

DMP NEWSLETTER

Division of Material Physics

In this Issue

- [Important Dates](#)
- [A Note from the Chair](#)
- [Division of Materials Physics Ovshinsky Student Travel Awards](#)
- [Richard L. Greene Dissertation Award in Experimental Condensed Matter Materials Physics](#)
- [Nominations for DMP Officers and Executive Committee Members](#)
- [Call for Submissions to the DMP-Sponsored Focus Topics](#)
- [List of DMP-Sponsored or Co-Sponsored Focus Topics and Sorting Categories for the 2016 APS March Meeting](#)

Important Dates

September 1, 2015 Nomination deadline for Richard L. Greene Dissertation Award in Experimental Condensed Matter Materials Physics.

November 6, 2015 (Friday) by 5pm EST. Abstract deadline for the 2015 APS March Meeting. Submission is via the web at <http://abstracts.aps.org>

May 2, 2016 DMP Deadline for APS Fellowship Nominations.

March 14 - March 18, 2016 (with tutorials, etc., March 12-13): APS March Meeting in Baltimore, Maryland.

August 17, 2015 (past) Deadline for submitting invited speaker suggestions for DMP Focus Topics.

A Note from the Chair

Summer is well upon us now and I hope many of you are enjoying a bit of 'downtime' with family and friends. Throughout the spring and summer months your DMP Executive Committee has been hard at work, and it is my pleasure to bring you an update on our activities as well as a call for your participation in upcoming important DMP activities.

At the top of this list is our preparation for the APS March Meeting to be held in Baltimore, March 14-18, 2016. Developing and running the strong slate of diverse DMP Focus Topics that comprise one of the largest blocs at the March Meeting is a year-long

process. This year, the Program is in the able hands of DMP Chair-Elect, Michael Flatté, with help from the entire Executive Committee. As detailed in this newsletter, Michael has assembled a strong line-up of 18 Focus Topics, each organized by leaders in their respective fields. From 2D Materials, to Complex Oxides, to superconductors to topological materials, 2016 is shaping up to be another outstanding showing for the DMP-led part of the program.

Now it's your turn: I encourage you to look over these Focus Topic descriptions and to please encourage your students and colleagues to contribute abstracts to those sessions most closely related to their work; contributed talks breathe life into the sessions and are an excellent opportunity for younger scientists among us to showcase their work to a receptive audience.

In addition to running an important part of the March Meeting, DMP sponsors or co-sponsors a number of awards, and we likewise depend on DMP membership to nominate or support candidates for receiving these awards.

For those of you who have nominated candidates for the James C. McGroddy Prize for New Materials, and the David Adler Lectureship in Materials Physics, I thank you: Nominations are time consuming and take considerable thought, and no one wins without strong backing.

This is the second year of the Richard L. Greene Dissertation Award in Experimental Condensed Matter Materials Physics. Having chaired last year's session where inaugural awardees Moureen Kemei and Matthew Reed presented outstanding work on spinel oxides and quantum computing to a sizeable crowd, I can attest to the value of such an award to the early career scientists it recognizes. We are grateful to Rick for this philanthropic contribution and expect to see many deserving candidates from which to choose the second annual award. The nomination deadline is September 1, 2015. Please see www.aps.org/programs/honors/dissertation/greene.cfm for full details.

DMP also recognizes the Young Scientist Prize in the Structure and Dynamics of Condensed Matter Physics. The International Union of Pure and Applied Physics (IUPAP), Commission 10, awards this prize and the winner is recognized with an invited talk in a DMP-sponsored Symposium, and at our Reception at the March Meeting.

Student presenters are invited to apply for a Stanford and Iris Ovshinsky Student Travel Award. These highly competitive and prestigious awards are available to students whose abstracts are submitted to DMP-sponsored contributed sessions. The award provides travel support, and the awardees will be publicly recognized in our Reception at the March Meeting.

Finally, this is my opportunity to thank the members of the DMP Executive Committee who have recently completed their service. I thank them for their generous donation of time and expertise in serving the DMP community. These are: Mark Hybertsen and Susanne Stemmer who have stepped down as Members at Large. I also want to give a

special thanks to David Cahill who has completed four years of leadership as Vice-Chair, Chair-Elect, Chair, and Past-Chair of the Division of Materials Physics. David has provided invaluable advice to me over the past couple of years, making my job a lot easier. Thank you, David!

Enjoy the rest of your summer, and I look forward to seeing you in Baltimore!

John Mitchell, DMP Chair

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

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

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

Students interested in being considered for an award must apply online (to be updated).

