

PCSI

Room Keauhou II - Session PCSI-WeM

Nanowires I/Nanowires II/Topological Properties I/Optical Studies of 2D Materials

Moderators: Ezekiel Johnston-Halperin, The Ohio State University, Paulina Plochocka, LNCMI, CNRS, Nicholas Harmon, University of Iowa

8:30am **PCSI-WeM-1 Bottom-up Grown Nanowire Quantum Devices, Erik Bakkers**, Eindhoven University of Technology, Netherlands **INVITED**

InSb nanowires are used to detect first signatures of quasi particles called Majorana fermions. Recently, different schemes for performing braiding operations and uncovering the non-Abelian statistics of Majorana fermions are proposed. Such operations are fundamental for topological quantum computing. For such a universal computational architecture the realization of a near-perfect nanowire network assembly is needed in which Majorana states are coherently coupled.

Here, we demonstrate a generic process by which we can design any proposed braiding device by manipulating an InP substrate and thereby the nanowire growth position and orientation [1]. This approach combines recent advances in materials growth and theoretical proposals. Our method leads to highly controlled growth of InSb nanowire networks with single crystalline wire-wire junctions. Additionally, nanowire "hashtag" structures are grown with a high yield and contacted. In these devices, the Aharonov-Bohm (AB) effect is observed, demonstrating phase coherent transport. These measurements reveal the high quality of these structures. This generic platform will open new applications in quantum information processing. Furthermore, these structures are well suited for epitaxial shadow growth of a superconductor on the nanowire facets. We study the growth of superconductors on nanowires and reveal the electronic properties.

9:00am **PCSI-WeM-7 Dopant Profiling in Semiconductor Nanowires by Atom Probe Tomography, A Rodil, R Plantenga, S Kolling, A Cavali, A Li, D Car, S Gazibegovic, E Bakkers, Paul M. Koenraad**, Eindhoven University of Technology, Netherlands

The controlled incorporation of doping atoms is essential for nearly all semiconductor devices. Devices such as transistors, light-emitting diodes, solar cells etc. are all impossible without the application of doping atoms that locally control the Fermi-level and the internal potential landscape. Nanowires comprise a relatively new class of highly interesting 3D semiconductor nanostructures in which doping also plays a crucial role. Due to their small size and special geometry it is very difficult to determine doping profiles in a straightforward manner by techniques such as SIMS and EDX. Also cross-sectional STM, which has an unprecedented capacity to determine the distribution of doping atoms in semiconductors is unfortunately not yet readily applicable for the study of doping atoms in nanowires.

At present the best and probably only technique that allows addressing this problem is Atom Probe Tomography. We have developed an improved approach [1] in which we have been able to measure doping concentrations with Atom Probe Tomography down the ppm-level or a doping level slightly below 10^{17} atoms/cm³. We have used this approach to examine Si (n-type) and Zn (p-type) doped InP nanowires and have been able to extract the doping profiles and check the dopant incorporation efficiency, see Figure 1a. Measurements like these allow to determine the doping efficiency. We noticed that this can vary from nanowire to nanowire and that at high doping concentrations the growth of the nanowire can become unstable. Under these conditions a strong local variation of the doping concentration can occur resulting in dopant clusters, see Figure 1b. Finally we have used the Atom Probe Tomography technique to analyze details in the doping profiles that allow us to retrieve important details in the incorporation process of doping atoms in nanowires. Figure 2 shows an example of a Si doping profile along the growth axis of the nanowire. The length and the height of both doping segments was supposed to be equal but as shown strong deviations can occur. Finally we have used Atom Probe Tomography to determine the background impurity level in core/shell GaP/Si nanowires.

[1] S. Koelling, et al, "Atom-by-Atom Analysis of Semiconductor Nanowires with Parts Per Million Sensitivity" Nano Letters DOI: 10.1021/acs.nanolett.6b03109.

