# Summer 2017 Newsletter

DMP NEWSLETTER
Division of Materials Physics

## In this Issue



## Important Dates

**August 29, 2017** Deadline for submitting invited speaker suggestions for DMP Focus Topics through ScholarOne site.
**November 3, 2017 (Friday)** Abstract deadline for the 2018 APS March Meeting. Submission is via the web at http://abstracts.aps.org
**November 21, 2017** Deadline DMP Ovshinsky Student Travel Awards.
**November 21, 2017** Deadline DMP Post Doctoral Travel Awards.
**March 5 - March 9, 2017** APS March Meeting in Los Angeles, California.

## A Note from the Chair

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 progress 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 Los Angeles, March 05-09, 2018. 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. Focus Topic sessions provide a high profile venue for contributed talks at the March Meeting as a typical Focus Topic session has one invited talk and twelve contributed talks, and ideally a series of sessions related by the topic will run sequentially in the same room. Chair-Elect Amanda Petford-Long is coordinating the process, utilizing input from you, the community, the members of the Executive Committee, and many volunteers from our community who are organizing the individual Focus Topics. We encourage you to review the topics, suggest invited speakers to the organizers, and plan to submit contributed talks to the topics that overlap with your

interests. A full list of the Focus Topics for this year's March Meeting is contained at the end of this newsletter.

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. This is the fourth year of the Richard L. Greene Dissertation Award in Experimental Condensed Matter Materials Physics. We are grateful to Rick for this philanthropic contribution and expect to see many deserving candidates from which to choose the fourth annual award. Please consider nominations for this award for March Meeting 2018. The nomination deadline is September 1, 2017. Please see the Richard L. Greene Dissertation Award page 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 as well as post-doctoral 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. Information is included below.

I want to also give a big round of thanks to 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 include Emilia Morosan and Jeff Neaton who have stepped down as Members at Large, Bob Nemanich who has completed a three-year term as Secretary/Treasurer, and last but not least, John Mitchell who has completed four years of leadership as Vice-Chair, Chair-Elect, Chair, and Past-Chair of the Division of Materials Physics. All have been extremely generous of their time and energy, and have made the DMP and the broader materials physics community much stronger and richer because of their efforts.

Most of you also know that we have recently lost a giant in our field, Professor Mildred "Millie" Dresselhaus, who passed away earlier this year. The DMP, working together

with the APS and other units, is exploring ways to honor and remember her. Your input on this is appreciated as well.

We look forward to seeing you in Los Angeles in March!

Dan Dessau, DMP Chair

## The DMP Executive Committee

**Chair:** Daniel Stephen Dessau, Univ of Colorado - Boulder (04/17 - 03/18)
**Chair Elect:** Amanda K Petford-Long, Argonne Natl Lab (04/17 - 03/18)
**Vice Chair:** Nitin Samarth, Pennsylvania State University (04/17 - 03/18)
**Past Chair:** Michael E Flatté, Univ of Iowa (04/17 - 03/18)
**Councilor:** Samuel Bader, Argonne Natl Lab (01/17 - 12/20)
**Secretary/Treasurer:** Charles Ahn, Yale University (4/17 - 3/20)

**Members-at-Large:**

Ezekiel Johnston-Halperin, Naval Research Lab (04/17-03/20)
Ni Ni, University of California, Los Angeles (04/17-03/20)
Peter M Gehring, NIST - Natl Inst of Stds & Tech (04/15 - 03/18)
John Singleton, Los Alamos Natl Lab (04/15 - 03/18)
Scott Chambers, Pacific Northwest Natl Lab (04/16 - 03/19)
Michelle Dawn Johannes, Naval Research Lab (04/16 - 03/19)

## The Division of Materials Physics March Meeting Post Doctoral Travel Awards

To recognize innovative materials physics research by post doctoral researchers, the Division of Materials Physics has initiated March Meeting Post Doctoral Travel Awards. The Awards are supported by the Division of Materials Physics.

We anticipate that there will be up to eight $800 Travel Awards in 2018 to support participation in DMP Focus Topic sessions at the APS March Meeting sessions. The selection will be based on the research quality, the impact of the research at the March Meeting and the innovative contribution of the post doctoral researcher, The selection committee will consist of members of the DMP Executive Committee.