The **Ovshinsky Student Travel Awards** for the 2015 March Meeting were presented to:

Urusa Alaan, Stanford University
Brian Capozzi, Columbia University
Ankit Disa, Yale University
Kurt Fredrickson, The University of Texas at Austin
Kenneth Gottlieb, University of California Berkeley
Alannah Hallas, McMaster University
Xu Han, University of Massachusetts, Amherst
Claire-Alice Hebert, University of California, Santa Barbara
James Lourembam, Nanyang Technological University
Evgeny Mikheev, University of California, Santa Barbara
Saima Siddiqui, Massachusetts Institute of Technology

The Richard L. Greene Dissertation Award in Experimental Condensed Matter Materials Physics - September 1, 2015 Nomination deadline

To recognize doctoral thesis research of exceptional quality and importance in experimental condensed matter or experimental materials physics. The award, to be given annually, will consist of \$2500, a certificate citing the contributions made by the recipient, and an allowance of up to \$1500 for travel to attend and give an invited talk at the annual APS March meeting at which the award will be presented.

The award was established in 2013 to honor the scientific and administrative contributions of Richard L. Greene to experimental condensed matter and materials physics. The Richard L. Greene Award is supported by a gift from his family.

Nominations will be accepted for doctoral dissertations written in English and submitted to any college or university, worldwide. Nominees must have submitted their dissertations after January 1, two years prior to the award. Nominations may be considered for up to two consecutive review cycles.

Nomination information: <http://www.aps.org/programs/honors/dissertation/greene.cfm>.

Photographs from the 2015 March Meeting Awards Reception



Dr. Robin Dibner joins Bob Nemanich and Laura Greene in presenting an Ovshinsky Student Travel Grant award to Saima Siddiqui of MIT. Dr. Dibner represented the Ovshinsky family who announced increasing their support of the Travel Grant program.
(photo credit: APS photo|Ken Cole)



2015 Ovshinsky Student Travel Award winners together with Laura Greene (DMP Chair, left) and Bob Nemanich (Secretary/Treasurer, back right). (photo credit|APS photo: Ken Cole)



2015 APS-DMP Fellows Awards Recipients together with, John Mitchell (Chair Elect, right), Bob Nemanich (Sec/Treas, back right) and Laura Greene (Chair, right). (photo credit: APS photo|Ken Cole)

Nominations for DMP Officers and Executive Committee Members

The DMP Officer election will be held late in 2015 to elect a Vice-Chair, and two new at-large Executive Committee Members. The Nominating Committee shall nominate at least two candidates for the ballot for each office. Suggestions for candidates can be made to the Chair of the Nominating Committee, Laura H. Greene (lhgreene@illinois.edu) by September 15, 2015.

In addition, candidates can be directly nominated by petition of five percent of the membership of the Division. Such petitions must be received by the Secretary/Treasurer, Robert Nemanich (robert.nemanich@asu.edu) by October 1, 2015.

DMP Focus Topics for the 2016 APS March Meeting

With this issue of the Newsletter, the Division of Materials Physics announces the program of DMP Focus Topics for the 2016 APS March Meeting (Baltimore, Maryland March 14 - March 18, 2016). 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. (*The deadline for invited speaker nominations was August 17, 2015.*)

For the 2016 March Meeting, DMP is the lead organization unit on 18 different Focus Topics and co-sponsoring unit for an additional 11. See lists below.

We encourage your contributed submissions to the DMP Focus Topics.

Finally, note that the contents of this Newsletter will be available electronically on the DMP website at <http://www.aps.org/units/dmp>. Corrections or updates will also be posted at this location.

List of DMP-Sponsored or Co-Sponsored Focus Topics and Sorting Categories for the 2016 APS March Meeting

6.1.3: Strongly spin-orbit coupled oxides/emergent entwinement (DMP)

Organizers:

James Analytis (UC Berkeley) analytis@berkeley.edu

Natalia Perkins (U. Minnesota) nperkins@umn.edu

Xingjiang Zhou (Institute of Physics, Beijing) XJZhou@aphy.iphy.ac.cn

Strong spin-orbit coupling (SOC) has played a central role in some of the most exciting discoveries in materials over the last few years. SOC is important for driving topologically non-trivial band structures, leading to spin-momentum locking in Rashba materials, protected surface states in topological insulators, and ultra-relativistic Dirac and Weyl quasi-particles in exotic metals. Moreover, SOC can strongly affect many-body phenomena, leading to complex broken symmetries in multi-ferroic systems or strong frustration in quantum magnets. Indeed, SOC materials are currently at the forefront of research into spin liquids, whose excitations are thought to be highly exotic, even having fractional quantum numbers. Research has largely focused on binary/ternary high-Z materials with weak correlations and mixed orbital character and transition metal oxides with strong correlations and complex competing interactions. The physics of SOC materials thus connects to some of the deepest problems in condensed matter, from topology to correlated electron phenomena. The scope of this Focus Topic will encompass 4d- and 5d-transition-metal compounds, rare earth compounds, and heavy chalcogenide compounds that exhibit a wide variety of SOC-related physical phenomena including metal-insulator transitions, Mott insulator formation, strong Rashba splittings, strong magnetic anisotropies and superconductivity.

7.1.1: Dielectric and Ferroic Oxides (DMP/DCOMP/DCMP)

Organizers:

Manfred Fiebig (ETH Zurich) manfred.fiebig@mat.ethz.ch

Dillon Fong (Argonne National Lab) fong@anl.gov

Complex oxides exhibit a rich variety of order parameters, such as polarization, magnetization, strain, charge and orbital degrees of freedom. The vast range of functional properties that emerge from their mutual coupling (e.g., ferroelectricity, magnetoelectricity, multiferroicity, metal-insulator transitions, defect-related properties) are the main topics of interest for this symposium. Examples of current grand challenges include:

- (i) Novel mechanisms to break inversion symmetry in heterostructures and layered oxides.
- (ii) Viable routes to achieve a strong coupling between polarization and ferromagnetism at room temperature.
- (iii) Band-filling and bandwidth control in complex oxides (a prerequisite to harnessing charge/orbital order, magnetic transitions and metal insulator transitions).
- (iv) Electric- or magnetic-field control of these phenomena - a very exciting prospect for both fundamental science and technology.
- (v) Structure and properties of magnetoelectric domains and domain walls of these materials.
- (vi) Emerging avenues to controlling polarization, magnetism and electronic properties via strain and/or strain gradients and/or defects.

Breakthroughs and progress in the theory, synthesis, characterization, and device implementations in these and other related topics are solicited for this Focus Topic.

7.1.2: Topological Materials: Synthesis and Characterization (DMP/DCMP)

Organizers:

Peter Armitage (Johns Hopkins U) npa@pha.jhu.edu

Feng Liu (U. Utah) fliu@eng.utah.edu

Sean Oh (Rutgers) ohsean@physics.rutgers.edu.

There has been explosive growth in the study of topological materials in which the combined effects of the spin-orbit coupling and fundamental symmetries yield a bulk energy gap with novel gapless surface states robust against scattering. Moreover, the field has expanded in scope to include topological superconductors, Dirac and Weyl semimetals, Kondo insulators and complex heterostructures capable of harboring exotic topologically nontrivial states of quantum matter. The observation of theoretical predictions depends greatly on sample quality and there remain significant challenges in identifying and synthesizing the underlying materials having properties amenable to the study of the surface and interface states of interest. This topic will focus on fundamental advances in the synthesis, characterization and modeling of candidate topological materials in various forms including bulk single crystals, exfoliated and epitaxial thin films, epitaxially modulated heterostructures, nanowires and nanoribbons, and theoretical studies that illuminate the synthesis effort and identify new candidate materials. Of equal interest is the characterization of these samples using structural, transport, magnetic, optical and other spectroscopic techniques, and related theoretical efforts aimed at modeling various properties

and the underlying spin-textures, spin-splittings and substrate effects, with particular focus on identifying samples whose properties are dominated by the surface and interface states.

8.1.2: Dopants and Defects in Semiconductors (DMP/FIAP)

Organizers:

Christoph Boehme (U. Utah) boehme@physics.utah.edu

Pat Lenahan (Penn State U) pmlesm@engr.psu.edu

Impurities and native defects profoundly affect the electronic and optical properties of semiconductor materials. Incorporation of impurities is nearly always a necessary step for tuning the electrical properties in semiconductors. In some cases, as in dilute III-V alloys, impurities even modify the band gap. Defects control carrier concentration, mobility, lifetime, and recombination; they are also responsible for the mass-transport processes involved in migration, diffusion, and precipitation of impurities and host atoms. The control of impurities and defects is the critical factor that enables a semiconductor to be engineered for use in electronic and optoelectronic devices as has been widely recognized in the remarkable development of Si-based electronics, the current success of GaN-based blue LED and lasers, and the emergence of ZnO for nanoelectronics sensors, and transparent conducting displays. The fundamental understanding, characterization and control of defects and impurities are essential for the development of new devices, such as those based on novel wide-band gap semiconductors, spintronic materials, and low dimensional structures.