9:05am **PCSI-WeM-8 How Can Band Offsets in III-V Nanowires be Determined Correctly by Scanning Tunneling Spectroscopy?, Philipp Ebert**, Forschungszentrum Jülich, Germany; P Capiod, ISEN; T Xu, Shanghai University, China; M Wei, A Díaz Álvarez, X Han, D Troadec, ISEN; J Nys, M Berthe, ISEN, France; G Patriarche, LPN-CNRS; L Lymerakis, J Neugebauer, MPIE; I Lefebvre, ISEN; S Plissard, LAAS-CNRS; P Caroff, Cardiff University, UK; R Dunin-Borkowski, Forschungszentrum Jülich, Germany; B Grandidier, ISEN, France

Scanning tunneling microscopy (STM) and spectroscopy (STS) allow a unique high resolution insight simultaneously into the structural and electronic properties of III-V semiconductor nanowires (NWs). Particularly interesting are heterostructured NWs with interfaces between different polytypes or different materials. Since the carrier transport through such NWs is expected to be affected by different band gaps and band offsets, the accurate determination of these values are critical. Although STM and STS is presented as the ideal technique for this, we demonstrate that STS measurements (and possibly other measurement techniques) are mostly wrongly interpreted and it is thus unclear if any of the published band offset values is reliable.

In this presentation we demonstrate that sidewall surfaces of III-V NWs regularly ex-hi-bit high step densities (or surface states as for III-nitrides), which induce a pinning the Fermi energy within the band gap. The pinning level is, however, different on every polytype or on every material. Hence, the relative band edge positions between different types of NW segments are extrinsically determined by the different pinning levels, but not by the intrinsic band offsets. Furthermore, extrinsic band offsets turn out to be much larger than intrinsic one. Hence, defect or surface states at the sidewall surface likely affect the carrier transport much stronger than intrinsic band offsets. Thus, it is of prime interest to determine pinning levels and extrinsic band offsets at the sidewall surfaces. We demonstrate these extrinsic band offsets using zinblend-wurtzite GaAs NW junctions.[1]

In order to nevertheless have experimental access to intrinsic band offsets, we developed a new methodology to determine accurate band offsets between different NW segments.[2] It uses a thin overgrown shell of a material with wider band gap. This allows electron tunneling through this thin shell directly into the core. The shell furthermore assures that the pinning of the overgrown and pure segments is identical. Then the differences between the band edge positions of both materials provide the correct band offset values. We applied this methodology to axial GaAs/GaAs_{0.81}Sb_{0.19}/GaAs heterostructure NWs.

[1] P. Capiod *et al.*, Appl. Phys. Lett. **103**, 122104 (2013).

[2] T. Xu *et al.*, Appl. Phys. Lett. **107**, 112102 (2015).

9:10am **PCSI-WeM-9 Lazarevite-type short-range ordering in ternary III-V nanowires, Michael Schnedler**, Forschungszentrum Jülich GmbH, Germany; I Lefebvre, Institut d'Electronique, de Microélectronique et de Nanotechnologie (IEMN), France; T Xu, Shanghai University, China; V Portz, Forschungszentrum Jülich GmbH, Germany; G Patriarche, Université Paris-Saclay, France; J Nys, ISEN, France; S Plissard, LAAS-CNRS; P Caroff, Cardiff University, UK; M Berthe, ISEN, France; H Eisele, Technische Universität Berlin, Germany; R Dunin-Borkowski, P Ebert, Forschungszentrum Jülich, Germany; B Grandidier, ISEN, France

Stabilizing ordering instead of randomness in alloy semiconductor materials is a powerful means to change their physical properties. We used scanning tunneling (STM) and transmission electron microscopy to reveal the existence of an unrecognized ordering in ternary III-V materials. The lazarevite short-range order (SRO), found in the shell of InAs_{1-x}Sb_x nanowires (NW), is driven by strong Sb-Sb repulsion along <110> atomic chains during Sb incorporation on unreconstructed {110} sidewalls. A preferred formation of lazarevite SRO under group-III-rich growing conditions is found as shown by the pair correlation function $c(x,y)$ and supported by our DFT calculations. Based on these observations, we present a growth model that offers the prospect to broaden the limited classes of ordered structures occurring in III-V semiconductor alloys. [1]

