Frontiers in Condensed Matter and Materials Physics:

A Symposium in Honor of the 70th Birthday of Steven G. Louie

University Club, California Memorial Stadium, Berkeley, CA

Saturday, March 2, 2019

Organizing Committee:
Li Yang (Co-Chair)
Jeffrey B. Neaton (Co-Chair)
Che Ting Chan
Jack R. Deslippe
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Angel Rubio
David A. Strubbe
David Vanderbilt
Felipe H. da Jornada
Diana Y. Qiu
Zhenglu Li
Arica Chhay

Co-Hosts:
Department of Physics
University of California at Berkeley

Molecular Foundry
Lawrence Berkeley National Laboratory

Materials Sciences Division
Lawrence Berkeley National Laboratory

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- PROGRAM -

MORNING SESSIONS

Registration and Breakfast (8:00 – 8:30 AM)

Welcome Session

8:30-8:40 AM	**Li Yang** (Washington University in St. Louis) Introduction Remarks/Logistics
8:40-8:50 AM	**Michael S. Witherell** (Director, Lawrence Berkeley National Laboratory) Welcoming Remarks

Scientific Session I – *Interaction and Topological Effects in 1D and 2D Materials*
Chair: Yves Pierre Petroff (Brazilian Synchrotron Light Laboratory, Brazil)

8:50-9:10 AM	**Michael F. Crommie** (University of California, Berkeley) Using Topology to Engineer the Electronic Structure of Bottom-Up-Synthesized Graphene Nanoribbons
9:10-9:30 AM	**Che Ting Chan** (Hong Kong University of Science and Technology, Hong Kong) Exploring Pseudospin-1 Physics Using Photonic Crystals
9:30-9:50 AM	**Tony F. Heinz** (Stanford University) To Be Announced
9:50-10:10 AM	**Felipe H. da Jornada** (Lawrence Berkeley National Laboratory) Universal Dispersionless Plasmons in Quasi-Two-Dimensional Metals

Coffee Break and Symposium Photo (10:10-10:40 AM)

Scientific Session II – *Methods Do Matter*
Chair: Sokrates Pantelides (Vanderbilt University)

10:40-11:00 AM	**James R. Chelikowsky** (University of Texas, Austin) Physics for the Generations: Steve Louie's Contributions in the 1970's
11:00-11:20 AM	**Mark S. Hybertsen** (Brookhaven National Laboratory) From the Band-Gap Problem in Semiconductors to a Canonical Tool for Materials Theory
11:20-11:40 AM	**Angel Rubio** (Max Planck Institute, Germany) Quantum Electrodynamical Density Functional Theory (QEDFT): Towards New States of Matter
11:40-12:00 PM	**Matthias Scheffler** (Fritz-Haber-Institute of the Max Planck Society, Germany) Modeling Materials Properties by Artificial Intelligence and Density-Functional Theory
12:00-12:20 PM	**Jack R. Deslippe** (Lawrence Berkeley National Laboratory) Exascale and Beyond: Challenges and Opportunities for the Materials Science Community

AFTERNOON SESSIONS

Lunch and Poster Session (12:20-1:40 PM)

Lunch and Poster Session is in the Stadium Club (4th floor), below the University Club (8th floor).

Scientific Session III – *Hetereostructures and Interfaces*
Chair: Zhi-Xun Shen (Stanford University)

1:40-2:00 PM	**Philip Kim** (Harvard University) Characterization of Atomic Scale Lattice Reconstruction in Twisted van der Waals Interfaces of Layered Materials
2:00-2:20 PM	**Young-Woo Son** (Korea Institute for Advanced Study, South Korea) Novel States in Stacked Two-Dimensional Crystals
2:20-2:40 PM	**Jeffrey B. Neaton** (Lawrence Berkeley National Laboratory and UC Berkeley) Photophysics of Point Defects in Transition Metal Dichalcogenides
2:40-3:00 PM	**Giulia Galli** (University of Chicago) On Giant's Shoulders: Some Progress in Understanding Excited State Properties of Heterogeneous Materials
3:00-3:20 PM	**Mei-Yin Chou** (Academia Sinica, Taiwan) Topics of Two-Dimensional Materials and their Heterostructures

Coffee Break (3:20-3:50 PM)

Scientific Session IV – *New Insights to Liquids and Solids*
Chair: Fu-Chun Zhang (University of Chinese Academy of Sciences, China)

3:50-4:10 PM	**Roberto Car** (Princeton University) Dielectric Properties of Water from Deep Molecular Dynamics
4:10-4:30 PM	**David Vanderbilt** (Rutgers University) From Two-Phonon Bound States to Dynamic Rashba Splitting
4:30-4:50 PM	**Andrew M. Rappe** (University of Pennsylvania) Theory and Modeling of Correlated Ionic and Electronic Motions in Hybrid Organic-Inorganic Perovskites
4:50-5:10 PM	**Susumu Saito** (Tokyo Institute of Technology, Japan) Accurate Theory of Donors and Acceptors in Semiconductors: GW Approximation Versus Density Functional Approach

Note: *All science talks are 15 minutes of presentation + 5 minutes of discussion*

EVENING SESSIONS

Refreshment and Poster Session (5:30-6:30 PM)
Refreshment and Poster Session is in the Stadium Club (4th floor).

Dinner and Short Talks (6:30-10:00 PM)
Dinner is in the University Club (8th floor).
Five-minute talks by:
Marvin L. Cohen, Stephen Fahy, Jeffrey B. Neaton, Diana Y. Qiu, Thomas Roitman, Alex Zettl.

POSTER TITLES

(Arranged in alphabetical order by authors)

	Presenter and Title
P1	**Ting Cao** (Stanford University) Excitons and Valley-Spin Physics in Quasi-2D Materials
P2	**Yang-Hao Chan** (University of California at Berkeley) Excitonic Effects in Shift Currents of Low Dimensional Materials from Time-Dependent Approach
P3	**Sangkook Choi** (Brookhaven National Laboratory) A Diagrammatically Motivated *Ab Initio* Theory of Strong Correlation in Real Materials
P4	**Sinisa Coh** (University of California at Riverside) First-Principles Approach to Phonon Dynamics with Broken Time-Reversal Symmetry and Einstein-de Haas Effect
P5	**Mehmet Dogan** (University of California at Berkeley) Modifying the Band Structure of Hexagonal Boron Nitride with Metal Electrodes
P6	**Cheng Gong** (University of California at Berkeley) Two Routes Towards 2D Antiferromagnetic Spintronics
P7	**Hung-Chung Hsueh** (Tamkang University, Taiwan) Polarization Dependent Optical Response and Layer-Controlled Band Gap of 2D Group IV Monochalcogenides
P8	**Jingwei Jiang** (University of California at Berkeley) Metallic Zero-Mode Superlattice Graphene nanoribbons and band engineering
P9	**Sheng Ju** (Soochow University, China) Quasiparticle Electronic Structure, Exciton, and Optical Absorption in Two-Dimensional Phosphorus Allotropes Based on BerkeleyGW Method
P10	**Leeor Kronik** (Weizmann Institute of Science) Screened Range-Separated Hybrid Functional and GW + GW-BSE Calculations of Prototypical Semiconductors: A Comparison
P11	**Hao-Kun Li** (University of California at Berkeley) Valley-Mechanical Coupling in Monolayer Semiconductors
P12	**Zhenglu Li** (University of California at Berkeley) Electron-Phonon Coupling from Ab Initio Linear-Response Theory within the GW Method: Method and Applications to Oxide Superconductors
P13	**Johannes Lischner** (Imperial College London, United Kingdom) Tuning Electronic Properties of Transition Metal Dichalcogenides via Defect Charge
P14	**Takashi Miyake** (National Institute of Advanced Industrial Science and Technology, Japan) Data-Driven Prediction and Analysis of Magnetic Materials
P15	**Yoshiyuki Miyamoto** (National Institute of Advanced Industrial Science and Technology, Japan) Coherent Electron Dynamics in Molecules Examined by the Real-Time TDDFT Calculations
P16	**David Prendergast** (Lawrence Berkeley National Laboratory) Revealing Many-Body Effects in X-ray Absorption Spectra
P17	**Diana Y. Qiu** (University of California at Berkeley) Defect-Induced Modification of Low-Lying Excitons and Valley Selectivity in Monolayer Transition Metal Dichalcogenides
P18	**Su Ying Quek** (National University of Singapore) Quasiparticle Levels at Large Interface Systems from Many-body Perturbation Theory