The physics of dopants and defects in semiconductors, from the bulk to the nanoscale, including surfaces and interfaces, is the subject of this focus topic. Abstracts on experimental and theoretical investigations are solicited in areas of interest that include: the electronic, structural, optical, and magnetic properties of impurities and defects in elemental and compound semiconductors, SiO₂ and alternative dielectrics, wide band-gap materials such as diamond including NV centers, SiC, group-III nitrides, two-dimensional materials including phosphorus and BN, oxide semiconductors, and the emerging organic-inorganic hybrid perovskite (e.g., MAPbI₃) solar cell materials are of interest. Likewise welcomed are abstracts on specific materials challenges involving defects, e.g., in processing, characterization, property determination, including imaging and various new nanoscale probes.

9.1.1 - Fe-based Superconductors (DMP/DCOMP)

Organizers:

Ian Fisher (Stanford U.) irfisher@stanford.edu

Peter Hirschfeld (University of Florida) pjh@phys.ufl.edu

Jenny Hoffman (Harvard U./U. British Columbia) jhoffman@physics.harvard.edu

Substantial experimental and theoretical progress has been made toward understanding the unusual normal and superconducting state properties of iron based superconductors (IBS). Yet, many challenges and controversies exist, often driven by recent discoveries of new or improved materials whose properties differ radically from the original set. Among the current challenges are the origin of the dramatically enhanced T_c in single-layer FeSe, and the reasons for nematicity without long range magnetic order in bulk FeSe. This Focus Topic will cover the latest experimental and theoretical issues pertaining to both normal and superconducting properties of IBS and their parent compounds, both pnictide and chalcogenide based. By better understanding the relationship between these two families, how the different crystalline, magnetic and electronic structures in IBS relate to the high critical temperatures, and how these systems compare to cuprates and other novel superconducting materials, the goal is to enhance the potential for discovering new superconducting systems with higher T_c 's.

12.1.1: 2D materials: synthesis, defects, structure and properties (DMP)

Organizers:

Manish Chhowalla (Rutgers) manish1@rci.rutgers.edu

Saptarshi Das (Argonne National Lab) das@anl.gov

Chongwu Zhou (USC) chongwuz@usc.edu

The interest in two dimensional (2D) materials is rapidly spreading across all scientific and engineering disciplines due to their exceptional chemical, mechanical, optical and electrical properties, which not only provide a platform to investigate fundamental physical phenomena but also promise solutions to the most relevant technological challenges. 2D materials find their immediate application in field effect transistors, gas sensors, bio-detectors, mechanical resonators, optical modulators and energy harvesting devices with superior performances that have already been demonstrated in prototype devices. However, the true impact will only be made if the initial breakthroughs are transformed into commercial technologies. A major challenge towards the commercialization of 2D materials is the large area, scalable and controllable growth of highly crystalline layers in a cost effective way. So far the best quality samples of 2D materials have been obtained through micromechanical exfoliation of naturally occurring single crystals. Chemical vapor deposition (CVD) is the most widely used bottom-up technique to grow large area 2D-materials. Several top-down approaches have also been adopted based on bulk liquid phase chemical and electrochemical exfoliation. The 2D focus topic will cover:

- Experimental, theoretical, and computational studies illuminating various aspects of the growth process including, e. g., layer number and stacking geometry control, the formation of topological and structural defects, grain

size and grain boundary control, and the effect of substrate chemistry, crystallography and strain

- Methods of doping
- Templated or bottom-up growth or top-down synthesis of nanostructures and integration with other materials
- Characterization and modeling of the structural, mechanical, electronic, and optical properties of the synthesized 2D materials

12.1.2 - 2D materials: semiconductors (DMP)

Organizers:

Jeanie Lau (UC Riverside) jeanie.lau@ucr.edu

Xiaodong Xu (U. Washington) xiaodongx@gmail.com

Xiaobo Yin (U. Colorado) Xiaobo.Yin@Colorado.EDU

Research exploring 2D semiconductors and their heterostructures are rapidly expanding to include a wide variety of layered material systems with diverse properties, including strong many body interactions, strong spin-orbit coupling effects, coupled spin-pseudospin physics, and topological physics etc. This Focus Topic will cover experimental and theoretical/computational work related to 2D semiconductors and their heterostructures, including large bandgap materials such as many chalcogenides (e.g., MoS₂, WSe₂, GaSe, ReSe, etc.), phosphorene and h-BN, and small gap materials with possible topological effects (such as silicene, germanene, stanene, and Bi₂Se₃ etc.). Important areas related to monolayers, few-layers and heterostructures include quantum transport properties, mobility engineering, spin and pseudospin physics, 2D exciton physics, defect engineering on optical and electronic properties, spin and valley Hall effects, understanding the role of the dielectric environment, many-body effects, and magnetic properties.

