Graphene and Related Materials Focus Topic
Room: 208 - Session GR+TF+ET-MoA

Graphene: Electronic Properties and Charge Transport
Moderator: L. Colombo, Texas Instruments Incorporated

2:00pm **GR+TF+ET-MoA1 Electronic and Magnetic Properties of a Graphene Line Defect**, ***D. Gunlycke***, Naval Research Laboratory **INVITED**

Although graphene exhibits excellent electron and thermal transport properties, it does not have an intrinsic band gap, required to use graphene as a replacement material for silicon and other semiconductors in conventional electronics. The band structure of graphene, however, offers opportunities to develop non-traditional applications. One such avenue is to exploit the valley degeneracy in graphene. In this presentation, I will present a two-dimensional valley filter based on scattering of electrons and holes off a recently observed extended line defect. The transmission probability depends strongly on the valley and the angle of incidence of the incident quasiparticles. Quasiparticles arriving at the line defect at a high angle of incidence lead to a valley polarization of the transmitted beam that is near 100%.

I will also discuss results showing that the extended line defect gives rise to ferromagnetically coupled local moments. This ferromagnetism can be understood from a symmetry analysis of the boundary-localized eigenstates. The symmetry requires that the principal moments couple ferromagentically both along and across the line defect, leading to approximately 2/3 more spin-up electrons and than spin-down electrons per repeat unit along the line defect.

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2:40pm **GR+TF+ET-MoA3 Hydrogenation Induced Graphene-Metal Contact - Observation of States at Fermi Level**, ***S. Rajasekaran***, Stanford University, *S. Kaya, T. Anniyev,* Stanford Synchrotron Light Source, *F. Yang, D. Stacchiola,* Brookhaven National Laboratory, *H. Ogasawara, A. Nilsson*, Stanford Synchrotron Light Source

Graphene has received tremendous interest due to its unique electronic structure. Manipulating its electronic structure has received considerable interest. Hydrogenating graphene to open a band gap has been proposed and certain groups have demonstrated hydrogenation induced band opening for graphene on metal substrates.

We employed carbon specific soft x-ray spectroscopy (X-ray photoelectron (XPS), X-ray absorption (XAS) and X-ray emission spectroscopy (XES)) and scanning tunneling microscopy (STM) to investigate how hydrogenation changes the geometric and electronic structure of graphene on Pt(111). Graphene growth on Pt(111) is accompanied with Moiré structure due to periodic rippling in the graphene overlayer due to lattice mismatch and weak interaction between graphene and Pt. Hydrogenation leads to complete disappearance of long range order, although STM indicates that ripple periodicity survives even after hydrogenation. We show that hydrogenation of the unit cell of Moiré nano-patterns is accompanied by pinning of the graphene layer to underneath metal substrate. Structural changes involved in the process of hydrogenation induce covalent graphene-metal interaction. Angle resolved XES and XAS make it possible to probe symmetry resolved states in σ and π bond geometry. XES-XAS indicates that the density of states (DOS) of graphene is very similar to that of graphite. Hydrogenation induces significant changes in the electronic DOS, most of which reflect the formation of C-H σ bonds. For disordered hydrogenated graphene, contrary to band opening, we observe states at the Fermi level after hydrogenation which we reason to arise due to graphene metal interaction and localized C-H bonds. This effect is proposed to be a way to tailor its electronic properties as a possible method to form better graphene-metal contact.

3:00pm **GR+TF+ET-MoA4 First-Principles Studies of Atomic and Electronic Structure of Graphene on Sn/Ni(111) Surface Alloy**, ***L. Adamska***, *R.Q. Addou, A. Dahal, M. Batzill, I.I. Oleynik*, University of South Florida

Graphene-substrate interactions can be exploited to modify the electronic structure of free-standing graphene. Although most of the efforts were directed towards investigation of graphene on pure metallic substrates, less is known about properties of graphene grown on surface alloys. Sn/Ni(111) surface alloy is of particular interest because this structure has the surface lattice constant of Ni(111), i.e. almost a perfect match with graphene's lattice constant, and its surface is highly corrugated due to the substantially large atomic radius of Sn compared to Ni. Here we present results of first-priniciples density functional theory investigations of structural and electronic properties of graphene on sqrt(3)xsqrt(3)R(30) Sn/Ni alloy substrate. It was found that the presence of Sn atoms (1/3 monolayer) results in substantial weakening of graphene-substrate interactions, as is evidenced by large graphene-substrate separation. Nevertheless, the electronic structure of graphene is substantially affected by the underlying substrate as is as seen on simulated STM images. The theoretical predictions for the atomic and electronic structures of graphene on Sn/Ni(111) substrate are compared with experimental results.

3:40pm **GR+TF+ET-MoA6 Charge Transport through Graphene: the Role of Metal Contacts**, *M.Y. Chou, M.E. Kindermann,* ***S. Barraza-Lopez***, Georgia Institute of Technology

Graphene is a flat form of carbon only one-atom tick. Formed by two interweaving triangular sublattices, it has two atoms on its unit cell. Under normal conditions the charge carriers in graphene can be described with an effective single-particle picture. They display an isotropic and linear (i.e., conical) electronic dispersion around the charge neutrality level. This dispersion is described by a Dirac-like equation with a pseudo-spin (related to the sublattice degree of freedom) instead of the standard electron spin. The pseudo-spin is responsible in great part for the strongly suppressed back-scattering in graphene that results in coherent quantum charge transport on lengths up to the micrometer scale, making graphene a relevant material for electronic applications. Yet for applications and for electrical measurements metal contacts are patterned onto graphene. Then the two following questions naturally arise: (i) How graphene interacts with these metal contacts? (ii) How this interaction affects the conductance of a metal/graphene/metal junction in comparison with the hypothetical conductance of pristine (and contactless, infinite) graphene?