P19	**John J. Rehr** (University of Washington) Cumulant Green's Function Approach for Excited States and Thermodynamics
P20	**Steven L. Richardson** (Howard University) Using Group IV Elements to Create New Color Centers in Diamond
P21	**Masahiro Sakurai** (The University of Texas at Austin) Implementation and Application of a Real-Space Pseudopotential Method for Calculating Magnetocrystalline Anisotropy
P22	**Sahar Sharifzadeh** (Boston University) Optoelectronic Properties of Point Defects in Gallium Nitride: A Many-Body Perturbation Theory Perspective
P23	**Sufei Shi** (Rensselaer Polytechnic Institute) Probing Excitonic Complexes in Monolayer WSe_2
P24	**David A. Strubbe** (University of California at Merced) Excited-State Forces in TDDFT and the Bethe-Salpeter Equation
P25	**Liang Z. Tan** (Lawrence Berkeley National Laboratory) Theory of Carrier Generation and Transport in Optoelectronic Materials
P26	**Meng Wu** (University of California at Berkeley) Giant Excitonic Effects in Insulating Two-Dimensional Magnets
P27	**Chao Yang** (Lawrence Berkeley National Laboratory) Using Low-Rank Approximation in the Solution of the Bethe-Salpeter Equation
P28	**Shengbai Zhang** (Rensselaer Polytechnic Institute) Vacuum Level in an Infinite Solid and the Built-in Potential
P29	**Fangzhou Zhao** (University of California at Berkeley) Topological Properties and Other Properties of Graphene Nanoribbons
P30	**Yi Chen** (University of California at Berkeley) Single-Layer Mott Insulator 1T-$TaSe_2$: Exotic Orbital Texture and Evidence for a Spin Liquid
P31	**Yu He** (Stanford University) Lock-Step Evolution of Electron-Phonon Coupling and Superconductivity in High-Tc Cuprates
P32	**Chaw Keong Yong** (University of California at Berkeley) Biexcitonic Optical Stark Effects in Monolayer Molybdenum Diselenide
P33	**Guang-Yu Guo** (National Taiwan University) On the Nature of π–electron Excitations in Graphene

Abstracts of Invited Talks

Using Topology to Engineer the Electronic Structure of Bottom-Up-Synthesized Graphene Nanoribbons

Michael F. Crommie

Department of Physics, University of California at Berkeley, Berkeley, CA
Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA

The idea of classifying materials by their topological properties is useful for predicting their behavior, especially at interfaces between insulators. When two topologically distinct insulators are fused together then metallic states arise at the interface between them. This concept, which has been so fruitful for 3D and 2D materials, was recently extended to 1D graphene nanoribbons (GNRs) in a theoretical prediction made by Steve Louie and coworkers [1]. While the 0D interface between two 1D GNRs of dissimilar topology cannot support a fully metallic phase like higher-dimensional topological insulators, it does generate the most basic constituent of a metal: a single, unpaired electron occupying a localized state within the GNR bandgap. Engineering topological interfaces in a GNR thus allows controlled placement of unpaired electrons that can interact to induce new electronic and magnetic behavior. Achieving the conditions that allow topological control of GNR behavior, however, requires atomically-precise control of the GNR structure. I will discuss how we have succeeded at experimentally confirming Steve Louie's prediction by creating and characterizing atomically-precise interfaces between topologically trivial and topologically nontrivial GNR segments, thus giving rise to topological interface states in new, controlled 1D geometries. We have used this technique in collaboration with Steve Louie and Felix Fisher to engineer the band structure of semiconducting GNRs, to create new metallic GNRs, and to synthesize new carbon-based quantum dot systems that are potentially useful for quantum information applications.

References:

[1] T. Cao, F. Zhao, and S. G. Louie. *Phys. Rev. Lett.* **119**, 076401 (2017).

Exploring Pseudospin-1 Physics Using Photonic Crystals

Che Ting Chan

Hong Kong University of Science and Technology, Hong Kong

We review some recent collaboration with Prof. Louie in the exploration of pseudospin-1 physics using dielectric photonic crystals (PCs). We show some physical implications of the PCs exhibiting an accidental degeneracy induced conical dispersion at $\mathbf{k} = 0$, such as the realization of zero refractive index medium. The photonic states of such PCs near the Dirac-like point can be described by an effective spin-orbit Hamiltonian of pseudospin 1. The transport of waves in such systems exhibits many interesting phenomena, including super Klein tunneling, robust super-collimation and unconventional Anderson localization.

Title: To Be Announced

Tony F. Heinz

Department of Applied Physics, Stanford University

Universal Dispersionless Plasmons in Quasi-Two-Dimensional Metals

Felipe H. da Jornada

Department of Physics, University of California at Berkeley
Materials Sciences Division, Lawrence Berkeley National Laboratory

Plasmons depend strongly on dimensionality: while plasmons in three-dimensional systems start with finite energy at wavevector **q** = 0, plasmons in traditional two-dimensional (2D) electron gas systems disperse strongly with *q* as $\omega_p \sim \sqrt{q}$. However, besides graphene, plasmons in *real*, atomically thin materials were not well understood. Using a combination of *ab initio* calculations and a microscopic analytical analysis, we show that the plasmon dispersion in real quasi-2D metals is qualitatively different, being virtually *dispersionless* for wavevectors of typical experimental interest. This stems from a lack of continuous translational symmetry, which leads to interband screening. So, dispersionless plasmons are a *universal* phenomenon in quasi-2D metals. Moreover, our *ab initio* calculations show that plasmons on monolayer metallic transition metal dichalcogenides (TMDs) are highly tunable, long lived and strongly localizable in real space (within ~20 nm) with no significant dispersion over practical measurement time. Their limited dispersion leads to field intensity enhancement factors exceeding 10^7 without requiring complicated nanopatterning or confined geometries, and opens the possibility of tracking plasmon wave packets in real time for novel imagining techniques in extended, atomically thin materials.

Scientific Session II – *Methods Do Matter*

Physics for the Generations: Steve Louie's Contributions in the 1970's

James R. Chelikowsky

Center for Computational Materials
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Much of our current thinking about the electronic structure of materials was formulated by Steve Louie's work as a graduate student. For example, computational methods to examine surfaces, defects, interfaces, and molecules based on supercell computations were pioneered at Berkeley during his tenure. This marked a sharp transition from traditional work that centered on the electronic structure of crystalline materials. I will give an overview of the activities of the Cohen group during this period that made this transition possible.

From the Band-Gap Problem in Semiconductors to a Canonical Tool for Materials Theory

Mark S. Hybertsen

Center for Functional Nanomaterials, Brookhaven National Laboratory

A feasible and predictive theory of electronic excitations is a canonical method in the tool-box for materials theory. I will briefly recall how many-body perturbation theory, specifically the feasible application of the GW approximation to real materials, emerged in the 1980's to enable accurate calculations of the energy bands in semiconductors, shortly after the first successful uses of density functional theory based approximations for material properties derived from the total electronic energy. Recent applications in nanoscience highlight the important role of this now fundamental tool. At the same time, on-going research seeks to refine and extend the theory towards more complex excitations and to address limitations of the perturbative approach.