[1] M. Schnedler *et al.*, Phys. Rev. B **94**, 195306 (2016)

9:15am **PCSI-WeM-10 III-V Nanowire Devices: A 3D Toolbox with Contact, Interface, and Heterostructure Engineering, Erik Lind, L Wernersson**, Lund University, Sweden **INVITED**

III-V nanowires are attractive for device applications. The small nanowire footprint reduces the number of propagating defects opening a path for integration of high-quality III-V materials on Si. The direct band gap and the wide range of wave lengths addressable makes the material suitable for

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optoelectronic applications including light emitting diodes, solar cells, and long wave length photodetectors. The advantageous transport properties find usage in transistors applications where the reduced scattering enhances the drive current. However, for the realization of these devices, processing strategies needs to be developed and the material carefully characterized to avoid detrimental parasitic effects on the device performance.

In this talk, III-V nanowire MOSFETs [1] and TunnelFETs [2] will be presented. State-of-the-art performance in terms of transconductance (g_m), drive current (I_{on}), subthreshold swing (S), and off-state leakage current (I_{off}) will be demonstrated. In particular, we will focus on InAs/InGaAs MOSFETs and InAs/InGaAsSb/GaSb TunnelFETs, where the nanowire growth technology allows for incorporation of materials with strong lattice mismatch into the transistor channel.

The transistor processing relies on understanding and control of the physics and chemistry at the transistor interfaces. Examples will be given including vertical TLM structures developed to evaluate the specific contact resistance [3]. Furthermore, a vertical gate-last process has been established to align the gate to the edges of the source and drain contact regions reducing access resistance [4]. The semiconductor/high- k interface has finally been evaluated and the growth and process technology optimized to reduce both interface state and border trap state densities [5].

[1] O.-P. Kilpi, et al Vertical InAs/InGaAs Heterostructure Metal–Oxide–Semiconductor Field-Effect Transistors on Si Nano Lett., (2017)

[2] E. Memisevic, et al, Individual Defects in InAs/InGaAsSb/GaSb Nanowire Tunnel Field Effect Transistors Operating below 60 mV/decade Nano Lett., 17, 4373 (2017)

[3] M. Berg, et al A transmission line method for evaluation of vertical InAs nanowire contacts Appl. Phys. Lett. 107, 232102 (2015)

[4] M. Berg, et al, Electrical Characterization and Modeling of Gate-Last Vertical InAs Nanowire MOSFETs on Si IEEE Electron Dev. Lett., 37, 966 (2016)

[5] J. Wu, et al Low Trap Density in InAs/High- k Nanowire Gate Stacks with Optimized Growth and Doping Conditions Nano Lett., 16, 2418 (2016)

9:45am **PCSI-WeM-16 The Zincblende/Wurtzite Interface in III-V Nanowires: Heterostructures with Atomically-abrupt Electronic Transition**, J Knutsson, S McKibbin, M Hjort, S Lehmann, Lund University; N Wilson, S Patel, C Palmstrom, University of California, Santa Barbara; K Dick, Lund University; A Mikkelsen, Rainer Timm, Lund University, Sweden
III-V semiconductor nanowires (NWs) have a large technological potential within energy harvesting and (opto)electronics [1]. In addition, they provide a unique playground in materials science, since their small footprint allows the formation of a wide range of radial and axial heterostructures with changes in material composition, doping, or crystal phase. Recently, it became possible to purposely tune the crystal structure between Zincblende (Zb) and Wurtzite (Wz) phase over InAs or GaAs NW segments of varying length [2].

Here, we use low-temperature scanning tunneling microscopy and spectroscopy (STM/S) to monitor both the atomic surface structure and the surface local density of states (LDOS) across Zb/Wz interfaces in InAs NWs. The NWs include Zb and Wz segments of varying length, down to the shortest possible insertion of Zb phase in a Wz matrix, i.e. a Zb single bilayer stacking fault. We compare STS spectra obtained at As atoms in the stacking fault with spectra from As atoms located 1 nm, 3 nm, and 5 nm away from it. Thereby we find similar Wz LDOS signal further away and in close proximity to the stacking fault, while the stacking fault itself shows a clear Zb signature. These results demonstrate that the atomically sharp structural transition between Zb and Wz phase is accompanied by an equally abrupt electronic transition. In addition, we analyze conduction band and valence band onsets from STS results obtained at Wz segments with Zb inclusions of varying length. We obtain strong valence band offsets and a nearly flat conduction band, in agreement with previous results on extended Wz and Zb segments [3], and we observe confinement energies of up to 30 meV with decreasing length of the Zb segment.

