Mini-symposium C3
Enhanced Spin-Orbit Coupling and Emergent Topological Phenomena in Graphene and Related Materials

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C3-01 Keynote
Topological Weyl semimetal and Axion Insulators
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We focus on describing the topological Weyl semimetal, this state is a three-dimensional analog of graphene with linearly dispersing excitations and provides a condensed-matter realization of Weyl fermions that obeys a two-component Dirac equation. It also exhibits remarkable topological properties manifested by surface states in the form of Fermi arcs, which are impossible to realize in purely two-dimensional band structures.

C3-02 Invited
Two-dimensional Valley Electrons and Excitons in 3R MoS2 Multilayers
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We find unique two-dimensional (2D) confinement for valley electrons and excitons in 3R stacked molybdenum disulfide (3R MoS2). Although the band structures of 3R and 2H MoS2 are very similar to each other, we first show that the charge of the valence states at K (and K') point in the hexagonal Brillouin zone are qualitatively different. By a group theoretical argument, we then show that the valley states have no interlayer hopping (hybridization) due to the symmetry of their Bloch functions. In fact, recent optical measurement has revealed that the reflectivity spectra for 3R and 2H MoS2 have appreciable differences. We find that these spectra can be well described in terms of the anisotropic hydrogen atomic model: The valley excitons in 3R (2H) MoS2 have 2D (3D) hydrogen-like spectral series. We also evaluate the spread of the exciton wave functions, and show that those for the former (latter) are smaller (larger) than the interlayer distance. Our results indicate that dimensional properties of the valley electrons and excitons can be controlled only by the stacking geometry, which can be exploited in future valleytronics.

C3-03 Invited
Spin-orbit coupling in graphene with adatoms
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Intrinsic spin-orbit coupling in graphene is relatively weak, some tens of micro eVs [1-3]. On one hand, this is good, as the projected intrinsic spin relaxation is also slow, on the order of microseconds. On the other hand, a greater value for the spin-orbit interaction is desired for spin manipulation and spin-orbit induced phenomena, such as the spin Hall effect. In this talk I will review the basics of the spin-orbit physics in graphene and show how to effectively increase the value of the spin-orbit interaction (to meVs) by adding adatoms. Specifically, our first-principles calculations show that hydrogen induces local spin-orbit coupling of about 1 meV [4], while fluorine up to 30 meV. I will also present our recent results on graphene on a copper substrate, as well as locally induced spin-orbit coupling due to copper adatoms and clusters. For each adatom I will present a minimal realistic hopping model explaining the first-principles results. Such models are useful for investigating model spin relaxation [5], spin and charge transport in functionalized graphene. I acknowledge collaboration with J. Fabian, M. Gmitra, S. Irmer, T. Frank, and S. Putz., as well as support from the DFG SFB 689, GRK 1570, and European Union Seventh Framework Programme under Grant Agreement No. 604391 Graphene Flagship.


C3-04
Quantum Anomalous Hall Effect in the Heterostructure of Graphene on an Antiferromagnetic Insulator
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Quantum anomalous Hall (QAH) effect, with potential applications in low-power-consumption electronics, is predicted in the heterostructure of graphene on the (001) surface of a real antiferromagnetic insulator RbMnCl3, from density-functional theory and Wannier function methods. Due to the interactions from the substrate, a much large exchange field (about 280 meV) and an enhanced Rashba spin-orbit coupling are induced in graphene, leading to a topologically nontrivial QAH gap opened in the system. How to tune the gap size is also discussed. Our work demonstrates that this graphene-based heterostructure is an appropriate system to experimentally observe the QAH effect and explore the promising applications.

C3-05
Dirac and Weyl Semimetal in XY Bi (X=Ba, Eu; Y=Cu, Ag and Au)
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Weyl and Dirac semimetals recently stimulate intense research activities due to their novel properties. Combining first-principles calculations and effective model analysis, we predict that nonmag-etic compounds BaY Bi (Y =Au, Ag and Cu) are Dirac semimetals. As for the magnetic compound EuY Bi, although the time reversal symmetry is broken, their long-range magnetic ordering cannot split the Dirac point into pairs of Weyl points. However, we propose that partially substitute Eu ions by Ba ions will realize the Weyl semimetal.