Research at the Center for Functional Nanomaterials, a U.S. DOE Office of Science Facility, at Brookhaven National Laboratory is supported under Contract No. DE-SC0012704.

Quantum Electrodynamical Density Functional Theory (QEDFT): Towards New States of Matter

Angel Rubio

Max Planck Institute for the Structure and Dynamics of Matter, Luruper Chaussee 149, 22761 Hamburg, Germany
Center for Computational Quantum Physics (CCQ), The Flatiron Institute, 162 Fifth avenue, New York NY 10010, USA
Laureate of the Max-Born-Prize 2018

Computer simulations that predict the light-induced change in the physical and chemical properties of complex systems usually ignore the quantum nature of light. Recent experiments at the interface between materials science and quantum optics have uncovered situations where both the molecular system and the photon field have to be treated in detail. In this talk, we show how the effects of quantum-photons can be properly included in the newly developed quantum electrodynamics density-functional formalism (QEDFT). We provide an overview of how well-established concepts in the fields of quantum chemistry and material sciences have to be adapted when the quantum nature of light becomes important. We identify fundamental changes in Born-Oppenheimer surfaces, conical intersections, spectroscopic quantities, and quantum control efficiency. We also show how periodic driving of many-body systems allow to design Floquet states of matter with tunable electronic properties on ultrafast time scales (and cavity induced-topology). This work paves the road for the development of two new fields, namely QED-materials and QED-chemistry.

Modeling Materials Properties by Artificial Intelligence and Density-Functional Theory

Matthias Scheffler

Fritz-Haber-Institut der Max-Planck-Gesellschaft, 14195 Berlin-Dahlem, Germany and
Department of Chemistry and Biochemistry, UC Santa Barbara, Santa Barbara, CA 93106, USA

Computational screening for new or improved functional materials relies on accurate and low-cost predictions of key properties such as structure, stability, energies, energy barriers etc. In this talk, I will describe a recently developed artificial-intelligence (AI) method [1, 2] to identify descriptors and analytical equations whose predictive power extends over a wide range of materials. Specifically I will address examples from heterogeneous catalysis. Here, for example, the approach identifies a descriptor equation for adsorption energies that outperforms so far and presently used methods. Furthermore, I will discuss an AI high-throughput screening study of the catalytic transformation of CO_2 into fuels and other useful chemicals. The work corrects previous models of CO_2 activation and leads to predictions of potentially good catalyst materials.

References:

[1] R. Ouyang, S. Curtarolo, E. Ahmetcik, M. Scheffler, and L.M. Ghiringhelli, SISSO: a compressed-sensing method for identifying the best low-dimensional descriptor in an immensity of offered candidates. *Phys. Rev. Mat.* **2**, 083802 (2018).

[2] R. Ouyang, E. Ahmetcik, Ch. Carbogno, M. Scheffler, L.M. M. Ghiringhelli, Simultaneous Learning of Several Materials Properties from Incomplete Databases with Multi-Task SISSO, submitted to *J. Phys. Materials* (2019), https://arxiv.org/abs/1901.00948 .

[3] M. Andersen, Sergey V. Levchenko, Matthias Scheffler, and Karsten Reuter, Beyond standard scaling relations for the description of catalytically active materials, *to be published*.

[4] A. Mazheika, Y. Wang, L. M. Ghiringhelli, F. Illas, S. V. Levchenko, M. Scheffler. *Ab initio* data-analytics study of carbon-dioxide activation on semiconductor oxide surfaces, *to be published*.

Exascale and Beyond: Challenges and Opportunities for the Materials Science Community

Jack R. Deslippe

The National Energy Research Scientific Computing Center (NERSC)
Lawrence Berkeley National Laboratory

The end of Dennard scaling (processor frequency increases) and the near end of Moore's Law (transistor area and power density) are leading to significant changes in computer architecture as the HPC community marches towards Exascale. The Top500 list is now dominated by supercomputers employing accelerators (e.g. GPUs) and so-called many-core energy efficient processors. Many experts in the field are predicting a diversity in computer architectures exemplified by recent hardware like Google TPUs, Amazon's custom ARM processors, Intel Nervana and the possibility of Neuromorphic and Quantum Computers on the horizon. How will all this affect the computational materials science community? I'll discuss the important trends and postulate on the challenges and opportunities that our community will need to take advantage of overcome to continue to push the limits of scale and fidelity in our scientific predictions.

Characterization of Atomic Scale Lattice Reconstruction in Twisted van der Waals Interfaces of Layered Materials

Philip Kim

Department of Physics, Harvard University

Control of the interlayer twist of van der Waals (vdW) interfaces has been widely used to engineer an artificial 2-dimensional (2D) electronic systems by the formation of a moiré superlattice. Many exotic physical phenomena occur associated with the incommensurability of the moiré superstructures where the wealth of the nontrivial topology of electronic band structures plays a key role to create exotic physical phenomena. In this presentation, we will discuss the engineered atomic scale reconstruction at twisted vdW interfaces using electron microscopy, optical spectroscopy, and electrical transport. We then will discuss emerging electronic and optoelectronic physics in the vdW interface between homojunctions.

Novel States in Stacked Two-Dimensional Crystals

Young-Woo Son

Korea Institute for Advanced Study, Seoul, South Korea

Recent advances in fabricating stacked two-dimensional crystals realize interesting electronic structure in low dimensions. I will first introduce a recent success in uniting the dodecagonal quasicrystalline order and relativistic Dirac fermions in bilayer graphene system with a twist angle of 30 degrees [1]. For this system, we have developed a new theory that can describe spatially localized 12 folded resonant states and their intriguing scaling behaviors [2]. If time allowed, I will also introduce a possible modification of magnetism through interlayer interactions in a certain magnetic van der Waals crystals [3].

References:

[1] S. J, Ahn *et al.*, Science **361**, 782 (2018).
[2] P. Moon, M. Koshino and Y.-W. Son, submitted [*arXiv*:1901.04701].
[3] S. Lee and Y.-W. Son, *in preparation*.

Photophysics of Point Defects in Transition Metal Dichalcogenides

Jeffrey B. Neaton

Lawrence Berkeley National Laboratory and University of California at Berkeley

Scientific Session III – *Hetereostructures and Interfaces*

On Giant's Shoulders:
Some Progress in Understanding Excited State Properties of Heterogeneous Materials

Giulia Galli

University of Chicago and Argonne National Laboratory

Building on methods developed by Steve Louie and collaborators to describe the excited state properties of solids, we developed a framework to carry out GW and Bethe-Salpeter equation (BSE) calculations of heterogeneous systems. In this talk we present recent results on solid/liquid interfaces and on liquids.

Topics of Two-Dimensional Materials and their Heterostructures

Mei-Yin Chou

Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei, Taiwan
School of Physics, Georgia Institute of Technology, Atlanta, Georgia, U.S.A.

It has become possible in recent years to fabricate and manipulate two-dimensional nanomaterials in the laboratory that are as thin as one to few atomic layers. The reduced dimensionality gives rise to unique physical and chemical properties that differ from those of traditional bulk materials, and intriguing physical properties have been found in these few-layer systems. Computational studies have played a central role in understanding and predicting these novel properties. In this talk, I will focus on a few representative systems, including graphene systems and monolayers of transition metal dichalcogenides that exhibit properties ranging from charge density waves [1] to the quantum spin-Hall effect [2]. The hybrid system of boron nitride and graphene (*h*-BNC) at low BN doping serves as an ideal platform for band-gap engineering and valleytronic applications. The calculations find a linear dependence of the band gap on the BN concentration at low doping, arising from an induced effective on-site energy difference at the two C sublattices as they are substituted by B and N dopants alternately. In addition, our calculations show that the Moiré patterns in van der Waals heterostructures will modify the local band gap, interlayer interaction, and structural parameters [3-5]. I will also discuss one-dimensional topological insulators manifested in graphene nanoribbons, in which localized spin states may exist at the end or near the junctions. A symmetry protected Z_2 topological classification is formulated for any type of termination with a π-quantized Berry phase when summed over all occupied bands [6].

