C5-01 Invited

Singular Electron–Phonon Interaction and Unconventional Superconductivity in Doped Topological Insulators
Xi Xiang Wang
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Understanding exotic, non-s-wave-like states of Cooper pairs is important and may lead to new superconductors with higher critical temperatures and novel properties. Their existence is known to be possible but has always been thought to be associated with non-traditional mechanisms of superconductivity where electronic correlations play an important role. Here we use a first principles linear response calculation to show that in doped Bi$_2$Se$_3$ an unconventional p-wave-like state can be favoured via a conventional phonon-mediated mechanism, as driven by an unusual, almost singular behaviour of the electron–phonon interaction at long wavelengths. This may provide a new platform for our understanding of superconductivity phenomena in doped band insulators.

C5-04 Invited

Simulations of Electronic Transport in Disordered Organic Semiconductors
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Scientific Computing Laboratory, Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia.
It remains a challenge to understand and predict the charge transport in organic electronic materials due to a lack of a simple model that links the chemical structure of the material to its measurable macroscopic electrical properties. We will review our methodology that has been developed to calculate the charge carrier mobility in disordered conjugated polymers starting from the atomic structure of the material [1]. The key ingredients of the method are the charge patching method [2] which is an efficient method for constructing the single-particle Hamiltonian, the overlapping fragments method [3] that is used to diagonalize such a Hamiltonian and a multiscale procedure which is used to link the electronic structure calculation to macroscopic conductivity [1]. Applications of the methods to the calculation of the density of states, the DC and the THz mobility in several polymers [polythiophenes, polyfluorenes, poly(aryl–ethynlylenes)] will be discussed [1, 4, 5] with special emphasis on insights that one obtains from such simulations.


C5-05 Invited

Anisotropic Electrical, Optical, and Thermal Properties of Few-Layer Black Phosphorus
Li Yang
Department of Physics, Washington University in St Louis, Saint Louis, Missouri, 63130, USA
I will present my group’s systematic studies of the electronic structures, excitons, and thermal conductance of a class of newly emerging two-dimensional semiconductors, few-layer black phosphorus (phosphorene). Using first-principles GW-Bethe-Salpeter (BSE) calculations, we incorporate the enhanced electron-electron and electron-hole interactions that substantially enlarge the quasiparticle band gap and magnify excitonic effects, which are consistent with recent experimental measurements. With these tools, we predict several unique anisotropic properties of few-layer black phosphorus. First, we show that the in-plane anisotropic electrical conductance can be rotated by 90 degrees under moderate strain conditions. Second, we...
predict that the optical absorption spectra of few-layer black phosphorus are highly anisotropic with respect to the polarization of the incident light. Third, we predict that not only the electrical conductance but also the lattice thermal conductance is anisotropic, making this material a promising candidate for thermoelectric applications. Lastly, we observe an unexpected merging of nonrelativistic and relativistic properties in few-layer black phosphorus, resulting in an unusual scaling law of the band gap in phosphorene nanoribbons.

C5-06 Invited
Electronic Structure and Electron Transport in Carbon-Based Nanosystems
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Nanoscale and molecular electronics promise to revolutionize computing, sensing, and harvesting of solar energy. However, molecular-scale control and manufacturing are difficult tasks, which require major advances to become practical in large-scale applications. The development of molecular electronics can thus be greatly enhanced by predictive simulation and by formulating design principles that will make molecular circuitry reproducible, more efficient and more reliable.

This talk describes three recent examples: (i) We discuss the electronic structure and spin polarization of nitrogen-doped carbon nanoribbons, which are candidate materials for ultrahigh speed electronics. It turns out that only certain classes of nearly perfect nanoribbons are suitable for devices. (ii) We consider molecular sensors based on carbon nanotubes and describe configurations based both on direct attachment (physisorption and chemisorption) and indirect functionalization via covalent and non-covalent linkers. (iii) We investigate electron transport in DNA and the effects of base-pair matching, solvent and counterions. All of these dramatically affect the conductivity of the system, which explains the wide range of results observed experimentally.

In collaboration with Y. Li, B. Tan, J. Jiang, M. Hodak, W. Lu and P. Boguslawski.

C5-07 Keynote
Complex Oxides for Charge-Based Electronics.
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Materials Department, University of California, Santa Barbara, C 93106-5050, USA

The formation of a two-dimensional electron gas (2DEG) at the interface between two insulators, SrTiO3 (STO) and LaAlO3 (LAO), has sparked huge interest in oxide electronics. In spite of almost a decade of research, the mechanisms that determine the density of this 2DEG are still controversial. The polar discontinuity at the STO/LAO interface can in principle sustain an electron density of 3.3x10^14 cm^-2 (0.5 electrons per unit cell). However, experimentally observed densities are more than an order of magnitude lower. We have used a combination of hybrid density functional calculations and Schrödinger-Poisson simulations to investigate the origin of the electrons in the 2DEG at the STO/LAO interface. The effects of different terminations of the LAO surface are examined. Our results apply to oxide interfaces in general, and explain why the SrTiO3/GdTiO3 interface has been found to exhibit the full density of 0.5 electrons per unit cell. I will also discuss how confinement effects in thin STO layers can trigger metal-insulator transitions.