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

## The 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 in, 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 that 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 and Honorable Mention Awards** were presented at the 2017 March Meeting and were listed in the 2016 Winter DMP Newsletter.

## Nominations for DMP Officers and Executive Committee Members

The DMP Officer election will be held late in 2017 to elect a Vice-Chair, a Secretary-Treasurer, a Divisional Councilor, and two new at-large Executive Committee Members. According to the Bylaws, the Nominating Committee shall nominate at least two candidates for the ballot for each office. We are inviting your suggestions for candidates, which should be emailed to the DMP Past Chair, Michael Flatté, (michael_flatte@mailaps.org) by September 15, 2017.

It is important to remember the membership of APS is diverse and global, so the Executive Committees of the APS should reflect that diversity. Nominations of women, members of underrepresented minority groups, and scientists from outside the United States are especially encouraged.

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 DMP Secretary/Treasurer, Charles Ahn (charles.ahn@yale.edu) October 1, 2017.

## DMP Focus Topics for the 2018 APS March Meeting

With this issue of the Newsletter, the Division of Materials Physics announces the program of DMP Focus Topics for the 2018 APS March Meeting (Los Angeles, California, March 5

– March 9, 2018). 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.

For the 2018 March Meeting, DMP is the lead organization unit on 20 different Focus Topics and co-sponsoring unit for an additional 15. See lists below.

We encourage Invited speaker nominations for the DMP-led Focus Topics. You will need an APS web account to log in to the system:

Deadline: Aug. 29, 2017
Submission: https://www.aps.org/meetings/abstracts

In suggesting speakers please keep in mind that speakers who gave an invited talk at the previous March Meeting are ineligible.

Your nomination will go to the organizers of the Focus Topic for which you have suggested a candidate and will aid the organizers in their selection of invited speakers.

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 2018 APS March Meeting

**7.1.1: Dielectric and Ferroic Oxides** (same as 11.1.1, 16.1.13)
***Organizers:***
**Seiji Kojima** (U Tsukuba) **kojima@ims.tsukuba.ac.jp**
**Nicholas Barrett** (CEA) **nick.barrett@cea.fr**
**Shi Liu** (Carnegie Inst for Science) **sliu@carnegiescience.edu**

Complex oxides can exhibit a rich variety of order parameters, such as polarization, strain, charge and orbital magnetization degrees of freedom. Their ordering phenomena give rise to a vast range of functional properties including ferroelectricity, polarity, pyroelectricity, electrocaloricity, magnetoelectricity, multiferroicity, metal-insulator transitions and defect-related properties, which are the principal topics of interest for this symposium. Understanding and harnessing these functional properties in view of new applications is a major challenge in our field:

- Photovoltaics and photo-induced phenomena such as strain and charge order
- Domain wall engineering
- Band-filling and bandwidth control for charge and orbital ordering
- Electric or mechanical control of ordering phenomena
- Energy harvesting

This focus topic therefore welcomes contributions on fundamental aspects of structure, ordering and functionality in complex oxides as well as on emerging avenues to controlling polarization, magnetism and electronic properties via strain and/or strain gradients and/or defects. Contributions on breakthroughs and progress in the theory, synthesis, characterization, and device implementations in these and other related topics are highly encouraged.

**7.1.2: Topological Materials: Synthesis, Characterization and Modeling**
***Organizers*:**
**Yong Chen** (Purdue Univ) chen276@purdue.edu
**Chaoxing Liu** (Penn State Univ) cxl56@psu.edu
**Zhiqiang Mao** (Tulane Univ) zmao@tulane.edu

There has been explosive growth in the study of topological insulators in which the combined effects of the spin-orbit coupling and time-reversal symmetry yield a bulk energy gap with novel gapless surface states that are robust against scattering. Moreover, the field has expanded in scope to include topological phases in superconductors, crystalline insulators, (semi)metals, Kondo systems, magnetic materials and complex heterostructures capable of harboring exotic topologically nontrivial state 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 that have properties amenable to the study of the bulk, 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 single crystals, exfoliated and epitaxial thin films and heterostructures, and nanowires and nanoribbons, in addition to 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, scanning probe, photoemission and other spectroscopic techniques, and related theoretical efforts aimed at modeling various properties both in the surface/interface and in the bulk.