References:

[1] P. Chen *et al., Nature Communications* **8**, 516 (2017).
[2] P. Chen *et al., Nature Communications* **9**, 2003 (2018).
[3] Q. Zhang *et al., Nature Communications* **7**, 13843 (2016).
[4] C. Zhang *et al., Science Advances* **3**, e16001459 (2017).
[5] Q. Zhang *et al., ACS Nano* **12**, 9355 (2018).
[6] K. Lin and M. Y. Chou, *Nano Letters* **18**, 7254 (2018).

Dielectric Properties of Water from Deep Molecular Dynamics

Roberto Car

Princeton University

Machine learning techniques greatly expand the time and size scales accessible to ab-initio molecular dynamics simulations. Here I will show that a deep neural network potential that includes information on the maximally localized Wannier centers allows us to compute the static dielectric constant of liquid water from first principles, including thermal and quantal fluctuations.

From Two-Phonon Bound States to Dynamic Rashba Splitting

David Vanderbilt

Department of Physics and Astronomy, Rutgers University

I will briefly review some work done with Steven and Marvin at Berkeley on two-phonon bound states in diamond, which sparked my interest in phonons in a way that has never quite dissipated. Jumping over 35 years, I will then give an overview of some recent work on the dynamic Rashba splitting of the band-edge states in strongly spin-orbit coupled semiconductors such as $CsPbCl_3$, originating from thermal fluctuations of zone-center phonon modes.

Theory and Modeling of Correlated Ionic and Electronic Motions in Hybrid Organic-Inorganic Perovskites

Andrew M. Rappe

University of Pennsylvania

The perovskite crystal structure hosts a wealth of intriguing properties, and the renaissance of interest in halide (and hybrid organic-inorganic) perovskites (HOIPs) has further broadened the palette of exciting physical phenomena. Breakthroughs in HOIP synthesis, characterization, and solar cell design have led to remarkable increases in reported photovoltaic efficiency. However, the observed long carrier lifetime and PV performance have eluded comprehensive physical justification. The hybrid perovskites serve as an enigmatic crossroads of physics. Concepts from crystalline band theory, molecular physics, liquids, and phase transitions have been applied with some success, but the observations of HOIPs make it clear that none of these conceptual frameworks completely fits. In this talk, recent theoretical progress in understanding HOIPs will be reviewed and integrated with experimental findings. The large amplitude motions of HOIPs will be highlighted, including ionic diffusion, anharmonic phonons, and dynamic incipient order on various length and time scales. The intricate relationships between correlated structural fluctuations, polar order, and excited charge carrier dynamics will also be discussed.

Accurate Theory of Donors and Acceptors in Semiconductors: GW Approximation Versus Density Functional Approach

Susumu Saito

Department of Physics, Tokyo Institute of Technology, Tokyo 152-8551, Japan

Impurity-induced states in semiconductors, namely donor states and acceptor states are the most important ingredients in semiconductor devices. Predicting their ionization energies and spatial distributions are therefore one of the most important issues in semiconductor physics. At the same time, however, it is still a challenging issue in the case of extended donor and acceptor states. Although the GW approximation should work in principle, the number of atoms to be included in the supercell for this issue is too large to be dealt with in the GW approximation. Much larger supercells can be dealt with in the density functional approaches with the standard approximations including the local-density approximation (LDA) and the generalized gradient approximation (GGA). On the other hand, results in the large supercell limit in LDA and GGA do not give the correct answers to this issue. The impurity-induced state to be obtained should be too delocalized and the ionization energy is therefore too small. In this talk I will discuss how one can overcome this difficulty in the density functional approach and can obtain much better results, and will show the results of our theory applied to diamond and boron nitride.

Abstracts of Posters

Poster Session – *P1*

Excitons and Valley-Spin Physics in Quasi-2D Materials

Ting Cao
Geballe Laboratory for Advanced Materials, Stanford University

Recent advances in the experimental and theoretical studies of atomically thin two-dimensional (2D) materials have opened up opportunities in exploring new phenomena and properties as well as related applications absent in conventional bulk materials. In this poster, we will present theoretical studies on the optical responses of gapped few-layer graphene and monolayer transition metal dichalcogenides. By *ab initio* GW-BSE calculations, we demonstrate unusual optical selection rules resulting from a valley-dependent nontrivial topological band effect [1, 2]. We then discuss the theory of dark excitons and trions, and how they could be brightened by applying an external magnetic field [3] or using other approaches. We further connect our theoretical discoveries to experimental results and explore their potential applications.

This work was supported by U. S. Department of Energy and National Science Foundation. I would like to acknowledge collaborations with Louie, McEuen, Wang, and Heinz groups, as well as support from a GLAM postdoctoral fellowship at Stanford University.

References:

[1] T. Cao, M. Wu, and S. G. Louie, Unifying Optical Selection Rules for Excitons in Two Dimensions: Band Topology and Winding Numbers, *Phys. Rev. Lett.* **120**, 087402 (2018).

[2] L. Ju, L. Wang, T. Cao, T. Taniguchi, K. Watanabe, S. G. Louie, F. Rana, J. Park, J. Hone, F. Wang, and P. L. McEuen, Tunable Excitons in Bilayer Graphene, *Science* **358**, 907-910 (2017).

[3] X.-X. Zhang, T. Cao, Z. Lu, Y.-C. Lin, F. Zhang, Y. Wang, Z. Li, J. C. Hone, J. A. Robinson, D. Smirnov, S. G. Louie, and T. F. Heinz, Magnetic brightening and control of dark excitons in monolayer WSe_2. *Nature Nanotech.* **12**, 883–888 (2017).

Poster Session – *P2*

Excitonic Effects in Shift Currents of Low Dimensional Materials from Time-Dependent Approach

Yang-Hao Chan,[1,2] Diana Y. Qiu,[1] Felipe H. da Jornada,[1] and Steven G. Louie[1]
[1]*Department of Physics, University of California at Berkeley and Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA*
[2]*Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei 10617, Taiwan*

Shift current is a DC current generated by optical excitations from a nonlinear response processes in a noncentrosymmetric material. It has been considered as a possible high efficiency photovoltaic mechanism. Although shift current in various materials is widely studied, the excitonic effects on shift current has not yet been discussed. We present first-principles studies on shift currents with excitonic effects in 2D materials using an adiabatic time-dependent GW approach. Using a newly developed real-time simulation method, we are able to include excitonic effects in the nonlinear responses from first principles, treating the complicated electron-hole interaction at the GW plus Bethe-Salpeter equation level for the first time. We applied this method to study shift currents in monolayer GeS and found strongly enhanced responses due to excitonic effects. Most interestingly, the dominant contributions to the shift currents here are generated at in-gap frequencies, which peaked at energies below the quasi-particle band gap by the exciton binding energies.