C3-06 Invited
Pseudospin order in 2D Dirac materials: the role of short vs long-range interactions
Jeil Jung
The advent of a new class of 2D Dirac materials, among which graphene is a paradigmatic example, has opened up a new frontier in materials research. Their reduced dimensionality makes these systems especially susceptible to electron-electron interactions and their simple stoichiometry makes them ideal platforms to explore in detail the complex role of many-body effects in configuring ordered phases. In this presentation I will use the example of single and few layers graphene to illustrate the role of short vs long-range electron-electron interactions in defining the ground-state properties in Dirac materials, where (layer/valley/spin) pseudospin order and band gap enhancements, and therefore of the spin-orbit coupling, can take place. Whereas short-range interactions that favor antiferromagnetic spin order can explain a number of experimental observations in zero and finite field Hall measurements, the non-locality of long-ranged interactions can lead to a competition between ground-states exhibiting spontaneous orbital moments that should be tunable through external system parameters and distinguished through transport and spectroscopy measurements.


C3-07 Invited
Anomalous Hall Effect and Orbital Magnetization Arising from Noncollinear Antiferromagnets
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Ferromagnetic conductors exhibit anomalous contributions to their transverse (Hall) conductivities that cannot be attributed to Lorentz force on electrons from a magnetic field. The anomalous Hall conductivity is often assumed to be proportional to the magnetization, allowing transport measurements to be used in spintronics as a convenient proxy for magnetometry. However, simple symmetry arguments demonstrate that the anomalous Hall effect requires only time-reversal symmetry breaking and spin-orbit coupling, not net magnetization, and we illustrate our ideas by examining a toy model of noncollinear antiferromagnet on a two-dimensional kagome lattice. This is further backed up with a realistic example based on first-principles calculations, predicting that single-crystals of Mn3Ir, a high-temperature antiferromagnet commonly used in spin-valve devices, have large anomalous Hall conductivities.

C3-08 Invited
Topological insulator gap in graphene with heavy adatoms
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The recent discovery of topological insulators (TIs) —hat act as insulators in the bulk yet possess quantized conducting edge or surface states—has triggered extensive interests in the field of condensed matter physics and materials science. Although graphene is the first predicted TI, the TI state in pure graphene is impossible to be realized in experiment, because the carbon’s spin-orbit coupling (SOC) is too weak. By depositing heavy adatoms on graphene, we proposed a few candidates for the realization of TI states in graphene. Firstly, p-valent adatoms such as In and Tl can transfer their strong SOC to graphene, so that huge TI gaps as large as 21 meV at Dirac point can be induced. Secondly, we found that the 5d orbitals hybridize with the graphene π bands, which generates a few impurity bands around the Fermi energy. Particularly, the Os/graphene system has giant TI gaps larger than 200 meV over a broad range of adatom coverage, and the Fermi level locates at the middle of the gap. Thirdly, Co adatoms on graphene can generate a new topological state—Chern half metal—which is a trivial metal in majority spin channel but a Chern insulator in minority spin channel.

C3-09
Electronic and topological properties in graphene-based heterostructures
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Using first-principles calculations, we study electronic and topological properties in heterostructures consisting of graphene and several other 2D materials (BiTe/graphene, Bi2Se3/graphene, graphene/graphene (i.e. bilayer graphene) and BN/graphene). We find topological phase transition either by decreasing the interlayer distance or by changing the stacking configuration of the heterostructures. Besides, the Fermi level and the metal-insulator-transition can be tuned by the interlayer distance. Our results provide a new way to control electronic properties of 2D materials and to realize multiple topological phases.