12.1.3 Devices from 2D materials: function, fabrication and characterization (DMP)

Organizers:

Xia Hong (U. Nebraska-Lincoln) xia.hong@unl.edu

Kin Fai Mak (Penn State U) kzm11@psu.edu

Douglas R. Strachan (U. Kentucky) doug.strachan@uky.edu

With the rapid progress in the research on 2D materials, including graphene and other layered material systems, a wide variety of properties and functionalities have emerged that have broad scientific and technological significance. The rational design of devices consisting of 2D materials calls for improved understanding of their intrinsic and extrinsic properties that are critical to the device functionality, as well as their integration with other device components.

The development of these 2D materials based devices also requires solutions to problems associated with material functionalization, structural fabrication, and device characterization. This Focus Topic will cover experimental and theoretical/computational work related to devices based on the growing array of 2D materials that exhibit a wide variety of behaviors – such as metallic, semiconducting, insulating, magnetic, superconducting, and various strongly correlated electronic phenomena. These 2D materials include (but are not limited to) graphene, transition-metal chalcogenides (e.g., MoS₂, WSe₂, NbSe₂, TaS₂, FeSe etc.), silicene, germanane, stannane, phosphorene, topological insulators (e.g., Bi₂Se₃, Bi₂Te₃, etc.), layered oxides (e.g., BSCCO), and large band gap materials such as h-BN. We invite contributions on topics including: (i) the functionalization, fabrication, measurements, and modeling of devices based on the unique properties of 2D materials in the single- or multi-layered forms as well as their heterostructures; (ii) proof-of-principle studies focusing on the electronic, magnetic, optical, mechanical, thermal, and chemical behaviors of 2D materials relevant for device applications; and (iii) interfacial, environmental, and system-based properties and behaviors inherent to the application of 2D materials in future devices.

12.1.4 - 2D materials: metals, superconductors, and correlated materials (DMP)

Organizers:

Alexey Bezryadin (U. Illinois Urbana-Champaign) bezryadi@illinois.edu

Yong P. Chen (Purdue) yongchen@purdue.edu

Xuan Gao (Case Western Reserve U.) xxg15@case.edu

After the discovery of graphene and other two-dimensional (2D) semiconductors and semimetals, research exploring 2D materials is rapidly expanding to include a wide variety of layered material systems with diversely different properties. There is enormous interest in building functional structures and devices based on these novel 2D materials, some possibly integrated with graphene or 2D semiconductors. This symposium will cover experimental and theoretical/computational work related to 2D materials that are metallic, superconductors, or have other correlated electronic phases such as charge or spin density waves, Mott insulators, etc. Examples of these 2D materials include various types of layered chalcogenides (eg. NbSe₂, TaS₂, FeSe) and oxides (eg. BSCCO, V₂O₅). Particular focus will be on the electronic, thermal, magnetic, and optical properties and functions of few-layers and monolayers of these materials and their heterostructures. Material synthesis (in either bulk or nanostructure form), device fabrication and integration are also included, as well as applications exploiting unique properties of these materials.

12.1.5: Carbon Nanotubes and Related Materials: Synthesis, Properties, and Applications (DMP/DCMP)

Organizers:

Zhihong Chen (Purdue) zhchen@purdue.edu

Shu-Jen Han (IBM) sjhan@us.ibm.com

Interest in the fundamental properties and applications of carbon nanotubes and related materials remains high. This is because of their unique combination of electrical, chemical, mechanical, thermal, optical, spectroscopic and magnetic properties. This focus topic addresses recent developments in the fundamental understanding of nanotubes and related materials, including synthesis, characterization, processing, purification, chemical, mechanical, thermal, electrical, optical, and magnetic properties. This session will highlight how these properties lead to new fundamental physical phenomena and existing or potential applications for interconnects, transistors, thermal management, composites, super-capacitors, nanosensors, nanopropes, field emitters, storage media, magnetic devices, etc.. Experimental and theoretical contributions are solicited in the following areas:

- Synthesis and characterization of nanotubes, nanohorns, nanocones, and related nanostructures;
- Control or optimization of growth, including helicity control and in-situ studies;
- Purification, separation, chemical functionalization, alignment/assembly;
- Structure and properties of hybrid systems, including filled and chemically modified carbon nanotubes and nanotube peapods;
- Mechanical and thermal properties of these nanostructures and their composites;
- Electrical and magnetic properties of these systems;
- Mesoscopic, structural, optical, opto-electronic and transport properties as well as their spectroscopic characterization.
- BN and other inorganic nanotubes; other 3D forms of sp²-carbon
- The focus topic will also cover the broad applications of these nanosystems, including:
 - Electronic devices including interconnects, supercapacitors, transistors, memory;
 - Thermal management applications;
 - Multifunctional nanotube composites;
 - Chemical and bio-sensing applications;
 - Field emission;
 - New generations of magnetic and electronic devices

12.1.6: Van der Waals Bonding in Advanced Materials (DMP) (DCMP)

Organizers:

Martin Head-Gordon (University of California, Berkeley)
mhg@cchem.berkeley.edu

Jamie L. Manson (Eastern Washington University) jmanson@ewu.edu

John Singleton (Los Alamos National Laboratory) jsingle@lanl.gov

Van der Waals interactions are ubiquitous in nature and play an important role in the structure, stability, and function of molecules and materials studied across all of the major disciplines of science, ranging from structural biology to supramolecular chemistry and condensed matter physics. While van der Waals interactions are considerably weaker than covalent bonds they have structure-directing ability and often control the physical properties of a material. These non-bonded interactions are inherently quantum mechanical in nature and result from dynamical correlation among collections of electrons, and remain a substantial challenge to experimentalists and theorists. Hence, the aim of this Focus Topic is to directly address this challenge by highlighting the current state-of-the-art in materials design and synthesis, as well as experimental and theoretical approaches to better understand van der Waals interactions. In doing so, we hope to lay the groundwork for future collaborative research - an approach that is necessary for describing these fundamental interactions in materials of increasing complexity.

12.1.7: Computational Discovery and Design of New Materials (DMP/DCOMP/DCMP)

Organizers:

Sahar Sharifzadeh (Boston University) ssharifz@bu.edu

Stephan Lany (NREL) stephan.lany@nrel.gov

Advances in algorithms, computational power, and the ability to predictively model physical phenomena are spurring the computational discovery and design of novel materials, allowing for virtual materials synthesis and characterization before their realization in the laboratory. This focus topic will cover studies at the frontier of computational materials discovery and design, ranging from quantum-level prediction to macro-scale property optimization. Topics of interest include, but are not limited to: Computational materials design and discovery, high-throughput computation and automatized data analysis, computational materials databases, materials informatics, data mining, machine learning, global structure and property optimizations, algorithms for searching the structure/composition space, first principles property prediction and methods for improved accuracy or efficiency, computational modeling of materials synthesis. Of particular interest are contributions that apply novel data/computation-intensive approaches to materials design, that feature a strong connection to experiment, and those that

translate physical insights gained from computation into advanced materials by design. The application focus broadly covers electronic materials, ranging from low-power electronics (Motttronics), energy conversion and storage materials (thermoelectrics, batteries, fuel cells, photovoltaics), to novel materials for non-linear optics and data processing (spintronics).

13.1.1: Nanostructures and Metamaterials (DMP/DCMP)

Organizers:

Vivian Ferry (U. Minnesota) veferry@umn.edu

Jeremy Munday (U. Maryland) jnmunday@umd.edu

Michael Naughton (Boston College) naughton@bc.edu

Recent experimental, theoretical and computational advances have enabled the design and realization of nanostructured materials with novel, complex and unusual electromagnetic properties. Such metamaterials and nanostructures provide unique opportunities to manipulate electromagnetic radiation over a broad range of frequencies, from the visible and infrared to terahertz and microwave. This focus topic will highlight recent progress in the fabrication and physical understanding of these designer materials. Topics of interest include, but are not limited to: nanophotonics, plasmonics, quantum optics, and the emerging interface of condensed matter and materials physics with the biological and neuro and energy sciences.

13.1.2 - Many-body perturbation theory for electronic excitations in materials (DMP)

Organizers:

Volker Blum (Duke) volker.blum@duke.edu

Claudia Draxl (Humboldt University of Berlin) claudia.draxl@physik.hu-berlin.de

Thomas Koerzdoerfer (U. Potsdam) thomas.koerzdoerfer@uni-potsdam.de

Noa Marom (Tulane) nmarom@tulane.edu

Many properties of functional materials, interfaces, and nano-structures derive from electronic excitations. For example, the ionization potential, the electron affinity, the fundamental gap, dielectric screening, charge transition levels of defects or dopants, and the energy level alignment at interfaces are associated with charged excitations. Conversely, the optical gap, absorption spectra, and exciton binding energies correspond to neutral excitations. These properties are critical parameters for the performance of devices, such as transistors, light emitting diodes, and solar cells.