Work performed in collaboration with L. Bjaalie, L. Gordon, B. Himmetoglu and A. Janotti, and supported by the ARO, SRC/DARPA, and NSF.

C5-08 Invited
Origins of the ferroelectricity of BiFeO3 studied from orbital selective external potential calculation
Chungang Duan

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By application of our recently developed orbital selective external potential (OSEP) method, we have studied the microscopic mechanism of the ferroelectricity of the most important multiferroic material—BiFeO3 (BFO). The OSEP method allows us to shift the energy level of specific atomic orbital, therefore is helpful to identify unambiguously the role of this orbital to the chemical and physical properties of the system we are interested in. We find that, in contrast to previous thought, stereochemically active lone pair of Bi ion has only limited contribution to the ferroelectricity of BFO. Fe-O hybridization plays very important role in the formation of large ferroelectricity of BFO, especially in the tetragonal phase of BFO.

C5-09
Impact of H-VZn defect complex on long lifetime of photocurrent in ZnO
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In MEMS and semiconductor process, plasma-etching employing fluorosulfur gas is widely used to make contact holes on a SiC surface. However, the nano-scale plasma-etching has serious problems such as a decrease in aspect ratio and generation of deformed holes. These failures are caused by side-etching and deposition of etchant species. To design an optimal etching, chemical reaction dynamics, which affects both side-etching and deposition, should be investigated. In this study, we developed an original etching simulator based on tight-binding quantum chemical molecular dynamics method [H. Ito et al., J. Phys. Chem. C, 118 (2014) 21580], and applied it to the elucidation of etching mechanisms. In etching simulations, 4H-SiC(0001)-surface is irradiated with SF6 and SF5 radicals which are the dominant species in SF6 plasma. During both etching simulations by SF6 and SF5, Si-F, C-F, Si-S, and C-S bonds and SiF4 and CF3 (x = 1-4) molecules, which are byproducts in experiments, are generated. Interestingly, there is the difference in etching efficiency, and SF5 makes a larger number of byproducts and dissociates more Si-C bonds of a SiC substrate than SF6. In conclusion, the surface reactions in SiC etching and an advantage of SF5 in etching rate are successfully revealed.

C5-10
Spin diffusion equations for strained hole-doped wells, and for cavity polaritons
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First we obtain the spin-orbit interaction and spin-charge coupled transport equations of a two-dimensional heavy hole gas under the influence of strain and anisotropy. In addition to the well-known cubic hole spin-orbit interaction, anisotropy causes a Dresselhaus-like term, and strain causes a Rashba term. We predict an enhanced spin lifetime associated with a spin helix standing wave similar to the Persistent Spin Helix which exists in the two-dimensional electron gas with equal Rashba and Dresselhaus spin-orbit interactions. These results may be useful both for spin-based experimental determination of the Luttinger parameters of the valence band Hamiltonian and for creating long-lived spin excitations.

Secondly we report on the spin dynamics of exciton polaritons, bosons with pseudo-spin 1/2 that occur within optical microcavities. Working in the diffusive limit of many scatterings, we calculate the coupled transport equations which describe diffusion, relaxation, and couplings between the polariton spin densities. We present experimentally observable polarization signals which manifest effects of both the ubiquitous TE-TM spin-orbit term and an external
magnetic field

C5-11
Origin and stability of ferromagnetism in Mg doped AlN: Bulk to Surface
Santhya Chintalapati, Ming Yang, Yongqing Cai, Shu Ping Lau, Yuan Ping Feng
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The mechanism of ferromagnetism in Mg doped AlN from bulk to different type of surfaces such as non-polar to polar and semi-polar surfaces has been investigated using first principle calculations. The Mg doping in the substitution of Al introduces a hole which results in a magnetic moment of ~ 1 µB. The magnetic moments are mainly derived from N atoms near Mg and the existence of partially filled spin down states of Mg-N cluster favors ferromagnetic coupling with the neighboring Mg-N clusters from bulk to surface of Mg doped AlN. The high to low stable ferromagnetic states have been realized from one surface to another surface. The mechanism and origin of different stable ferromagnetic states for various surface orientations of Mg doped AlN has been analyzed based on energy level splitting and charge hopping between Mg-N clusters. The existence of strong localized nature and lower bandwidth of defect state in Mg doped AlN non-polar (11-20) surface allowed the high stable ferromagnetism compared to polar and semi-polar surfaces.