**7.1.3: Dirac and Weyl semimetals: prediction, synthesis, characterization and new phenomena** (same as 12.1.10)
***Organizers*:**
**Ken Burch** (Boston College) ks.burch@bc.edu
**Andrei Bernevig** (Princeton Univ) bernevig@princeton.edu
**Johnpierre Paglione** (Univ Maryland) paglione@umd.edu

The field of topological semimetals has developed dramatically over the past few years. After the initial prediction and discovery of Dirac and Weyl semimetals – materials whose low energy excitations can be described by the Dirac or Weyl equation of high-energy physics – the field has now expanded to include new low-energy excitations not possible in a high-energy setting. Semimetals with different degeneracy at crossing points or lines have been predicted. Transport theories and effects have been predicted and proposed in order to measure a small subset of the topological characteristics of the semimetals (such as Chern numbers). Furthermore, semimetals whose existence is guaranteed by filling constraints derived from the presence of certain orbitals at certain points in specific lattices have also been mentioned in the literature.

Distinct from conventional low carrier density systems, Dirac, Weyl and other semimetals are expected to possess exotic properties due to the nontrivial topologies of their electronic wavefunctions. A subset of the novel properties predicted include Berry phase contributions to transport properties, chiral anomaly, quantized nonlinear transport under circularly polarized

light, protected Fermi arc surface states, suppressed scattering, optical control of topology, landau level spectroscopy, superconductivity, and non-local transport. While promising candidate materials exist for many but certainly not all of the topological semimetals, many phenomena have yet to be clearly resolved.

This focus topic aims to explore Dirac, Weyl and other new semimetals and the novel phenomena associated with them. We solicit contributions on predictions, new materials synthesis and characterization, new phenomena in topological semimetals, as well as studies on both conventional and unconventional semimetals, both in the bulk and on the surfaces of samples that accentuate the non-trivial topological character of the new semimetals.

**7.1.4: Hybrid Organic-Inorganic Halide Perovskites** [Same as 12.1.11]

***Organizers*:**

**Yan Li** (Univ Utah) sarahli@physics.utah.edu
**Hanwei Gao** (Florida State Univ) h-gao@physics.fsu.edu

Organometallic halide perovskites have recently caused a surge of interest in their optoelectronic properties and applications due to their remarkable performance as semiconductor light absorbers in solar cells. As a anew class of semiconductors, these materials are interesting not only because of the hybrid organic-inorganic structure, but also for their superior properties such as high defect tolerance, strong optical absorption, low recombination rate, ambipolar charge transport, and tunable physical properties. Rapid progress has been made in the demonstration of photoelectronic perovskite devices for photovoltaics, light emission, lasing and photodetection. Possible structural asymmetry, due to lattice distortion by organic cations, gives rise to ferroelectricity and large Rashba spin-orbit coupling in the hybrid perovskites, which provides more functionality to devices with electric field control and/or utilization of spin. However, the underlying physics of many unusual properties remains elusive, such as the hysteretic current-voltage relationships, low recombination rate, long spin lifetime and ferroelectric behavior. The practical use of these hybrid perovskite calls for more in-depth understanding of their fundamental properties and versatile strategies to tune and optimize the materials properties. In this Focus Topic we expect contributions on broadly-defined experimental and modeling studies of the optical, electronic, structural and defect properties of the organometallic halide perovskites. Advancements in materials engineering and the development of practical applications are also encouraged.