A proper description of electronic excitations requires theoretical approaches that go beyond ground state density functional theory (DFT). Methods originating from Green's function based many-body perturbation theory are a natural choice.

In this framework, the random phase approximation (RPA) accounts for dynamic and long-range correlation effects (e.g., van der Waals interactions) manifested in the dielectric function and in the energetics of weakly bonded systems. The GW approximation, where G is the one-particle Green's function and W is the screened Coulomb interaction that derives from the dielectric function, provides an accurate description of charged excitations and the Bethe-Salpeter equation (BSE) of neutral excitations (including charge transfer excitations).

This focus topic is dedicated to recent advances in many-body perturbation theory methods for electronic excitations, their scalable implementations in electronic structure codes, and their applications to functional materials, interfaces, molecules, and nano-structures.

13.1.3: Electron, Ion, and Exciton Transport in Nanostructures (DMP/DCMP)

Organizers:

Pierre Darancet (Argonne National Laboratory) pdarancet@anl.gov

Alec Talin (Sandia National Laboratories) aatalin@sandia.gov

Understanding the transport of electrons, ions, and excitons in nanostructures is critical for realizing the potential of nanoscience and next generation device technologies. Of particular challenge, and opportunity, for understanding transport in nanostructures is the impact of interfaces, shapes, electronic confinement, interactions and quantum effects. This is particularly true of hybrid, complex nanomaterials of different compositions and phases that can have varying degrees of electronic and optical couplings and interactions. Depending on the composition and geometry, couplings (electromagnetic, Coulomb, ballistic, tunnel, etc) can be weak or strong. Structural components used in hybrid nanostructures can be made of semiconductors, metals, molecules, liquids, etc. Correspondingly, elementary excitations responsible for optical and transport responses of such nanostructures include excitons, plasmons, electrons and ions.

Contributions are solicited in areas that reflect recent advances in experimental characterization and theory of transport mechanisms in inorganic and hybrid nanoscale structures. Specific topics of interest include, but are not limited to:

- Excitonic nanomaterials with light-harvesting and lighting properties utilizing both solid-state and molecular components
- Plasmonic nano- and meta-structures for light harvesting and concentration
- Hybrid structures with interacting exciton and plasmon resonances
- Energy transfer in hybrid nanomaterials including dots, wires, plates, polymers, etc
- Charge and exciton transport through metal-semiconductor interfaces

- Ultrafast dynamics of charge and exciton transport in nanostructures and across nanoscale interfaces
- Dynamics of energy and charge flow in nanostructured hybrid materials
- Hybrid nanomaterials for photo-catalytic applications utilizing excitons and plasmons
- Nanomaterials with bio-sensor properties
- Externally driven nanomaterials interacting with bio-matter
- Theoretical models of hybrid nanostructures with migration of charge and energy
- Experimental and theoretical correlation of nanoscale structure with electronic transport properties.
- Influence of dimensionality on charge and exciton transport

13.1.4: Complex Oxide Interfaces and Heterostructures (DMP/DCMP)

Organizers:

Sergei V. Kalinin (ORNL) sergei2@ornl.gov

James M Rondinelli (Northwestern U.) jrondinelli@northwestern.edu

Complex oxide heterostructures display a range of impressive multi-functionality, encompassing superconductivity, colossal magnetoresistance, magnetism, multiferroicity, and strongly correlated Mott-Hubbard insulator-type behavior in addition to novel interface-stabilized ground states such as two-dimensional electron gases (2DEGs), 2D superconductivity, novel magnetism, and topological phases. The extreme sensitivity of these phenomena to composition and interface structure offers endless possibilities for fundamental studies of the interactions between the structural and electronic degrees of freedom that give rise to these fascinating phenomena, and thus providing many insights into materials physics in addition to the capability to design completely new devices. Local symmetry breaking, charge transfer, magnetic and electrostatic interactions, and coupling between structural modes are just some of the many mechanisms that can lead to the appearance of novel interfacial functionalities and can be employed for rational design of artificial materials with desirable structural, electronic and magnetic properties.