Poster Session – *P3*

LQSGW+DMFT:
A Diagrammatically Motivated *Ab Initio* Theory of Strong Correlation in Real Materials

Sangkook Choi
Condensed Matter Theory CMPMS Department, Brookhaven National Laboratory

The *first principles* description of strongly-correlated materials is currently regarded as one of the greatest challenges in condensed matter physics. In contrast to the weakly correlated materials, the application of one-particle picture based on the Fermi liquid theory to strongly correlated materials fails qualitatively since electrons are neither fully localized on the atomic sites nor fully itinerant in the crystal. Among various theoretical approaches to overcome the limitation of one-particle picture, one of the candidates to most successful approaches is the dynamical mean field theory (DMFT). In combination with density functional theory, it has described many features of strongly-correlated materials successfully. These successes revived the interest in the long sought goal of achieving a diagrammatically controlled approach to the quantum many body problems of solids. In this approaches, the free energy functional can be expressed in terms of the Green's function *G* and the screened Coulomb interactions *W*. The lowest order perturbation theory in this functional gives rise to the GW approximation while the local approximation applied to the most correlated orbitals gives rise to an extended DMFT approach to the electronic structure problem. In this presentation, I'll give an introduction to our new methodology within GW+DMFT, so called LQSGW+DMFT, and its application to the strongly correlated materials containing open-*d* shells. I will also show how GW+DMFT approaches improve the spectral properties of materials in comparison to other theories.

Poster Session – *P4*

First-Principles Approach to Phonon Dynamics with
Broken Time-Reversal Symmetry and Einstein-de Haas Effect

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I will present a first-principles approach to computing the effect of time-reversal symmetry breaking on phonon dynamics in a ferromagnet such as iron. On one hand, these effects are small in magnitude in comparison with the non-time-reversal effects included in the force-constant matrix. On the other hand, these effects are leading terms when it comes to the analysis of effects such as Einstein-de Haas effect.

Poster Session – *P5*

Modifying the Band Structure of Hexagonal Boron Nitride with Metal Electrodes

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Tuning the large band gap of BN to make it functional in a given device configuration has been challenging. Theoretical attempts via an external electric field, strain, and changing the interlayer distance have produced promising results, however, at unrealistically high electric field and strain values. In this DFT-based study, we propose an alternate scheme for tuning the electronic states in BN. We investigate systems in which a few layers of BN are sandwiched between two metals with different work functions, such as Cu/BN/K, creating a large electric field through the BN slab. We find that the energy gap among the BN states can be significantly decreased in such configurations. We also report on the dependence of this effect on the different metals used and the number of BN layers, as well as the BN stacking order, as the controlled growth of an alternative (Bernal) stacking order was recently reported (S. M. Gilbert et al., arXiv:1810.04814) and thus became available for such applications.

Poster Session – *P6*

Two Routes Towards 2D Antiferromagnetic Spintronics

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Intrinsic long-range ferromagnetic order has recently been discovered in 2D atomic crystals. However, the prospect of 2D magnets remains largely hindered by the scarcity of 2D ferromagnets. In this context, creative ways to exploring 2D antiferromagnetic spintronics are significant for both fundamental physics and device applications. Here we show two routes towards 2D antiferromagnetic spintronics: (1) inducing half metallicity in 2D antiferromagnets, and (2) converting 2D antiferromagnetism to ferromagnetism. Our work paves the new paths towards the high-efficiency 2D antiferromagnetic spintronics.

Poster Session – *P7*

Polarization Dependent Optical Response and Layer-Controlled Band Gap of 2D Group IV Monochalcogenides

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Sharing with the same bulk-like flake crystal structure of black phosphorus and phosphorene, group IV monochalcogenides exhibits unique many-electron effects in its electronic and optical properties. Few-layer group IV monochalcogenides absorbs light polarized along the structures' armchair direction and is transparent to light polarized along the zigzag direction, making them potentially viable linear polarized for applications. In this work, we employ first-principles excitation calculations based on the combined GW+BSE approach to explore the electronic structure and optical response with respect to different polarizations of few-layer layered group IV monochalcogenides. In addition to the strong polarization dependence of the optical absorption spectra, the band gap, excitation binding energies, and optical absorption spectrum of group IV monochalcogenides can also be broadly tuned by changing the number of stacked layers. This scenario serves as a convenient and efficient method for engineering the layered material's excited-state properties.

Poster Session – *P8*

Metallic Zero-Mode Superlattice Graphene nanoribbons and band engineering

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The ability to fabricate metallic graphene-based materials at arbitrarily small length scales is a long-standing challenge since quantum confinement and other possible perturbations tend to generate electronic band gaps in nanostructures. Thanks to recent developments in bottom-up synthesis, we are able to realize graphene nanoribbons (GNRs) structures as designed at atomically-precise level. As predicted by our tight-binding model, we have designed metallic GNRs via introducing symmetric zero-modes superlattice. The metallicity remains unchanged under first-principles calculation and is further confirmed by scanning tunneling microscopy and spectroscopy (STM/STS). Our results also reveal that by controlling the sublattice polarization and mixing of the substituent zero-mode wavefunctions, the 1D metallic bandwidth can be varied by more than an order of magnitude.

Poster Session – *P9*

Quasiparticle Electronic Structure, Exciton, and Optical Absorption in Two-Dimensional Phosphorus Allotropes Based on BerkeleyGW Method

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Two-dimensional (2D) van de Waals layered materials have attracted wide interest in condensed matter physics, materials science, chemistry, and engineering. Among them, phosphorus displays many allotropes. Besides the narrow band gap black phosphorus, a nonplanar honeycomb structure (i.e. blue phosphorus) was proposed recently. Here, by considering many-body effects arising from strong electron-electron and electron-hole interactions in 2D, we have studied the quasiparticle electronic structure, excitonic properties, and optical absorption of this 2D structure. It is revealed that the intrinsic indirect quasiparticle band gap of monolayer is 3.41 eV, with a strong bright exciton located at 2.84 eV. The strain is found to tune the electronic and optical properties effectively. However, both the band gap and the first optical absorption are found to reduce significantly with the increasing the layers thickness. Given recent advances in the successful fabrication of atomically thin blue phosphorus crystals, we expect the potential application of monolayer blue phosphorus in photonsenser, solar, and lighting technologies.

Poster Session – *P10*

Screened Range-Separated Hybrid Functional and GW + GW-BSE Calculations of Prototypical Semiconductors: A Comparison

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We present band structure and optical absorption spectra obtained from density functional theory (DFT) and linear response time dependent DFT (TDDFT) calculations using a screened range-separated hybrid (SRSH) functional, including spin-orbit coupling, for seven prototypical semiconductors. The results are compared to those obtained from highly converged many-body perturbation theory calculations using the GW approximation and the GW plus Bethe-Salpeter equation (GW-BSE) approaches. We use a single empirical parameter for our SRSH calculations, fit such that the SRSH band gap reproduces the GW band gap at the Γ point. We then find that ground-state generalized Kohn-Sham SRSH eigenvalues accurately reproduce the band structure obtained from GW calculations, typically to within 0.1-0.2 eV, and optical absorption spectra obtained using TDDFT with the SRSH functional agree well with those of GWBSE, with peak position agreement to within 0.1 eV, at a fraction of the computational cost.

Poster Session – *P11*

Valley-Mechanical Coupling in Monolayer Semiconductors

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University of California at Berkeley

The interaction of macroscopic mechanical object with electron charge and spin plays a vital role in today's information technology and fundamental studies of the quantum-classical boundary. Recently emerged valleytronics encodes information to the valley degree-of-freedom and promises exciting applications in communication and computation. Here, we realize valley-mechanical coupling in a monolayer MoS_2 resonator and demonstrate transduction of valley information to the mechanical states. The valley and mechanical degrees-of-freedom are coupled through the magnetic moment of the valley carriers under a magnetic field gradient. We identify the valley-actuated mechanical motion by optical interferometry and attain a transduction confidence level near unity. Our experiment lays the foundation for a new class of valley-controlled mechanical devices and facilitates realization of hybrid valley-mechanical systems.