Furthermore, we present initial tests on utilizing NWs with Wz and Zb segments for the creation of advanced 3D heterostructures with atomic precision: We expose GaAs NWs with both Wz and Zb segments to Sb and monitor the incorporation of individual Sb atoms in the surface due to Sb-for-As exchange reactions. Thereby we find a preferential incorporation of Sb in the Zb {110} surface facets, as compared to Wz {11-20} surface segments (see Fig. 1), which is also verified by density functional theory

calculations [4]. Such preferential incorporation, prior to subsequent radial overgrowth, opens up a path towards atomically thin quantum rings of tunable diameter and height.

[1] J. Wallentin et al., Science 339, 1057 (2013); E. Lind et al., IEEE J. El. Dev. Soc. 3, 96 (2015).

[2] S. Lehmann et al., Nano Lett. 13, 4099 (2013).

[3] M. Hjort et al., ACS Nano 8, 12346 (2014).

[4] M. Hjort et al., Nano Lett. 17, 3634 (2017).

9:50am **PCSI-WeM-17 Selective-area Epitaxy and Electronic Transport in in-plane InAs One-dimensional Channels**, JoonSue Lee, S Choi, M Pendharkar, A McFadden, C Palmstrøm, University of California, Santa Barbara

One-dimensional (1D) semiconductor nanowire proximitized by a superconductor could exhibit topological superconducting phases, which host Majorana zero modes at the ends of the proximitized region. Based on the hybrid superconductor/1D nanowire systems, scalable designs for topological quantum computing processes by braiding of Majorana zero modes have been proposed [1]. Experimental efforts have been made to realize the complex nanostructures consisting of multiple Majorana zero modes: bottom-up synthesis of self-assembled nanowire networks with predefined superconducting islands has been recently reported [2], and top-down processing of the large-scale nanostructures has been suggested on a two-dimensional material platform of epitaxial superconductor/semiconductor heterostructures [3].

In this work, we study a new bottom-up approach of selective-area growth of semiconductor 1D channel networks. This approach is advantageous for scalability and for minimizing damages from further fabrication processes. We employ chemical beam epitaxy to selectively grow in-plane InAs 1D channels on pre-patterned SiO₂/InP(001) substrates. For electronic transport, InAs Hall bars with channel width of 50-500 nm and length of 500-2000 nm are selectively grown and measured with a perpendicular magnetic field at cryogenic temperatures. In order to achieve optimal transport properties, we vary 1) substrate preparation process, 2) growth conditions, such as substrate temperature, growth rate, and V/III ratio, 3) 1D channel dimensions of width and height, 4) crystallographic orientations, 5) buffer layers, and 6) capping layers. The resulting electron mobility is observed up to a few thousand cm²/Vs with electron density of low 10¹² cm⁻². Magnetoresistance also reveals universal conductance fluctuations and weak antilocalization. Further transport studies of electrostatic gating and Aharonov-Bohm oscillations will be discussed.

[1] T. Karzig *et al.*, Phys. Rev. B 95, 235305 (2017).

[2] S. Gazibegovic *et al.*, Nature 548, 434 (2017).

[3] J. Shabani *et al.*, Phys. Rev. B 93, 155402 (2016).