The aim of this focus session is to provide a forum for the discussion of recent experimental and theoretical results on complex-oxide heterostructures and their interfaces. The topics covered in this session will include advances in the growth and characterization of complex-oxide heterostructures, development of interface-related measurement techniques, theory and modeling of oxide heterostructures and interfaces, experimental investigation and tuning of interface-related properties in conducting, insulating and magnetic oxides, chemical and electrochemical effects in manifestation of physical functionalities,

applications based on interface-related phenomena in complex-oxide heterostructures, and new phenomena appearing in complex oxides owing to heterostructuring.

13.1.6: Thermoelectric Phenomena, Materials, Devices, and Applications (DMP/GERA/FIAP/DCOMP/DCMP)

Organizers:

Pramod Reddy (U. Michigan) pramodr@umich.edu

Eric Toberer (Colorado School of Mines) etoberer@mines.edu

Jeffrey Urban (LBNL) jjurban@lbl.gov

Thermoelectrics have emerged as a new frontier of materials research for energy conversion applications, with the dramatic increases in ZT over the past twelve months adding to the excitement. Physics associated with charge carrier, spin, photon, and phonon transport is of particular interest. This focus topic addresses recent developments in the fundamental understanding of thermoelectric materials, including theory, synthesis, characterization, processing, mechanical, thermal, and electrical properties. This sessions will also highlight the latest application advances in waste heat recovery, high efficiency heating/cooling, and how application related requirements lead to new avenues of fundamental research. Both Experimental and theoretical contributions are solicited.

13.1.7: Mesoscopic Materials and Devices (DMP/DCMP)

Organizers:

David Lederman (West Virginia U) dlederma@wvu.edu

Jeremy Levy (U. Pittsburgh) jlevy@pitt.edu

Nina Markovic (Johns Hopkins University) ninazagreb@gmail.com

This Focus Topic covers materials and devices with physical dimensions that are comparable to the quantum phase coherence length of the electrons. In this regime, the properties of the system can be manipulated and novel phenomena can be uncovered by controlling the size, shape, configuration and boundary conditions. The focus topic spans two main areas: (i) facilities, tools and methods needed to make, characterize and describe mesoscale materials, and (ii) new mesoscale phenomena and functionality.

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

- Mesoscale fabrication: For example, lithographic techniques based on high-resolution electron beams, scanning- force-microscopy (SFM), and imprinting; SFM-stimulated growth; self-assembly; focused ion beam (FIB) manufacture; electron-beam-induced deposition (EBID); ion-beam-induced deposition (IBID) and other novel fabrication and synthesis methods.

- Mesoscale characterization: Some examples are ballistic-electron emission microscopy (BEEM), SFM, optical microscopy and spectroscopy, time- and frequency-resolved measurements, tunneling spectroscopy, transport properties and electro-luminescence studies in small structures.
- Mesostructures and devices: This includes quantum wires and dots; mesoscale FETs and single-electron transistors (SETS); photonic and plasmonic structures; ferromagnetic, multiferroic, and spin-based devices; superlattice arrays; new developments in graphene devices, topological states of matter at the mesoscale; molecular electronic systems; and meso-electromechanical devices.
- Correlated electron systems at the mesoscale: Relevant phenomena include non-equilibrium transport, instabilities; competition between phases at the mesoscale; and quantum critical phenomena in metallic systems.
- Quantum coherence at the mesoscale: The systems include the quantum Hall effect in mesoscale devices; ballistic quantum systems; quantum chaos; quantum-computing implementations and theory, phase coherence and breaking of coherence in electronic and spin systems.

DMP Co-Sponsored Focus Topics led by other APS Units (submit invited talk nominations through primary sponsoring Unit)

01.1.8 Organic Electronics and Photonics (DPOLY/DMP)

10.1.1 Magnetic Nanostructures: materials and phenomena (GMAG/DMP)

10.1.2 Emergent properties in bulk complex oxides (GMAG/DMP)

10.1.3 Magnetic oxide thin films and heterostructures (GMAG/DMP)

10.1.4 Spin transport and magnetization dynamics in metals-based systems (GMAG/DMP/FIAP)

10.1.5 Spin dependent phenomena in semiconductors (GMAG/DMP/FIAP)

10.1.6 Frustrated magnetism (GMAG/DMP)

10.1.7 Spin-orbit mediated chiral spin textures (GMAG/DMP)

10.1.8 Low-dimensional and molecular magnetism (GMAG/DMP)

16.1.2 Predicting and Classifying Materials Via High-Throughput Databases and Machine Learning (DCOMP/DMP)

16.1.7 Materials in Extremes: Bridging Simulation and Experiment (DCOMP/DMP/GSCCM)