C5-12 Invited
GaN as an Interfacial Passivation Layer: Tuning Fermi Level Pinning for III-V MOS Devices
Zhaofu Zhang, Changhong Wang, Ruyue Cao, Haobo Li, Hui Liu, Kyeongjae Cho, Robert Wallace, and Weichao Wang
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The use of an interfacial passivation layer is one of the important strategies to achieve a high quality interface between high-K and III-V materials integrated into high-mobility metal-oxide-semiconductor field-effect transistor (MOSFET) devices. Here, we propose GaN as the interfacial layer between III-V materials and HfO₂. Utilizing first-principles calculations, we explore the structural and electronic properties of the GaN/HfO₂ interface with respect to the interfacial oxygen contents. In the O-rich condition, an O₈ interface (eight oxygen atoms) displays the most stability. By reducing the interfacial O concentration from 100% to 25%, we find that the interface formation energy increases; the interface becomes even more stable when the interfacial oxygen vacancy exists compared with O₈. A strong band offsets dependence on the interfacial oxygen concentration is also observed. Further analysis of the electronic structure shows that no interface states are present at the O₈ interface. These findings indicate that O₈ interface serves as a promising candidate for high-quality MOS III-V devices. Moreover, interfacial states are present when such interfacial oxygen is partially removed. The interface states, leading to Fermi-level pinning, originate from the unsaturated interfacial Ga atoms.

C5-13
Theory for the time-resolved two-photon photoemission spectroscopy on GaAs and InP - Photogeneration of the Fermi surface in the electron vacuum
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1Yamagata University, 2Tsuruoka College of Technology, 3Institute of Materials Structure Science

A time-resolved two-photon photoemission spectroscopy is a valuable experiment through which we can trace dynamics of electrons near the Fermi surface. Recently, the relaxation process of a macroscopic number of photoexcited electrons in GaAs and InP[1] has been clarified. Being inspired by this experiment, we have developed theory on the relaxation process for photoexcited electrons in the insulating system to form Fermi degeneracy.

In the experiment, only 0.3 percent of electrons are excited to the conduction band. Therefore, the Coulombic scattering is rather a rare event, and furthermore, it does not work as an energy reservoir. Electrons relax by emitting phonons. We employ the following Hamiltonian as

\[ H = H_e + H_p + H_{e-p} + H_{e-e} \]

The first two terms represent the one-body electron and phonon parts, while the last two terms denote the electron-phonon couplings. Here, we consider the both the acoustic and optical phonons.

We will show that the relaxation consists of two time regions, femtosecond avalanching region, where the electron temperature is not determined, and critical slowing down region, where the electron system continue relaxing by emitting only acoustic phonons. The present result well explain the experiment and indicates that Fermi degeneracy is never realized in the exact sense.


C5-14
Tunable Magnetic Semiconductor Behavior Driven by Half-Filled One Dimensional Band in Zigzag Phosphorene Nanoribbons
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An antiferromagnetic insulating state has been found in the zigzag phosphorene nanoribbons (ZPNRs) from a comprehensive density functional theory calculations. Comparing with other one-dimensional systems, the magnetism in ZPNRs displays several surprising characteristics: (i) the magnetic moments are antiparallel arranged at each zigzag edge; (ii) the magnetism is quite stable in energy (about 29 meV/magnetic-ion) and the band gap is big (about 0.7 eV); (iii) a moderate compressive strain will induce a magnetic to nonmagnetic as well as semiconductor to metal transition. All of these phenomena arise naturally due to one unique mechanism, namely the electronic instability induced by the half-filled one dimensional bands which cross the Fermi level at around \( \frac{1}{2} I \). The unusual electronic and magnetic properties in ZPNRs endow them great potential for the applications in nano electronic devices.

C5-15
Plasma-Etching of SiC by Fluorosulfur Radicals: Tight-Binding Quantum Chemical Molecular Dynamics Simulation
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In MEMS and semiconductor process, plasma-etching employing fluorosulfur gas is widely used to make contact holes on a SiC surface. However, the nano-scale plasma-etching has serious problems such as a decrease in aspect ratio and generation of deformed holes. These failures are caused by side-etching and deposition of etchant species. To design an optimal etching, chemical reaction dynamics, which affects both side-etching and deposition, should be investigated. In this study, we developed an original etching simulator based on tight-binding quantum chemical molecular dynamics method

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[H. Ito et al., *J. Phys. Chem. C*, 118 (2014) 21580], and applied it to the elucidation of etching mechanisms. In etching simulations, 4H-SiC(000-1) surface is irradiated with SF$_3$ and SF$_5$ radicals which are the dominant species in SF$_6$ plasma. During both etching simulations by SF$_3$ and SF$_5$, Si-F, C-F, Si-S, and C-S bonds and SiF$_x$ and CF$_x$ (x = 1-4) molecules, which are byproducts in experiments, are generated. Interestingly, there is the difference in etching efficiency, and SF$_5$ makes a larger number of byproducts and dissociates more Si-C bonds of a SiC substrate than SF$_3$. In conclusion, the surface reactions in SiC etching and an advantage of SF$_5$ in etching rate are successfully revealed.