9:55am **PCSI-WeM-18 Writing Gallium Oxide on GaN Nanowires With The AFM Tip**, Jovana Colvin, R Ciechonski, J Ohlsson, A Mikkelsen, R Timm, Lund University, Sweden

Superior inherent properties of gallium nitride (GaN) semiconductor nanowires (NWs) such as defect free nature, high surface to volume ratio, wide band gap, large break-down voltage, high electron saturation velocity and mobility, high-temperature operation make them highly promising for the future metal-oxide-semiconductor (MOS) based high power and high temperature devices. However, much work will have to be done in order to achieve high quality gate oxide. Gallium (III) oxide, the native oxide of GaN, has a potential of fulfilling the aforementioned requirement [1].

Here, we study a continuous GaN film formed from GaN NWs [2]. The NWs are grown first at a low V/III ratio (1:1), and radially overgrown using a high V/III ratio on the order of 1000:1. Amplitude-modulated atomic force microscopy (AFM) characterization shows that the top c-plane of the NWs is defect free. In addition, we simultaneously monitor topography and conductivity of the GaN film. In agreement with the intended doping levels, we find significant conductivity only at the position of the GaN cores. Importantly, we observe both a height increase (see Fig. 2) and a drop in conductivity at the GaN cores upon imaging the film with a bias of 6 V or more applied between the sample and the AFM tip. This demonstrates that we can locally induce a thin gallium oxide barrier over the GaN cores, where the rest of the surface is unaffected, see Figure 2. We will present a systematic investigation of the oxide thickness as a function of growth parameters, as well as the tip loading force and applied voltage and polarity.

[1] H. Oon, K. Materials Science in Semiconductor Processing, 16, 5, 2013

[2] W Seifert, US Patent 9,024,338, 2015

10:00am **PCSI-WeM-19 Recombination processes and localization effects in GaNAsP** **Recombination Processes and Localization Effects in GaNAsP Nanowires**, *M Jansson, S Chen*, Linköping University, Sweden; *R La*, University of California, San Diego; *J Stehr*, Linköping University, Sweden; *C Tu*, University of California, San Diego; *W Chen, Irina A. Buyanova*, Linköping University, Sweden

The GaNAsP material system, belonging to the family of dilute nitride alloys, has shown significant promises as a candidate for intermediate band solar cells (IBSCs), due to its high band gap tunability and an attractive band structure. Owing to very recent advances in fabrication techniques, it has become possible to fabricate GaNAsP in the nanowire (NW) geometry, which may reduce costs for device fabrication and also opens a door for integration of the IBSC concept with the promising NW architecture.

In this work we perform systematic optical studies of such novel GaNAsP NWs grown by molecular beam epitaxy on Si substrates, combined with comprehensive structural characterization of the wires. Based on the performed transmission electron microscopy and Raman studies, we show that the fabricated NW arrays have good structural and optical quality, in spite of a large difference in electronegativity and sizes between N and replaced As/P atoms. The arrays are also found to exhibit excellent compositional uniformity among individual wires. Based on temperature-dependent photoluminescence (PL) studies, we show that random alloy disorder causes localization of photo-generated carriers at low temperatures. The localization potential increases in N-containing wires as compared with reference GaAsP NWs. In some regions, it leads to three-dimensional carrier confinement, based on the observation of sharp and discrete PL lines in μ -PL spectra from individual NWs. Localization effects, however, are found to have negligible influence on carrier recombination at room temperature (RT) owing to thermal activation of the localized carriers to extended states. From time-resolved PL measurements, the prolonged roomtemperature carrier lifetime at RT was found in N-containing wires. As the carrier lifetime under these conditions is typically governed by non-radiative recombination via surface states, this finding implies N-induced suppression of surface recombination. The presented results, therefore, show that GaNAsP NWs hold great promises for future applications of this material system in nano-optoelectronic and photonic devices.

