Mini-symposium C5
Computational Semiconductor Materials Science

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C5-01 Keynote

Theory of Emerging Electronic Materials and Their Defect Properties

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Recent history of electronic materials research has witnessed a rapid development of new materials ranging from monolayer semiconductors, their three-dimensional assemblies, to organic-inorganic hybrid perovskite solar materials. I will present three examples from our own research: (a) MB_4 layers where the boron honeycombs are stabilized by a single metal M layer [S.-Y. Xie, et al., Phys. Rev. B **90**, 035447 (2014)]. MoB_4 possesses double Dirac cones offset by about 100 meV, one donating whereas the other accepting electrons. It could be a natural place to form exciton condensate. In contrast, MnB_4 can sustain superconductivity while simultaneously being ferromagnetic. (b) Carbon Kagome lattice (CKL) which borderlines the physics of graphene and orbital frustration [Y. Chen, et al., Phys. Rev. Lett. **113**, 085501 (2014) (Editor's Suggestion)]. We predict that here a metal-insulator transition occurs, leading to the formation of direct gap elemental semiconductor with strong visible absorption in the blue. And (3) $MAPbI_3$ whose defect physics resides heavily on the strong covalency of I and Pb, despite the ionic nature of iodine. [M. L. Agiorgousis, Y.-Y. Sun, H. Zeng, and S. Zhang, JACS (in press)]. By forming the I trimers and Pb dimers, deep recombination centers develop in such a material.

C5-02 Invited

Theoretical studies on the NV(-) defect in diamond

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The NV(-)center of diamond is being under intense investigation lately due to its potential for application in quantum information technology, nano-sensing and bio-labeling. Controlled formation in high concentration and stable luminescence are key issues. Based on calculations with a hybrid exchange functional in a bulk supercell, we discuss here the basic formation mechanisms and conclude that NV centers are primarily produced directly by the irradiation of N-doped diamond, and concentration enhancement in the subsequent annealing is limited by divacancy (V_2) formation. To ensure a high concentration of negative NV centers, V_2 has to be annealed out, i.e., the annealing temperature must be higher than the ones used so far. Since most applications require the NV(-) center to be near the diamond surface, the effect of the latter can be critical. Based on calculations similar to the ones above, but on (001) slabs of diamond, we show that the completely hydrogenated or hydroxylated surface leads to bleaching, while a much too strong oxygenation to blinking of the luminescence. Ideally, the surface should be terminated by a mixture of H, OH and bridging O, which can be achieved by mild oxidation of a hydrogenated surface or by oxidation with an acid.

C5-03 Invited

Singular Electron--Phonon Interaction and Unconventional Superconductivity in Doped Topological Insulators

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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_2Se_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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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–ethynylenes)] will be discussed [1, 4, 5] with special emphasis on insights that one obtains from such simulations.

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[3] N. Vukmirovic and L. W. Wang, J. Chem. Phys. 134, 094119 (2011).
[4] N. Vukmirovic, C. S. Ponseca, Jr., H. Nemec, A. Yartsev and V. Sundstrom, J. Phys. Chem. C 116, 19665 (2012).
[5] N. Vukmirovic, Phys. Chem. Chem. Phys. 15, 3542 (2013).

C5-05 Invited

Anisotropic Electrical, Optical, and Thermal Properties of Few-Layer Black Phosphorus

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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