**7.1.5: 5d/4d Transition Metal Systems**

***Organizers:***

**Vivien Zapf** (Los Alamos National Lab) vzapf@lanl.gov
**Natalia Perkins** (Univ Minnesota) nperkins@umn.edu

Materials with 5d and 4d orbitals occupy a unique niche due to the competition between the crystal-field, spin-orbit coupling and Coulomb repulsion energy scales, as well as exchange interactions. These materials pose a challenge for observing and calculating behavior in the strongly spin-orbit coupled regime due to competing spin, charge and lattice degrees of freedom. As a consequence of the intricate interplay between various interactions, 5d and 4d materials exhibit intriguing properties that have been observed in experiment and theory, including unexpected insulating behavior, topological spin liquids and unconventional superconductivity. This focus topic covers experimental and theoretical work on compounds containing 5d/4d elements, e.g. iridium, osmium, rhodium or ruthenium and others. These materials can be found for a variety of two- and three-dimensional lattices with varying degree of frustration and

correlations. Emergent phases include magnetism, topological behavior, spin liquids, superconductivity and metal-to-insulator transitions. The topic is not limited to oxides.

**8.1.2: Dopants and Defects in Semiconductors** [same as 16.1.14]

***Organizers*:**

**Jack Lyons** (Naval Research Lab) john.lyons@nrl.navy.mil
**Evan Glaser** (Naval Research Lab) evan.glaser@nrl.navy.mil
**Greg Fuchs** (Cornell Univ) gdf9@cornell.edu

Impurities and native defects profoundly affect the electronic and optical properties of semiconductor materials. Impurity incorporation is often a necessary step for tuning the electrical properties in semiconductors. Defects control carrier concentration, mobility, lifetime, and recombination; they are also responsible for the mass-transport processes involved in the migration, diffusion, and precipitation of impurities and host atoms. Controlling the presence of impurities and defects is a critical factor in semiconductor engineering, and has enabled the remarkable development of Si-based electronics, GaN-based blue light-emitting diodes and lasers, semiconducting oxides for transparent conducting displays, and the promise of next-generation sensors and computing based on individual defects like the NV center in diamond. The fundamental understanding, characterization and control of defects and impurities will also be essential for developing 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 and including surfaces and interfaces, is the subject of this focus topic. Abstracts on experimental, computational 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; wide band-gap materials such as diamond, aluminum nitride, and gallium oxide; single-photon defect emitters including NV centers and their analogues; defects in two-dimensional materials including phosphorene, h-BN and transition metal dichalcogenides; and the emerging organic-inorganic hybrid perovskite (e.g., MAPbI3) solar cell materials are of interest. Abstracts on specific materials challenges involving defects, e.g., in processing, characterization, property determination, including imaging and various new nanoscale probes are also welcomed.

**9.1.1: Fe-based Superconductors**

***Organizers*:**

**Jiun-Haw Chu** (U. Washington) jhchu@uw.edu
**Qimiao Si** (Rice U.) qmsi@rice.edu
**Jiaqiang Yan** (Oak Ridge National Lab) yanj@ornl.gov

Fe-based superconductors (FeSCs) continue to fascinate the materials and condensed matter physics communities as we move into a new decade of their study. While the field started from the iron pnictides, new efforts have increasingly been directed towards the iron chalcogenides. Recent advances in the synthesis and control of the FeSCs are giving us renewed hope for even higher superconducting transition temperatures. At the same time, considerable progress is being made in the understanding of these materials, including the bad-metal normal state and the degree of electron-electron correlations, the order and excitations of the various electronic degrees of freedom (spin, orbital, charge and nematic), the role of quantum criticality in the phase diagram, and the amplitude and structure of the multi-orbital superconducting pairing. In addition, there is progress in understanding the unifying principles that may optimize

superconductivity of the FeSCs and connect them with other unconventional superconductors such as the cuprates, heavy fermions and organic charge-transfer salts. Finally, the FeSCs may connect to broader issues on superconductivity, such as BCS-BEC crossover and topological superconductivity. This focus topic will cover the pertinent recent developments in the materials growth, experimental measurements and theoretical understandings, and survey the potential for discovering new superconducting systems with still higher transition temperatures.