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11:00am **PCSI-WeM-31 Quantum Anomalous Hall Effect in the Magnetic Topological Insulator Thin Films**, **Cui-Zu Chang**, The Pennsylvania State University

INVITED

The quantum anomalous Hall (QAH) effect can be considered as the quantum Hall (QH) effect without external magnetic field, which can be realized by time reversal symmetry breaking in a topologically non-trivial system [1, 2]. A QAH system carries spin-polarized dissipationless chiral edge transport channels without the need for external energy input, hence may have huge impact on future electronic and spintronic device applications for ultralow-power consumption. The many decades quest for the experimental realization of QAH phenomenon became a possibility in 2006 with the discovery of topological insulators (TIs). In 2013, the QAH effect was observed in thin films of Cr-doped TI for the first time [3]. Two years later in a near ideal system, V-doped TI, contrary to the negative prediction from first principle calculations, a high-precision QAH quantization with more robust magnetization and a perfectly dissipationless chiral current flow was demonstrated [4]. In this talk, I will introduce the route to the experimental observation of the QAH effect in aforementioned two systems [3, 4], and discuss the demonstration of the dissipationless chiral edge state as well as the origin of the dissipative channels in the QAH state [5]. Finally I will talk about our recent progress on the QAH insulator-Anderson insulator quantum phase transition and its scaling behaviors [6].

[1] F. D. M. Haldane, Phys. Rev. Lett. 61, 2015 (1988).

[2] R. Yu et al, Science 329, 61 (2010).

[3] Cui-Zu Chang et al, Science 340, 167(2013).

[4] Cui-Zu Chang et al, Nat. Mater. 14, 473(2015).

[5] Cui-Zu Chang et al, Phys. Rev. Lett. 115, 057206 (2015).

[6] Cui-Zu Chang et al, Phys. Rev. Lett. 117, 126802 (2016).

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11:30am **PCSI-WeM-37 Molecular Beam Epitaxy of Near Surface InAs_xSb_{1-x} Quantum Wells for Topological Quantum Computation**, **Mihir Pendharkar**, *J Lee, A McFadden, C Palmstrom*, University of California, Santa Barbara

Topological quantum computation based on Majorana Zero Modes (MZMs) promises to be a reliable approach to fault tolerant quantum computation.^[1] MZMs, created at the interface of a 1D chain of electrons with an s-wave superconductor, on application of an in-plane magnetic field, are predicted to be protected from external perturbations by the size of the topological energy gap, thus induced.^[2] The size of this energy gap, can be increased by increasing the spin-orbit coupling and mobility of the semiconductor host.

In this work, we report on the Molecular Beam Epitaxy (MBE) growth of near surface, inverted, InAs_xSb_{1-x} (0.4 > x > 0.2) quantum wells strained to Al_{0.3}InSb barrier layers and compare them to InAs and InSb quantum wells. Due to band gap bowing, certain compositions of InAs_xSb_{1-x} (centered around x ≈ 0.36) are predicted to have a higher g-factor and lower electron effective mass than either of the constituent binary compounds of InAs and InSb. Such compositions of InAsSb are hence ideal candidates for hosting MZMs providing a substantial enhancement in the topological protection. Near surface inverted QW structures with the doping layer below the 2DEG, are necessary for effective top gate control and transparent coupling to an epitaxial superconductor layer above the QW. While previous work has demonstrated MZMs in InAs and InSb nanowires and InAs QWs, demonstration of a near surface 'inverted' InAsSb QW to host MZMs had remained a challenge.

These structures were grown on GaSb and InSb substrates to study the effect of interfacial strain (compressive from GaSb and tensile from InSb) on the effective mass of electrons in the 2DEG. This work is also believed to be the first demonstration of an InAsSb QW on an InSb substrate allowing for hetero-epitaxy with drastically reduced lattice mismatch as compared to GaSb and GaAs.

The depth of the quantum well from the surface was also varied to study the effect of surface pinning on the 2D electron density. The surface of InAs is believed to be pinned at 0.2eV above the conduction band minima (electron accumulation) while InSb surface is believed to be pinned mid-gap (~0.12eV below the conduction band minima). A systematic reduction in sheet carrier density was observed with reducing depth from the surface, which also correlated to a reduced doping efficiency of n-type dopants near the surface, indicating the presence of a surface depletion layer.

This understanding of the surface pinning and the first demonstration of InAsSb QWs on InSb substrates is now expected to provide a new platform for the measurement of MZMs and consequent development of InAsSb based robust topological quantum networks.