In this talk I will discuss quantitatively –within a single-particle description– the quantum transport of charges through graphene, with a focus on the signatures that metal/graphene interfaces imprint on the conductance features. The metals considered are normal (i.e., not superconducting), and spin unpolarized. A crucial observation is that not all metal form covalent bonds to graphene. The conductance is obtained as a function of the separation between contacts, the width of the junctions, as well as the thickness of the metal layers when necessary. From these calculations we are able to extract the basic physics involved in transport for all normal metals [1]. Our studies aim towards a comprehensive modeling of graphene devices at the quantitative level.

[1] S. Barraza-Lopez, M. Vanevic, M. Kindermann, and M.-Y. Chou. "Effects of metallic contacts on electron transport through graphene." *Phys. Rev. Lett.* **104**, 076807 (2010); S. Barraza-Lopez, M. Kindermann and M.-Y. Chou. "Charge transmission through short two-terminal graphene junctions with normal bonding metal contacts." (In preparation.)

4:00pm **GR+TF+ET-MoA7 Layer Number Determination and Thickness-dependent Properties of Graphene Grown on SiC**, ***W. Zhu***, *C. Dimitrakopoulos, M. Freitag, Ph. Avouris*, IBM T.J. Watson Research Center

The electronic properties of few-layer graphene grown on the carbon-face of silicon carbide (SiC) are found to be strongly dependent on the number of layers. The carrier mobility is larger in thicker graphene because substrate-related scattering is reduced in the higher layers. The carrier density dependence of the mobility is qualitatively different in thin and thick graphene, with the transition occurring at about 2 layers. The mobility increases with carrier density in thick graphene, similar to multi-layer graphene exfoliated from natural graphite, suggesting that the individual layers are still electrically coupled. The Hall coefficient peak value is reduced in thick graphene due to the increased density of states. A reliable and rapid characterization tool for the layer number is therefore highly desirable. To date, AFM height determination and Raman scattering are typically used since the optical contrast of graphene on SiC is weak. However, both methods suffer from low throughput. We show that the scanning electron microscopy (SEM) contrast can give similar results with much higher throughput.

4:20pm **GR+TF+ET-MoA8 Graphene: Scratching the Surface**, ***M. Fuhrer***, University of Maryland at College Park **INVITED**

Graphene is of interest for its unique electronic structure: electrons in graphene obey the Dirac equation for massless particles, complete with a two-component spinor degree of freedom that mimics the spin of a relativistic particle. But graphene is also composed entirely of surface atoms, making the techniques of surface science useful in studying its properties. I will discuss experiments which combine ultra-high vacuum (UHV) surface science with electronic transport measurements to understand graphene and the adsorbed species on its surface. Surface science techniques can be used to controllably modify graphene's properties: potassium atoms can be deposited to form charged impurity scatterers; ice can be deposited to modify the dielectric environment of graphene and tune the electron-electron interaction strength; and ion irradiation can be used to create atomic vacancies which act as Kondo impurities. Graphene's transport properties are extraordinarily sensitive to surface adsorbates, and can be used to detect e.g. correlations in the positions of potassium atoms at concentrations below 1/1000th of a monolayer, and phase transitions in few-monolayer water.

5:00pm **GR+TF+ET-MoA10 Metallic and Insulating Adsorbates on Graphene**, ***K.M. McCreary***, *R.K. Kawakami*, University of California, Riverside

While several experiments have separately investigated the doping of graphene by metallic and insulating adsorbates, the transition from metallic to insulating behavior of the adsorbates has not yet been explored. We directly compare the effect of metallic titanium (Ti) and insulating titanium dioxide (TiO_2) on the transport properties of single layer graphene. The deposition of Ti results in substantial *n*- type doping and a reduction of graphene mobility by charged impurity scattering. Subsequent exposure to oxygen largely reduces the doping and scattering by converting Ti into TiO_2. In addition, we observe evidence for short-range scattering by TiO_2 impurities.

5:20pm **GR+TF+ET-MoA11 Electron Transport in Carbon Nanotube - Graphene Contacts**, *B. Cook*, *W. French*, ***K. Varga***, Vanderbilt University

Graphene and carbon nanotubes are two of the most promising materials for future applications due to their unique properties. Devices combining the two materials are expected to be particularly advantageous. The interface of carbon nanotubes and various metal electrodes has been previously studied, both experimentally (Chen et al. Nano Lett. 2005, Zhang et al. Nano Lett. 2007) and theoretically (Shan et al. PRB 2004, Zhu et al. APL 2006, He et al. APL 2009). These studies focus on the search for materials with a low p-type Schottky barrier. Hybrid graphene-carbon nanotube structures have been previously demonstrated (Tung et al. Nano Lett. 2009). We propose the use of graphene as a electrode material for carbon nanotube based FET devices. To this end the carbon nanotube - graphene contact is investigated with first-principles calculations within density functional theory of the Schottky barrier height (SBH) and transport properties. Total energy and electronic structure calculations are carried out with a plane-wave basis set and the transport characteristics are calculated with a localized atomic orbitals basis within the non-equilibrium Green's function framework. We consider only the side-contact geometry, nanotubes laying atop graphene. The SBH for (5,0), (8,0) and (10,0) nanotubes on graphene is calculated. The transport characteristics of a combined graphene - nanotube device are considered. In the case of small diameter nanotubes (~0.6nm) a SBH of ~0.09 eV is found when graphene contacts are used, much lower than the typical reported values (0.3 eV and higher).

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