### 9.1.2 Topological Superconductivity

***Organizers:***

**Matthew Gilbert** (Univ Illinois Urbana-Champaign) matthewg@uiuc.edu
**Eun-Ah Kim** (Cornell Univ) eun-ah.kim@cornell.edu
**Nadya Mason** (Univ Illinois Urbana-Champaign) nadya@illinois.edu

Topological superconductors are superconductors characterized by topological invariants associated with the band-structure of the Bogoliubov quasi-particles. They have been a focus of significant experimental and theoretical effort due to their potential relevance to both fundamental physical and mathematical concepts, and practical implementations of topological quantum computation. Although the early focus in the search for topological superconductors was on bulk materials, there has been much recent progress in studies of atomically thin materials, artificially engineered structures, and the surfaces of new bulk materials. This Focus Topic will cover topological superconductivity and closely related non-centrosymmetric superconductivity in new experimental settings such as transition metal dichalcogenides, topological insulators, Weyl semi-metals, FeSe-based systems, graphene, engineered heterostructures, semiconducting nanowires, Shiba states, junctions with ferromagnets, quantum Hall states, and Floquet systems. This Focus Topic will also cover new developments in the understanding of $Sr_2RuO_4$ and other known candidate systems, as well as advances in strategies for quantum information processing using topological superconductivity.

### 12.1.1: 2D Materials: Synthesis, Defects, Structure and Properties

***Organizers***:

**Connie Li** (Naval Reseach Lab) connie.li@nrl.navy.mil
**Marc Bockrath** (Ohio State Univ) bockrath.31@osu.edu
**Eric Stinaff** (Ohio Univ) stinaff@ohio.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** [Same as 8.1.7]

***Organizers*:**

**Junqiao Wu** (UC Berkeley) wuj@berkeley.edu
**Ian Appelbaum** (Univ Maryland) appeli@physics.umd.edu
**Di Xiao** (Carnegie Mellon Univ) dixiao@cmu.edu

Research exploring 2D semiconductors and their heterostructures is rapidly expanding to include a wide variety of layered material systems with diverse properties, including strong many-body interactions, strong spin-orbit coupling effects, spin- and valley-dependent physics, and topological physics. This Focus Topic will cover experimental and theoretical/computational work related to 2D semiconductors and their heterostructures, including large bandgap materials such as the chalcogenides (e.g. $MoS_2$, $WSe_2$, GaSe and ReSe), phosphorene and h-BN, small bandgap materials with possible topological properties (such as silicene, germanene, stanene and $Bi_2Se_3$), and magnetic semiconductors (e.g. $CrGeTe_3$, $CrI_3$, Mn:$MoS_2$). We encourage abstracts discussing important topics related to monolayers, few-layers and heterostructures, including quantum transport properties, mobility engineering, spin- and valley-dependent phenomena, 2D exciton physics, the effect of defect engineering on optical and electronic properties, understanding the role of the dielectric environment, and many-body effects, in addition to magnetic, thermal and mechanical properties.

**12.1.3: Devices from 2D Materials: Function, Fabrication and Characterization**

***Organizers***:

**Jim Hone** (Columbia Univ) jh2228@columbia.edu
**Joshua Robinson** (Penn State Univ) robinson@matse.psu.edu
**Andrea Young** (UC Santa Barbara) andrea@ucsb.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., $MoS_2$, $WSe_2$, $NbSe_2$, $TaS_2$, FeSe etc.), silicene, germanane, stanene,

phosphorene, topological insulators (e.g., $Bi_2Se_3$, $Bi_2Te_3$, 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**

***Organizers***:

**Luis Balic**as (High Field Magnet Lab, Tallahassee) balicas@magnet.fsu.edu
**Tony Heinz** (Stanford Univ) tony.heinz@stanford.edu

In the last few years, there has been an explosion of activities in the field of two-dimensional materials beyond graphene. Much of the effort focused on the rich optoelectronic properties of semiconducting compounds like the transition metal dichalcogenides (TMDs) or black phosphorus. Some of the TMDs display an insulating to metal transition upon gating which seems to be driven by electronic correlations. Others are metallic (or semi-metallic) over the entire temperature range while presenting gapped electronic ground states, such as superconductivity or charge-density waves. Semi-metallic $WTe_2$ and orthorhombic $MoTe_2$ (or $ZrTe_5$) are claimed to possess unique topological features in their electronic band structures apparently leading to anomalous transport properties and perhaps also to an unconventional superconducting state. For monolayer $NbSe_2$ superconductivity was shown to survive the application of extremely high magnetic fields when applied along its planar direction, while electronic correlations are likely to be important for the high superconducting transition temperature observed in monolayer FeSe. Surprisingly, the suppression of inter-planar coupling was claimed to enhance the charge-density wave transition in monolayers of TMDs. But with the exception of bilayer graphene, and probably also the quantum Hall-effect seen in transition metal dichalcogenides, InSe or black-phosphorus, to date there are relatively few examples of mono- or few-layered compounds, for which correlations seem to play a fundamental role.