C3-10 Invited
Dirac and Weyl Superconductors in Three Dimensions
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Inspired by the recent discovery of Dirac and Weyl semimetals, we explore their analogues in superconducting systems. In this work, we introduce the concept of 3D Dirac (Weyl) superconductors (SC), which have protected bulk four(two)-fold nodal points and surface Andreev arcs at zero energy. We provide a sufficient criterion for realizing them in centrosymmetric SCs with odd-parity pairing and mirror symmetry. In the Bogliubov-de Gennes (BdG) description of SCs, the particle-hole redundancy leads to a natural half-filling and an intrinsic particle-hole symmetry (PHS). Compared to the cases of semimetals, the former feature simplifies our task to focus on the nodal points at zero energy, whereas the latter feature poses an additional symmetry constraint which plays intriguing roles in stabilizing the nodes. Specifically, we find that a 3D Dirac SC can be realized in a nodal phase of a centrosymmetric SC with odd-parity pairing and mirror symmetry. Pairs of Dirac nodes would appear in a mirror-invariant plane when the mirror winding number is nontrivial. Each Dirac node is protected locally by the combination of mirror symmetry, TRS, and an inversion-gauge symmetry. Breaking mirror symmetry may gap Dirac nodes producing a topological SC. Each Dirac node evolves to a nodal ring when inversion-gauge symmetry is broken, whereas it splits into a pair of Weyl nodes only when time-reversal symmetry is broken. Our physics might be realized in the nodal phase of Cu-doped Bi2Se3.

C3-11 Invited
Nontrivial topological states with large gap in Bi (111) passivated with hydrogen or halogen
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Large bulk band gap is critical for the application of the quantum spin Hall (QSH) insulators in spintronic devices operating at room temperature (RT). Based on the first-principles calculations, here we predict a group of 2D topological insulators BiX/ShX (X = H, F, Cl, and Br) with extraordinarily large bulk gaps from 0.32 to a record value of 1.08 eV. Using tight-binding methods in combination with first-principles calculations, we systematically derive a low-energy
effective Hamiltonian for these huge QSH insulators. We find that the low-energy Hilbert subspace mainly consists of $p_x$ and $p_y$ orbitals from the group-V elements Bi and Sb, and the giant first-order effective intrinsic spin-orbit coupling is from the on-site atomic spin-orbit interaction. These systems represent the first real 2D honeycomb lattice materials in which the low-energy physics is associated with $p_x$ and $p_y$ orbitals. Via introduction of an exchange field, quantum anomalous Hall effect emerges in these otherwise huge-gap QSH insulators. These features make the Bi (111) passivated with hydrogen or halogen an ideal platform to realize many exotic phenomena and fabricate new quantum devices operating at RT.

C3-12
Optimal curvilinear transport of a spin-polarized electron with Rashba and Dresselhaus spin-orbit coupling in a uniform magnetic field
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The spin-polarized transport of an electron along a curved-one dimensional wire with Rashba and Dresselhaus spin-orbit couplings (SOCs) and a uniform perpendicular magnetic field is considered in this study. Here we analytically derived the appropriate eigenenergies and eigenvalues of the system and numerically determine the output transmission coefficients. Spin polarization, probability current density and conductance are then obtained using transfer matrix approach to examine the dependence of spin transport on the radius, R, of curved wire, on the external magnetic field, B, and on the SOCs strengths.

From our results, we find the condition, $B \approx R^{1/3}$, at which there would be no spin switching regardless of the SOC strengths. A value of R beyond this condition will no longer have a spin reversal. Moreover, for a material with sufficiently strong SOCs, regardless of its type, the effective SOC strength follows the standard form equation of a circle in which the Rashba SOC and the Dresselhaus SOC are the component coordinates. From here, we optimize the probability current density by properly tuning the Rashba coupling strength for a given value of B, R and Dresselhaus SOC.

C3-13
Quantum Spin Hall and Z2-Metallic States in a Real Organic Material
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Motivated by recently searching for topological states in organic materials as well as successfully experimental synthesis of a graphite-like metal-organic framework Ni3(C18H12N6)2 (Sheberla et al. J. Am. Chem. Soc. 136, 8859 (2014)), we systematically investigated the electronic and topological properties of the Ni3(C18H12N6)2 monolayer using an ab-initio method combined with a tight-binding model. Our calculations demonstrate that the material can be in a quantum spin Hall or Z2-metallic state in different electron-doped concentrations, which are experimentally accessible with currently electrostatic gating technologies. The tight-binding model also shows that the real next-nearest-neighbor interaction is essential to drive the Z2-metallic phase in Ni3(C18H12N6)2-type lattices.