Wednesday Morning, January 22, 2020

PCSI

Room Canyon/Sugarloaf - Session PCSI-1WeM

Optical Properties of 2D Materials

Moderator: Wanyi Nie, Los Alamos National Laboratory

8:30am **PCSI-1WeM-1 Metals at the Atomic Limit***, **Joshua Robinson**,* Penn State University **INVITED**

The last decade has seen an exponential growth in the science and technology of two-dimensional materials. Beyond graphene, there is a huge variety of layered materials that range in properties from insulating to superconducting that can be grown over large scales for a variety of electronic devices and quantum technologies, such as topological quantum computing, quantum sensing, and neuromorphic computing. In this talk I will discuss our pioneering work in confinement heteroepitaxy (CHet) that enables the creation of 2D forms of 3D materials (e.g. 2D-Ga, In, Sn) and *decouples* the growth of the metals from other 2D layers, thereby enabling a new platform for creating artificial quantum lattices (AQLs) with atomically sharp interfaces and designed properties. As a specfic example, we synthesize plasmonic layers that exhibit >2000x improvement in nonlinear optical properties, and 2D-superconductors combined with topological insulators as the building block of next generation "2D" topological superconductors. Confinement heteroepitaxy opens up avenues for enabling a virtual "legoland" of hybrid quantum materials.

9:10am **PCSI-1WeM-9 Tuning the Spontaneous Emission of Monolayer Wse$_2$ by Optical Environment Control – Cavity Coupling and Substrate Manipulation***, J Lee, **Hyunseung Lee**,* Ajou University, Republic of Korea

Atomically thin layer of transition metal dichalcogenides (TMDs) such as monolayer WSe2 exhibit direct bandgaps ranging from visible to near-infrared with strong exitonic effect. Thanks to its optical characteristics, these materials can be used for integrated functional devices such as light emitting devices, photodetectors and optical modulators. In these applications, device performances can be improved by engineering the material thicknesses and doping levels, applying external fields, or modulating optical environment. In particular, tailoring the optical environment has been demonstrated by coupling monolayer TMDs to various types of optical microcavities such as Bragg reflectors or photonic crystals.

In this work, we utilize microspheres on planar substrates to manipulate the emission properties of monolayer WSe2. First, we show the enhancement of the photoluminescence (PL) emission which is controlled by the size of the coupled microsphere which ranges from 2 to 7 µm. Time-resolved PL measurement supports the cavity-induced emission rate enhancement of monolayer WSe2 coupled to a microsphere. The PL enhancement is further increased by increasing the thickness of the oxide layer between the microsphere and silicon substrate, which is supported by finite-time domain method (FDTD) simulations. Both microsphere coupling and substrate manipulation provide convenient pathways to modulate 2D material-based photonic devices.

9:15am **PCSI-1WeM-10 First Principles Study on Optical Properties of Monolayer Bismuthene under an Electric Field***, **Wei-Chieh Liu**, L Xu, M Lin,* Hanyang University, South Korea*; T Leung, H Hsu,* National Taipei University of Technology, Republic of China

Monolayer bismuthene has extraordinary optoelectronics, catalytic and biocompatible properties, and potential as a 2D topological insulator. When monolayer bismuthene is deposited in a sufficiently thin layer on an object, it possesses a stable low-buckled hexagonal structure and it has the property of semiconducting, which could be a promising low-dimensional thermoelectric material. Monolayers bismuthene is p-type semiconductors, but the hole concentration arising from the intrinsic defects is very low and hard to control. In this work, the band structure, density of states and optical constant of monolayer bismuthene have been calculated using first-principle calculations based on density functional theory (DFT). The results are compared to those calculated from the tight-binding model. With an applied external electric field, it is found that the electric and optical properties will be dramatically changed. Monolayer bismuthene can be calculated may generate some applications in optoelectronics, either combined with other 2D materials or topological materials.

9:20am **PCSI-1WeM-11 Formation of Coherent Phase Domain Heterojunctions in Single Layer MoS$_2$ on Au(111)***, **Fanglue Wu**, Z Liu,* Texas A&M University*; M Chandross,* Sandia National Laboratories*; Q Moore,* Texas A&M University*; N Argibay, J Curry,* Sandia National Laboratories*; J Batteas,* Texas A&M University

Two-dimensional (2D) transition metal dichalcogenides (TMDs) have attracted tremendous attention over the past decade due to their exciting mechanical, electronic and frictional properties [1-5]. Heterojunctions of semiconductors and metals are the fundamental building blocks of modern electronics. Coherent heterostructures between dissimilar materials can be achieved by composition, doping or heteroepitaxy of chemically different elements. Here we report, the formation of coherent single-layer MoS heterostructures (Figure 1), which are chemically homogenous with matched lattices, but show electronically distinct semiconducting (1H phase) and metallic (1T phase) character, when deposited by mechanical exfoliation on Au(111). The facile exfoliation technique here eliminates tape residues usually found in many exfoliation methods, and yields single-layer MoS with millimeter (mm) size. Raman spectroscopy, X-ray photoelectron spectroscopy (XPS), scanning tunneling microscopy (STM) and scanning tunneling spectroscopy (STS) have collectively been employed to elucidate the structural and electronic properties of MoS monolayers on Au substrates. Our work provides a basis to produce macroscale two-dimensional heterostructures, which represent unique candidates for future electronic devices and applications.

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9:25am **PCSI-1WeM-12 UPGRADED: Effects of Electromechanical Coupling in Locally Strained Monolayer MoS$_2$***, **Alex De Palma**, G Cossio, K Jones, J Quan,* The University of Texas at Austin*; X Li,* Univ of Texas at Austin*; E Yu,* The University of Texas at Austin

Strain in atomically thin transition metal dichalcogenides (TMDs) has a broad range of consequences, and can be used for tuning of their optical and electronic properties [1, 2]. In particular, the use of localized strain to engineer these effects, such as in exciton funneling, has been demonstrated [3]. Additionally, TMDs exhibit intrinsic piezoelectricity in monolayer and few layer form originating from a lack of centrosymmetry [4]. The presence of piezoelectricity in TMD systems with strain and strain gradients can also have appreciable effects, which have only begun to be explored. Understanding these effects is necessary for engineering of TMD-based structures in which strain is present.

In this work, we examine the effects of piezoelectricity on MoS$_2$ in the presence of strain and strain gradients. Samples consisting of monolayer MoS2 suspended over 800nm-diameter cavities were fabricated by exfoliation and transfer of MoS$_2$ onto a patterned substrate. Suspended MoS$_2$ was deformed via atomic force microscope (AFM) indentation, and Photoluminescence (PL) measurements were simultaneously performed as a function of indentation force to determine the effects of the strain gradient on exciton bandgap and exciton diffusion (Fig. 1a, b). Additionally, we show through calculations that spatially varying strain, can be a source of electrostatic potentials due to the piezoelectric effect. According to a mechanical model for indentation [5], the charge density can be as high as 10^{12} e/cm^2 at the points of highest strain gradient - significant enough to generate electrostatic potential variations on the order of ±0.1V over the MoS$_2$ (Fig. 1c). The relationship between strain and the potential generated by piezoelectricity, and the impact of this effect on excitons, will be discussed.

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