This focus topic will concentrate on two-dimensional materials displaying gate induced phase-transitions or ground states with either non-trivial topologies or broken-symmetries for which new and relevant physical phenomena is likely to emerge.

**12.1.6: Van der Waals Bonding in Advanced Materials** [same as 16.1.17]

***Organizers***:

**Evan Reed** (Stanford Univ) evanreed@stanford.edu
**Aaron Lindenburg** (Stanford Univ) aaronl@stanford.edu
**Alejandro Rodriguez** (Princeton Univ) arod@princeton.edu

Whether binding two-dimensional materials, organic components, or defining surface energies, van der Waals interactions are central to structure, stability and function. While these forces are typically weaker than the internal (covalent) bonds that hold a molecule together, they still span a few orders of magnitude and thus present a unique challenge to both theory and experiment. Electromagnetic Casimir effects are closely related but are commonly studied and engineered by separate communities. This focus session aims to bring together theorists and experimentalists from a wide range of materials and electromagnetic disciplines to discuss the

key challenges, opportunities, and recent progress in the characterization and engineering of van der Waals bonded complexes/materials and Casimir forces in structured media.

We hope to increase participation by some members of the Casimir community for cross fertilization of ideas.

**12.1.7: Computational Design and Discovery of Novel Materials** [same as 16.1.1]
***Organizers***:
**Qimin Yan** (Temple University) qiminyan@temple.edu
**Anderson Janotti** (University of Delaware) janotti@udel.edu
The development of predictive computational simulation for accelerating the discovery and rational design of functional materials is a challenge of great contemporary interest. Advances in algorithms and predictive power of computational techniques are playing a fundamental role in the discovery of novel functional materials, with successful examples in catalysis, batteries, and photoelectrochemistry. High-throughput computation and materials databases have recently enabled rapid screening of both molecules and solid-state compounds with multiple properties and functionalities. This focus topic will cover research efforts to accelerate materials discovery and/or development by building the fundamental knowledge base and applying novel data driven approaches to design materials with specific and targeted functional properties from first principles.
Abstracts are solicited in the areas of interest that include computational materials design and discovery; development of accessible and sustainable data infrastructure; development of new data analytic tools and statistical algorithms; advanced simulations of material properties in conjunction with new device functionality; data uncertainty quantification; advances in predictive modeling that leverage machine learning and data mining; algorithms for global structure and property optimizations; and computational modeling of materials synthesis. The technical applications include but are not limited to electronic and optoelectronic materials, magnetic materials and spintronics, energy conversion and storage materials (thermoelectrics, batteries, fuel cells, photocatalysts, photovoltaics, ferroelectrics), metallic alloys, and two-dimensional materials. Contributions that feature strong connection to experiments are of special interest.

**13.1.1: Nanostructures and Metamaterials**
***Organizers***:
**Jay Foley** (William Patterson Univ) jayfoley.iv@gmail.com
**Hayk Harutyunyan** (Emory Univ) hayk.harutyunyan@emory.edu

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

**13.1.3: Electron, Exciton, and Phonon Transport in Nanostructures**
***Organizers*:**
**Pierre Darancet** (Argonne National Lab) pdarancet@anl.gov

**Alexander Weber-Bargioni** (Lawrence Berkeley National Lab) afweber-bargioni@lbl.gov
**Pramod Reddy** (Univ Michigan) pramodr@umich.edu

Understanding and controlling how heat, charge, and energy flow at the nanoscale is critical for realizing the potential of nanomaterials in next generation device technologies. Of particular challenge, and opportunity, is understanding how elementary excitations such as phonons, electrons, holes, excitons, and plasmons interact with each other and are influenced by interfaces, confinement, and quantum effects in nanostructures. This is particularly true for heterogeneous nanoscale materials and interfaces with varying degrees of electronic and phononic couplings, and distinct thermal and electrical impedances. Structural components used in hybrid nanostructures can be made of semiconductors, metals, molecules, liquids, etc.