Poster Session – *P12*

Electron-Phonon Coupling from Ab Initio Linear-Response Theory within the GW Method: Method and Applications to Oxide Superconductors

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We present a first-principles linear-response theory of changes due to perturbations in the quasiparticle self-energy operator within the GW method. This approach, named GW perturbation theory (GWPT), is applied to calculate the electron-phonon (e-ph) interactions with the full inclusion of the GW non-local, energy-dependent self-energy effects, going beyond density-functional perturbation theory. Unlike the frozen-phonon approach, GWPT gives access to e-ph matrix elements at the GW level of all phonons, and the computational cost scales linearly with the number of phonon modes (wavevectors and branches) investigated. We present results of correlation-enhanced superconductivity in $Ba_{0.6}K_{0.4}BiO_3$ and of e-ph physics in other oxide superconductors where many-electron effects are strong.

This work was supported by the Center for Computational Study of Excited-State Phenomena in Energy Materials (C2SEPEM) as part of the Computational Materials Sciences Program and by the Theory of Materials Program at the Lawrence Berkeley National Laboratory, both funded by the U.S. Department of Energy, Office of Basic Energy Sciences under Contract No. DE-AC02-05CH11231, and by the National Science Foundation under Grant No. DMR-1508412. Computational resources have been provided by NERSC and XSEDE.

Poster Session – *P13*

Tuning Electronic Properties of Transition Metal Dichalcogenides via Defect Charge

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Defect engineering is a promising route for controlling the electronic properties of monolayer transition-metal dichalcogenide (TMD) materials. Here, we demonstrate that the electronic structure of MoS2 depends sensitively on the defect charge, both its sign and magnitude. In particular, we study shallow bound states induced by charged defects using large-scale tight-binding simulations with screened defect potentials and observe qualitative changes in the orbital character of the lowest lying impurity states as function of the impurity charge. To gain further insights, we analyze the competition of impurity states originating from different valleys of the TMD band structure using effective mass theory and find that impurity state binding energies are controlled by the effective mass of the corresponding valley, but with significant deviations from hydrogenic behaviour due to unconventional screening of the defect potential.

Poster Session – *P14*

Data-Driven Prediction and Analysis of Magnetic Materials

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Machine-learning-aided computational screening is attracting interest as a powerful tool for materials discovery. The basic idea is to construct a machine-learning model from calculated data and estimate material properties quickly using the model. The reliability of this scheme depends on the prediction accuracy of the model. We propose a descriptor for crystals, called orbital field matrix (OFM) [1, 2], which is based on Voronoi partition and electron configuration of constituent atoms. Application to thousands of transitionmetal compounds reveals that the kernel ridge regression using OFM reproduces both the formation energy and magnetic moments in good accuracy. We will present virtual screening of iron-based rare-earth compounds using this technique. We also discuss how machine learning can be used to extract important descriptors of magnetic properties. We present *subgroup relevance analysis* of Curie temperature of rare-earth transition-metal bimetals [3].

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Poster Session – *P15*

Coherent Electron Dynamics in Molecules Examined by the Real-Time TDDFT Calculations

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We propose possibility of observing coherent electron dynamics in an isolated molecule by shinning two short laser-pulses with anti-phases [1]. We have tested benzene, naphthalene, and anthracene molecules monitoring the potential increase by the first pulse and decrease by second anti-phase pulses, as illustrated by Fig. 1.

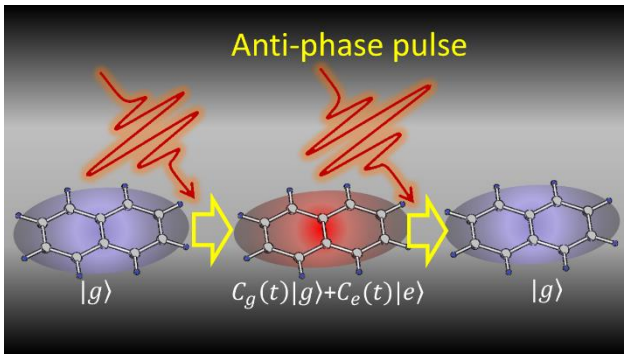

Fig. 1. Schematic of a naphthalene molecule irradiated by two anti-phase laser pulses. The electronic structure change is indicated as equations

As illustrated by Fig.1, the electronic structure changes from the ground state to dynamically beating state between ground and excited state by the first pulse. When the beat remains with coherence, the electronic state becomes to the ground state by the second pulse with anti-phase. When the interval between first and second pulses are elongated, the decrease was not seen indicating the finite lifetime of the coherence. We will also discuss molecular size dependence as well as lattice vibration effect. All calculations were performed based on the time-dependent density functional theory [2].

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Poster Session – *P16*

Revealing Many-Body Effects in X-ray Absorption Spectra

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X-ray absorption spectroscopy reveals element-specific details of local electronic structure. In the case of simple 1s excitations of light-atoms, the response of the valence electron density to core electron excitations can be accurately modeled using a static core-hole within orbital-occupancy constrained density functional theory. However, within such final state approaches, care must be taken in the evaluation of Fermi's golden rule expressions to account for both the correct time-ordering and many-electron effects present in the valence response. Using an efficient Slater determinant formalism we can accurately reproduce the oxygen K-edge spectra of a wide variety of transition metal oxides, improving upon single-particle core-hole approaches. We also can approximate the spectral signature multiple electron-hole pair excitations in metallic oxides. This approach further extends the ability of density functional theory to interpret the X-ray absorption spectra of materials.

Poster Session – *P17*

Defect-Induced Modification of Low-Lying Excitons and Valley Selectivity in Monolayer Transition Metal Dichalcogenides

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We study the effect of point-defect chalcogen vacancies on the optical properties of monolayer transition metal dichalcogenides using ab initio GW and Bethe-Salpeter equation calculations. We find that chalcogen vacancies introduce unoccupied in-gap states and occupied resonant defect states within the quasiparticle continuum of the valence band. These defect states give rise to a number of strongly-bound defect excitons and hybridize with excitons of the pristine system, reducing the valley-selective circular dichroism. Our results suggest a pathway to tune spin-valley polarization and other optical properties through defect engineering.

Poster Session – *P18*

Quasiparticle Levels at Large Interface Systems from Many-body Perturbation Theory

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Accurate prediction of quasiparticle levels at interface systems is required for determining energy barriers for electron tunneling across the interface, and lays the foundation for an accurate description of optical properties. However, predicting quasiparticle levels at the interface remains a challenging problem. Formally, Kohn-Sham density functional theory (DFT) approaches are not expected to give quantitative predictions of quasiparticle levels, which are best predicted using many-body perturbation theory within the GW approximation. Yet, GW calculations are typically intractable for large interface systems, primarily because of the large memory and computational cost associated with the computation of the fully non-local dielectric matrix. In this work, we develop a GW-based approach (which we call XAF (expand-addchi-full)-GW) to compute the ELA of large interface systems without strong covalent interactions. Our only assumption is that the polarizability matrix (chi) of the interface system can be approximated by the sum of chi for the individual components. We show that this approximation is sufficiently general to allow cases where the interface wavefunction is a linear combination of wavefunctions from individual components, as well as cases where bonding and antibonding states are formed between the individual components. Further, very large, computational savings are obtained by noting that the chi matrices for individual components of the interface can often be computed for much smaller sub-unit cells, and using an expansion (unfolding) procedure to obtain exactly the chi matrices in the actual supercell. Finally, with the chi matrix, the quasiparticle levels can be computed either for the individual components only (XA-noF-GW) or where necessary, for the full interface system (XAF-GW). Unlike previously developed embedding approaches for GW, use of full XAF-GW enables a proper treatment of weakly hybridized systems and even interfaces with charge transfer. We illustrate our method using PTCDA monolayers on Au(111) and Ag(111) systems, which have more than 3000 electrons per unit cell. The predicted ELA is in good agreement with experiment, for both the physisorbed PTCDA/Au system, and the more strongly chemisorbed PTCDA/Ag system where interface charge transfer is important. Our approach is easy to implement and enables tractable GW calculations for large interface systems, including self-assembled monolayers of molecules on substrates, Moire superlattices in 2D materials, and twisted bilayer systems.