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[1] M. H. Freedman, Found. Comput. Math. 1, 183 (2001)

[2] J. D. Sau, et al., Phys. Rev. Lett. 104, 040502 (2010)

[3] J. Shabani, et. al., Phys. Rev. B 93, 155402 (2016)

[4] H. J. Suominen, et. al., arXiv:1703.03699 (2017)

11:45am **PCSI-WeM-40 Exploring the Bright Side and the Dark Side of Excitons in Atomically-thin Transition Metal Dichalcogenides**, **Alex High**, University of Chicago

INVITED

In this talk, we will explore fundamental properties of bright and dark exciton transitions in Transition Metal Dichalcogenides (TMDs). On the bright side, we will probe a simple question: can TMDs act as an atomically-thin mirror at the bright exciton resonance? Such an experimental realization places a stringent demand on the excitons – the radiative linewidth should dominate the total transition linewidth, a criteria rarely fulfilled in solid-state systems. Remarkably, we observe resonant reflection of up to 85% of incident light from a monolayer of MoSe₂, indicating that the radiative decay rate of excitons can be up to an order of magnitude larger than the non-radiative and dephasing rates. Furthermore, we demonstrate that these mirrors can be electronically switched, and exhibit strong power- and wavelength-dependent hysteresis. On the dark side, because of strong spin-orbit coupling the lowest-energy excitonic states in some TMD monolayers (such as WSe₂ and WS₂) involve nominally spin-forbidden optical transitions and are thus optically dark. Probing and understanding these dark excitons provides crucial insights into the fundamental properties of TMD monolayers, however their presence typically can only be inferred through indirect measurements. We will introduce a method for probing the optical properties of two-dimensional

(2D) materials via near-field coupling to surface plasmon polaritons (SPPs). This coupling selectively enhances optical transitions with dipole moments normal to the 2D plane, enabling direct detection of dark excitons in TMD monolayers. When a WSe₂ monolayer is placed on top of a single-crystal silver film, its emission into near-field-coupled SPPs displays new spectral features whose energies and dipole orientations are consistent with dark neutral and charged excitons.

12:15pm **PCSI-WeM-46 Structure and Peierls Transition of the Indium/Si(111) 1D Model System: A Microscopic View from Raman Spectroscopy**, *Norbert Esser*, *E Speiser*, *S Chandola*, Leibniz-Institut für Analytische Wissenschaften-ISAS e.V., Germany; *S Wippermann*, Max-Planck-Institut für Eisenforschung, Germany; *S Sanna*, Institut für Theoretische Physik, Justus-Liebig-Universität, Germany; *W Schmidt*, Universität Paderborn, Germany

Raman spectroscopy can be used for the analysis of surface structures by recording surface confined vibrational modes. In recent years we have demonstrated for various clean and adsorbate modified semiconductor surfaces that the related Raman signals are a general feature of solid surfaces [1], which does not depend on plasmonic/chemical Raman enhancement like for SERS.

As one example of a 1D surface structure, In nanowires on Si(111) have been analysed thoroughly by Raman spectroscopy [2]. In/Si(111) is a one-dimensional metallic nanostructure which undergoes a Peierls transition into an insulating structure upon cooling below 125K. We have recorded surface specific phonon spectra related directly to the atomic nanowire structures above and below the phase transition temperature. By performing ab-initio calculations of the structures and their vibrational properties we are able to assign Raman lines to individual surface phonon modes and verify atomic structure models. Moreover, we can follow the Peierls transition and find a clear indication of phonon softening of some particular modes, associated with a first order phase transition in the 1D-nanostructures. A microscopic picture of the whole process is achieved from ab-initio DFT based calculations.

Moreover, in 1D systems collective modes (phason, amplitudon), should arise as characteristic excitations of the correlated electron system. Such excitations have been observed with Raman spectroscopy in other correlated systems [3,4] and should also appear in the In/Si nanowire Raman spectra. We discuss the spectral signatures of such excitations in the surface Raman spectra and also their microscopic origin as a coupled electronic/vibronic excitations.