Contributions are solicited in areas that reflect recent advances in experimental measurement, theory, and modeling of transport mechanisms in nanoscale materials and interfaces. Specific topics of interest include, but are not limited to:

- Electron-phonon coupling and heat generation by hot charge carriers
- Dynamics of energy and charge flow in nanostructured hybrid materials
- Ultrafast dynamics of charge carriers, excitons and phonons in nanostructures and across nanoscale interfaces
- Charge, heat, and exciton transport through metal-semiconductor interfaces
- Correlating nanoscale interface structure & chemistry with charge, heat, and exciton transport
- Non-equilibrium heat transport and phonon-bottlenecks effects
- Influence of dimensionality and nanostructuring on charge, heat, and exciton transport
- Energy transfer in hybrid nanomaterials including dots, wires, plates, polymers, etc
- 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
- Near-field heat transfer and energy conversion in nanogaps and nanodevices
- Hybrid structures with interacting exciton and plasmon resonances
- Hybrid nanomaterials for photo-catalytic applications utilizing excitons and plasmons

### 13.1.3: Complex Oxide Interfaces and Heterostructures

***Organizers***:

**Adam Hauser** (Alabamu Univ) ahauser@ua.edu
**Divine Kumah** (North Carolina State Univ) dpkumah@ncsu.edu
**Xifan Wu** (Temple Univ) XifanWu@temple.edu

When complex oxides are prepared as thin films and heterostructures, they exhibit additional properties that cannot be realized in the constituent materials alone. These novel properties arise as a result of interfacial charge transfer, exchange coupling, orbital reconstructions, proximity effects, dimensionality as well as the mechanical and electric boundary conditions. Emergent electronic and magnetic states at oxide interfaces raise exciting prospects for new fundamental physics and technological applications. This Focus Topic is dedicated to progress in the fabrication, methodologies, and knowledge in the field of complex oxide thin films, heterostructures, superlattices, and nanostructures. Synthesis, characterization, theory, and novel device physics are emphasized. Specific areas of interest include, but are not limited to, growth of oxide thin films and heterostructures (with special emphasis on new materials/interfaces), control of properties (magnetic, electronic, ordering, interfacial

superconductivity, multiferroicity, magnetotransport, spin-orbit coupling), and developments in theoretical prediction and materials-by-design approaches. Advances in techniques to probe and image electronic, structural and magnetic states at heterostructure interfaces are also emphasized. Note that overlap exists with other DMP and GMAG focus sessions. As a rule of thumb, if complex oxides and their heterostructures are at the core of the investigation, then the talk is appropriate for this focus topic.

**13.1.4 Materials for Post-Moore Computing**
***Organizers***:
**Shriram Ramanathan** (Purdue Univ) shriram@purdue.edu
**Joshua Yang** (Univ Massachusetts) jjyang@umass.edu

Information processing is at a cross-roads. Traditional approaches to CMOS scaling and dimensionality reduction are nearly at the physical limits with diminishing returns on performance. The bottleneck of von Neumann architecture has become an increasing limiting factor on the throughput of traditional computing paradigms. Exponential growth in mobile devices amidst a rapid pace of global connectivity through internet and satellites creates new opportunities for condensed matter physics and devices. New materials and new physical properties / collective excitations should be exploited going forward to continue seamless innovations and breakthroughs in electronic materials and devices for unconventional computing. Close collaboration between physicists, materials scientists and electrical engineers may be particularly fruitful. In this context, a symposium focusing on new materials and structures for computing coupled with fundamental physical understanding of properties and phenomena is being explored in APS for the first time. Given this topic is highly exploratory in nature, we solicit presentations in broadly defined areas below as well as related topics that would be considered to be in early stages of research:

- 2D materials and electronics
- New materials (e.g. non-Silicon CMOS) such as oxides, chalcogenides, compositionally complex systems for information storage, logic
- Memristors and two-terminal computing devices
- Ionotronics: use of ions for computing and memory
- Metals and other exotic spin systems for spintronics
- Magnetic materials for domain wall electronics
- Hybrid electronics, e.g. liquid-solid interfaces for ionic-gated devices
- New approaches to computing non-charge state variables, e.g. topological order, spin
- Optical computing materials and devices
- Biological, polymer or inorganic materials for neuromorphic computing
- First principles theory/simulations of emerging electronic materials/devices
- New computing approaches for non-equilibrium systems, e.g. materials under electric fields
- Other ideas that may be exploratory and less well defined at this time

**13.1.5 Assembly and Behavior of Hierarchical Materials**
***Organizers****:*
**Steve Whitelam** (Lawrence Berkeley National Lab) swhitelam@lbl.gov
**Dmitri Talapin** (U Chicago) dvtalapin@uchicago.edu

Hierarchical materials can have properties much different to those of their constituents arranged in a simple way. For instance, tooth enamel and bone have properties of strength and durability that far outstrip those of simple crystals of their constituent minerals. Nature's ability to build

functional hierarchical materials extends to virus capsids and proteins, and provides inspiration for synthetic hierarchical nanomaterials self-assembled in the laboratory. This DMP Focus Topic will explore the assembly and properties of hierarchical materials, both synthetic and biological.

**14.1.1: Surface Science of Organic Molecular Solids, Films, and Nanostructures**

***Organizers*:**

**Mina Yoon** (Oak Ridge National Lab and U Tennessee) myoon@ornl.gov
**Chenggang Tao** (Virginia Tech) cgtao@vt.edu
**Wai-Lun Chan** (Univ Kansas) wlchan@ku.edu

Organic molecular solids are a challenging materials class since numerous "weak" interactions, all of comparable strength, control structures and functional properties. The promise of high performance optoelectronics, designer sensors, electrode work function control, and bioelectronic devices make the payoff for addressing this challenge high. Moreover, there is great scientific value in addressing complex systems with hierarchical interactions and a strong tension between localized and delocalized phenomenon such as found in organic molecular solids. This Focus Topic will bring together Surface Scientists to report and discuss new experimental and theoretical/computational results aimed at the basic physics underpinning this material class. Research of interest includes the structure, properties, electron dynamics, and applications of organic adsorbates, monolayer assemblies, thin films, crystals and nanostructures.

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

**01.1.9: Organic Electronics and Photonics (DPOLY/DMP)**
**08.1.8: Organic Electronics and Photonics (DPOLY/DMP)**
**10.1.1: Magnetic Nanostructures: Materials and Phenomena (GMAG/DMP)**
**10.1.2: Emergent Properties of Bulk Complex Oxides (GMAG/DMP/DCOMP)**
**10.1.3: Magnetic Oxide Thin Films and Heterostructures (GMAG/DMP/DCOMP)**
**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/DCOMP)**
**10.1.6: Frustrated Magnetism (GMAG/DMP)**
**10.1.7: Spin-orbit Mediated Chiral Spin Textures, including Skyrmions (GMAG/DMP)**
**10.1.8: Low-dimensional and Molecular Magnetism (GMAG/DMP)**
**16.1.1: Petascale Science and Beyond: Applications and Opportunities for Materials, Chemical and Bio Physics (DCOMP/DMP/DCMP/DCP/DBIO)**
**16.1.2: Electrons, Phonons, Electron Phonon Scattering and Phononics (DCOMP/DMP)**
**12.1.3: First-Principles Modeling of Excited-State Phenomena in Materials (DCOMP/DMP)**
**16.1.4: Materials in Extremes: Bridging Simulation and Experiment (DCOMP/DMP/GSCCM)**
**16.1.8: Free Energy Mapping in Biology and Materials Science (DCOMP/DMP)**
**21.1.1: Thermoelectric phenomena, materials and devices (GERA/DMP)**