Poster Session – *P19*

Cumulant Green's Function Approach for Excited States and Thermodynamics

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A quantitative treatment of electronic excitations and response functions in condensed matter has long been challenging. Physically, these properties depend on many-body correlation effects and require treatments beyond the independent particle approximation. Quasiparticle (QP) approaches yield significant improvements, as in GW and GW/Bethe-Salpeter equation methods, but still ignore inelastic losses due to multi-electron excitations. Recently there has been considerable interest in cumulant Green's function approaches [1-3] which address this behavior. In contrast to GW, the cumulant approach naturally explains multiple-plasmon satellites and charge-transfer excitations observed in XPS, as well as inelastic losses in XAS. We also discuss the finite temperature (FT) extension [4], with a cumulant that yields finite temperature DFT exchange-correlation potentials and energies of the electron gas in good agreement with quantum-Monte Carlo calculations. The method has also been extended to FT-TDDFT [5]. Applications such as thermodynamic properties of the homogeneous electron gas over a wide range of densities and temperatures up to the warm dense matter (WDM) regime are briefly discussed [4].

Supported by DOE BES TCMP Grant DE-FG02-97ER45623.

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Poster Session – *P20*

Using Group IV Elements to Create New Color Centers in Diamond

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The NV^- vacancy in diamond is an important example of a solid-state single photon emitter or color center whose optical and spin properties can be exploited for important applications in quantum cryptography, metrology, and quantum information processing. [1] Despite the long coherence times observed for NV^- centers, their non-zero electronic dipole moments lead to inhomogeneous broadening of their fluorescent signals. Color centers like the SiV^- center in diamond have inversion symmetry and while they are not as susceptible to local fluctuations, they unfortunately have short coherence times which impede their performance as ideal solid-state single photon emitters. [2] Recently, there have been a number of interesting efforts in the literature to use other Group IV elements of the Periodic Table beside silicon to form color centers in diamond (e.g. GeV [3], SnV [4], and PbV [5]) in an effort to find new candidates for solid-state single photon quantum emitters. A number of important questions need to be asked about these Group IV color centers. What are their ground state geometries? Which charge states are more stable? Thermodynamically, how easy it is to prepare these color centers? How susceptible are these color centers to recombination with other vacancies in the host diamond material, such as the omnipresent carbon vacancy (V_C)? In this presentation we shall use density-functional theory to address these questions and compare our predictions with experimental results where available.

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Poster Session – *P21*

Implementation and Application of a Real-Space Pseudopotential Method for Calculating Magnetocrystalline Anisotropy

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We present a real-space pseudopotential method for calculating magnetocrystalline anisotropy within relativistic density-functional theory. Our formalism is implemented in our real-space pseudopotential code, PARSEC, which is explicitly designed for an efficient implementation on a parallel computing platform [*Phys. Rev. Materials* **2**, 084411 (2018)]. We demonstrate that our formalism works well for prototypical transition-metal compounds, such as YCo_5 and Mn_2Ga, yielding an accurate magnetization and a magnetocrystalline anisotropy constant consistent with previous work. We also use our method to explore possible candidate materials for rare-earth-free permanent magnets. We find that $ZrCo_5$ compounds can provide moderate magnetocrystalline anisotropy and sufficient saturation magnetization [*Phys. Rev. Materials* **2**, 084410 (2018)]. Our work is supported by the National Science Foundation (NSF), DMREF-1729202. HPC resources were provided by the Texas Advanced Computing Center (TACC).

Poster Session – *P22*

Optoelectronic Properties of Point Defects in Gallium Nitride: A Many-Body Perturbation Theory Perspective

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An accurate and detailed knowledge of the influence of defects in semiconductors is central to the design of new high-performance materials. We employ first-principles many-body perturbation theory within the GW/BSE approximation to investigate the influence of point defects on the electronic properties of bulk wurtzite Gallium Nitride (GaN). For a+1 charged nitrogen vacancy within bulk GaN, we develop an approach to systematically identify defects and their energies from GW/BSE calculations. By analysis of the bandstructure and optical absorption spectrum, we predict that this particular defect does not significantly alter the excited-state energies of GaN. However, analysis of the low-energy exciton wavefunctions shows that the defect significantly influences the nature of the excitonic states.

The authors acknowledge funding support from the Department of Energy (Award #DE-SC0018080).

Poster Session – *P23*

Probing Excitonic Complexes in Monolayer WSe_2

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Strong Coulomb interactions in single-layer transition metal dichalcogenides (TMDCs) results in the emergence of strongly bound excitons, trions and biexcitons. In particular, tungsten based TMDCs can host a dark exction due to the spin-orbit coupling induced splitting in the conduction bands. These emerging excitonic quasi-particles possess valley degree of freedom, which can be exploited for quantum optoelectronics. By constructing high quality boron nitride encapsulated monolayer WSe_2 devices, we are able to identify the photoluminescence peaks of different excitonic complexes through gate dependent and magnetic field dependent PL spectroscopy. The determination of the characteristic energy of the excitonic complexes not only helps us to unveil the detailed configuration of excitonic complexes but also reveals important information about interactions such as exciton-phonon coupling.

Poster Session – *P24*

Excited-State Forces in TDDFT and the Bethe-Salpeter Equation

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Excited-state forces are useful to study phenomena such as light-induced structural changes, photovoltaic degradation, and Stokes shifts. I will show efficient approaches for excited-state forces for the Bethe-Salpeter equation and time-dependent density-functional theory (TDDFT) within the Tamm-Dancoff approximation. Building on the work of Ismail-Beigi and Louie [*Phys. Rev. Lett.* **90**, 076401 (2003)], we use the Hellman-Feynman theorem and a direct representation of the effective Hamiltonian in plane waves or real space, and have a more accurate GW-force approximation using the diagonal approximation. These formulations are implemented in BerkeleyGW and Octopus, and are applied to pentacene self-trapped excitons and photoisomerization of organic molecules for energy storage as “solar thermal fuels”.

Poster Session – *P25*

Theory of Carrier Generation and Transport in Optoelectronic Materials

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Here we present theory and simulation of carrier generation and transport processes in optoelectronic materials, focusing on halide and oxide perovskites, including bulk, two-dimensional, and one-dimensional varieties. We examine the impact of nanostructuring on the control of these processes, explaining the results of transport and optical experiments.

Poster Session – *P26*

Giant Excitonic Effects in Insulating Two-Dimensional Magnets

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The magneto-optical (MO) effects, such as the magneto-optical Kerr effect (MOKE) and the Faraday effect, have been intensively investigated in a variety of magnetic materials serving as a highly sensitive probe for electronic and magnetic properties. Recent experiments using MOKE have discovered a few two-dimensional magnets, and demonstrated their rich magnetic behaviors. In particular, a giant Kerr response has been measured in insulating monolayer and few-layer CrI_3. However, by far, the microscopic origin of such MO signals is still unknown, because the sizable spin-orbit coupling and excitonic effects that are essential for such an understanding are beyond the capability of existing first-principles methods. With newly developed GW and GW-BSE methods, we show, for the first time, that the exceedingly large optical and MO responses in insulating ferromagnetic monolayer CrI_3 per se arise from the strongly bound exciton states consisting of spin-polarized electron-hole states. Comparison between bulk and monolayer CrI_3 reveals the pivotal role of quantum confinement in enhancing the excitonic effects and MO responses.

