surface, from solar to exosolar planets. The main interest lies in the exploration of ices, fluids, minerals as well as complex/imperfect materials over the appropriate 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, progress in laser-based spectroscopy, the second- and third-generation synchrotron sources, static and dynamic compression techniques, and advanced theoretical methods combined with rapidly increasing computer power has fundamentally altered how we investigate Earth materials and their interaction with the environment. Of particular importance is that we now have *in situ* methods capable of determining the properties and behavior of materials under conditions ranging from deep-earth temperatures and pressures to ambient conditions. The goal of these sessions will be to explore the science and the technological advances that inspire research in this area.

Organizers:

Renata M. Wentzcovitch Dept of Chem Engr & Mater Sci Univ of Minnesota 421 Washington Ave SE Rm 151 Minneapolis, MN 55455 Phone: (612) 625-6345 Fax: (612) 626-7246 Email: wentzcov@cems.umn.edu

Hokwang Mao Geophysical Lab, CIW 5251 Broad Branch Rd, NW Washington, DC 20015 Phone: (202) 321-8899 Email: <u>mao@gl.ciw.edu</u>

Eric R. Schwegler Lawrence Livermore National Laboratory PO Box 808, MS L-415 Livermore, CA 94550 Phone: (925) 424-3098 Fax: (925) 373-3542 Email: <u>schwegler@llnl.gov</u>

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

A wide variety of phenomena, such a solid compressed by a shock wave, planetary interiors, a nanoparticle subjected to an intense radiation field, or a cell membrane under large strain, all represent matter under extreme conditions. Matter at extreme conditions is characterized by a strong perturbation of structure and dynamics far from ambient equilibrium by environmental factors. Despite the diversity of applications, strong commonality exists among the methods employed in the description of strongly perturbed matter. This focus session concerns recent advances in theoretical and computational methodologies applied to metallic, organic, inorganic, and biological materials, as well as liquids, plasmas, and atomic or molecular clusters exposed to high pressures, strain rates (including shock loading), temperature extremes, or intense external fields. Presentations will include such diverse computational approaches as atomistic (quantum, semi-classical, and classical), mesoscopic (grain-scale), continuum, and multi-scale techniques. Representative scientific areas of interest are: (1) equations of state; (2) dynamical response of materials; (3) inelastic deformation, fracture, and spall; (4) high-pressure phase transitions; (5) electrical, optical, and other properties of shocked materials; (6) energetic materials; (7) shock-induced chemistry; (8) high energy density conditions; (9) intense external field interactions; and (10) biological or geophysical applications.

Organizers:

Timothy C. Germann X-7, MS-F699 Los Alamos National Laboratory Los Alamos, NM 87545 Phone: (505) 665-9772 Fax: (505) 665-6722 Email: tcg@lanl.gov

Laurence E. Fried L-282 Lawrence Livermore National Laboratory 7000 East Avenue Livermore, CA 94550 Phone: (925) 422-7796 Fax: (925) 424-3281 Email: <u>fried1@llnl.gov</u>

Sandro Scandolo The Abdus Salam International Center for Theoretical Physics Strada Costiera 11 34014 Trieste (Italy) Phone: +39 040 2240 209 Fax: +39 040 224163 Email: scandolo@ictp.it