This work was supported by NSF Grant No. DMR-1508412 and No. EFMA-1542741, and by the U.S. Department of Energy under Contract No. DE-AC02-05CH11231. Computational resources have been provided by the the NSF through XSEDE resources at NICS and Lawrence Berkeley National Laboratory's High Performance Computing Services.

Poster Session – *P27*

Using Low-Rank Approximation in the Solution of the Bethe-Salpeter Equation

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We present an efficient way to solve the Bethe-Salpeter equation (BSE), a method for the computation of optical absorption spectra in molecules and solids that includes electron-hole interactions. Standard approaches to construct and diagonalize the Bethe-Salpeter Hamiltonian require at least $O(N_e^5)$ operations, where N_e is the number of electrons in the system, limiting its application to small systems. Our approach uses the interpolative separable density fitting (ISDF) technique to construct low rank approximations to the bare exchange and screened direct operators associated with the BSE Hamiltonian. This approach reduces the complexity of the Hamiltonian construction to $O(N_e^3)$ with a smaller pre-constant, and allows for a faster solution of the BSE.

Poster Session – *P28*

Vacuum Level in an Infinite Solid and the Built-in Potential

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Built-in potential is an old concept but until now is an ill-defined quantity. Here, we present an unambiguous universal definition of built-in potential that allows a unified quantitative description of the properties at any type of heterojunction interfaces. Based on the theory [1], a new school of thought emerges: built-in potential is determined by the bulk properties of constituent materials, but only if the system is allowed to reach electronic equilibrium. Key to our finding is identifying the vacuum-level position in an infinite solid, which will serve as the common energy reference among dissimilar bulk materials. The magnitude of the built-in potential is explicitly given by the electrostatic potential, rather than, as generally believed, the charge density. Using metal-metal, metal-semiconductor, and semiconductor-semiconductor interfaces as examples, we show that this unified theory of built-in potential provides new perspectives into the study of interface science.

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Poster Session – *P29*

Topological Properties and Other Properties of Graphene Nanoribbons

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Graphene nanoribbons (GNRs) have recently been shown to possess distinct topological phases in general, characterized by a Z_2 invariant. Cove-edged and chevron GNRs moreover are chemically and structurally diverse, quasi-one-dimensional (1D) nanostructures whose structure and electronic properties can be rationally controlled by bottom-up synthesis from precursor molecules. We present the value of the topological invariant of the different types of cove-edged and chevron GNRs, and we present the electronic properties of various junctions formed by these GNRs, as well as such GNRs with the more common armchair or zigzag GNRs. We extend the explicit categorization of topological invariants of GNRs beyond the previously demonstrated armchair GNRs and provide new design rules for novel GNR junctions as well as future GNR-based nanoelectronic devices. We also present our study on boron-doped GNRs with flat dopant bands. We use first-principles calculations to investigate the strong interaction between the boron-doped GNR and the gold substrate. The calculation result explains the scanning tunneling microscopy measurement well.

Poster Session – *P30*

Single-Layer Mott Insulator 1T-$TaSe_2$: Exotic Orbital Texture and Evidence for a Spin Liquid

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Mott insulating behavior is induced by strong electron correlation and can lead to exotic states of matter such as unconventional superconductivity and quantum spin liquids. Recent advances in van der Waals material synthesis enable the exploration of novel Mott systems in the two-dimensional (2D) limit. Here we report characterization of the local electronic properties of the single-layer Mott insulator 1T-$TaSe_2$ via spatial- and momentum-resolved spectroscopy involving scanning tunneling microscopy (STM) and angle-resolved photoemission. Our combined experimental and theoretical study indicates that electron correlation induces a robust Mott insulator state in single-layer 1T-$TaSe_2$ that is accompanied by novel real-space orbital texture. By placing single-layer 1T-$TaSe_2$ onto a metal, we observe a strong Kondo resonance peak at the Fermi level, verifying the existence of local moments in this 2D Mott insulator. Finally, STM dI/dV imaging at the Hubbard band edges reveals a new incommensurate superstructure with a wavevector close to $2k_F$ of a half-filled spinon band, indicating a possible formation of a spinon-related density wave.

Poster Session – *P31*

Lock-Step Evolution of Electron-Phonon Coupling and Superconductivity in High-Tc Cuprates

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Lattice vibrations are known to have strong presence in many cuprate high-Tc systems. I will first demonstrate a low-energy phonon hybridization that may act as a precursory instability to the charge order in cuprates. Then I will demonstrate how a particular lattice vibrational mode can be activated via broken local symmetry and reduced doping in high-Tc cuprate $Bi_2Sr_2CaCu_2O_8$, subsequently helping double the superconducting Tc amid strong electronic correlation effects.

Poster Session – *P32*

Biexcitonic Optical Stark Effects in Monolayer Molybdenum Diselenide

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Floquet states, where a periodic optical field coherently drives electrons in solids, can enable novel quantum states of matters. A prominent approach to realize Floquet states is based on the optical Stark effect. Previous studies on the optical Stark effect often treated the excited state in solids as free quasi-particles. However, exciton-exciton interactions can be sizeably enhanced in low-dimensional systems and may lead to light-matter interactions quantitatively different from those in the non-interacting picture. Here we use monolayer molybdenum diselenide ($MoSe_2$) as a model system to demonstrate that the driving optical field can couple a hierarchy of excitonic states, and the many-body inter-valley biexciton state plays a dominant role in the optical Stark effect. Specifically, the exciton-biexciton coupling in monolayer $MoSe_2$breaks down the valley selection-rules based on the non-interacting exciton picture. The photon-dressed excitonic states exhibit energy redshift, splitting or blueshift as the driving photon frequency varies below the exciton transition. We determine a binding energy of 21 meV for the inter-valley biexciton and a transition dipole moment of 9.3 Debye for the exciton-biexciton transition. Our study reveals the crucial role of many-body effects in coherent light-matter interaction in atomically thin two-dimensional materials.

Poster Session – *P33*

On the Nature of π–electron Excitations in Graphene

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Graphene, a two-dimensional (2D) material with carbon atoms arranged in a single-layer honeycomb lattice possessing an unusual band structure with a linear spectrum, hosts 2D Dirac fermions. It provides a great opportunity to investigate novel phenomena in low-dimensional Dirac fermion systems. Furthermore, the easy manipulation of the Fermi level by an applied gate voltage makes graphene an excellent candidate for technological applications. Therefore, the elementary electronic excitations (plasmons, electron-hole pairs and excitons) in graphene have been intensively investigated theoretically and experimentally (see [1] and references therein). For example, the plasmon excitations of the 2D electrons were found to form a $\sqrt{q}$ –dependent dispersion at 0-1 eV, being characteristic of the plasmon excitations of non-relativistic 2D electron gas [2] and distinctly different from the linearly dispersed Dirac cones. Surprisingly, recent *ab initio* calculations and electron energy loss spectroscopy (EELS) studies reported a linear π–plasmon dispersion above ~4 eV, characteristic of the plasmon excitations of one-dimensional electron systems [3]. Strangely, Nelson *et al.* recently claimed that π- and π+σ peaks in EELS are not plasmons but rather single-particle interband transitions [4]. To clarify the nature of the electronic excitations of π-electrons, we have scrutinized the π–electron excitations by high *q*-resolution EELS experiments and *ab initio* calculations [1]. In contrast to previous studies, we find a $\sqrt{q}$ –dependent dispersion for q < 0.5 Å^{-1}, characteristic of 2D plasmon exciations, and a quasilinear dispersion above q = 0.5 Å^{-1}, characteristic of a non-vertical $\pi \rightarrow \pi^*$ interband transitions.

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