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Refs.:

- [1] N. Esser, W. Richter, Topics in Applied Physics 76, Springer-Verlag (2000)
- [2] E. Speiser, N. Esser, S. Wippermann, W.G. Schmidt, Phys. Rev. B 94, 095417 (2016)
- [3] S. Sugai et al, Phys. Rev. Lett. 96, 137003 (2006)
- [4] D.H. Torchinsky et al, Nature Materials 12, 387 (2013)

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12:20pm **PCSI-WeM-47 Charge Transfer Dynamics in Graphene-Inorganic 'hybrids' with Transition Metal Oxides Using In-Situ Raman Spectroelectrochemistry**, *Sanju Gupta*, *S Carrizosa*, Western Kentucky University

We report on the electrochemical assembled two- and three-dimensional graphene variants with nanostructured cobalt oxide (CoO and Co₃O₄) polymorphs that synthesize hybrids with optimal loading and chemical attachment of cobalt oxides micro/nano particles on the functionalized graphene surface, creating tailored interfaces crucial to electrochemical property enhancement. In-situ Raman spectroscopy integrated with electrochemistry was employed to investigate ion transport and charge transfer dynamics and to determine the concomitant electrochemical tuning of Fermi level. The variation of structural bonding in these hybrids dipped in aqueous alkaline electrolyte (e.g. KOH) with electrochemical biasing was monitored. It is because Raman spectroscopy can detect changes in graphene/metal and graphene/metal oxide bond through various spectral features. Two of the transverse optical phonons and corresponding longitudinal optical (LO) phonons of Co₃O₄ (and CoO) above 500 cm⁻¹ are observed depending on the surface morphology and particle size as well as carbon-carbon bonding via G and 2D bands at 1590 cm⁻¹ and 2670 cm⁻¹, respectively. Consistent reversible and substantial variations in Raman intensity and band positions of these modes induced by electrode potential point at the fine and continuous tuning, indicative of

emptying/depleting or filling of the specific bonding and antibonding states which become electroactive. The results were explained in terms of changes in the electron density of states arising due to alterations in the overlap integral of bonds between the s and p (and d) orbitals of the adjacent carbon and metal oxide atoms. We estimated the extent of variation of the absolute potential of the Fermi level and overlap integral between the nearest-neighbor atoms from modeling the electrochemical potential dependence of Raman intensity thus corroborating the synergistic coupling of graphene and cobalt oxide polymorphs. The interplay of heterogeneous basal and edge plane sites graphene and crystalline spinel cobalt oxides reinforce density of states in the vicinity of Fermi level and efficient interfacial electron transfer. We acknowledge KY NSF EPSCOR RSP, WKU Research Foundation and Graduate School internal awards in parts for financial support.

12:25pm **PCSI-WeM-48 Rydberg Excitons & Dielectric Environment Effects in Monolayer Semiconductors: Insight from High Magnetic Fields**, *A Stier*, Los Alamos National Laboratory; *N Wilson*, University of California, Santa Barbara; *J Kono*, Rice University; *X Xu*, University of Washington; **Scott Crooker**, Los Alamos National Laboratory

Excitons in atomically-thin semiconductors necessarily lie close to a surface, and therefore their properties are expected to be strongly influenced by the surrounding dielectric environment. However, systematic studies exploring this role are challenging, in part because the most readily accessible exciton parameter—the exciton's optical transition energy—is largely unaffected by the surrounding medium. In this work we show that the significant role of the dielectric environment on 2D materials can be directly revealed through its systematic influence on the size of the exciton, which can be measured via the diamagnetic shift of the exciton transition in high magnetic fields [1].

Using exfoliated Wse₂ monolayers affixed to single-mode optical fibers, we tune the surrounding dielectric environment by encapsulating the flakes with different materials [2] and perform polarized low-temperature magneto-absorption studies to 65 T. The systematic increase of the exciton's size with dielectric screening, and concurrent reduction in binding energy (also inferred from these measurements), is quantitatively compared with leading theoretical models based on the Keldysh potential for 2D materials. These results demonstrate how exciton properties and the free-particle bandgap can be tuned in 2D van der Waals heterostructures, via the surrounding dielectric environment. We also present recent 65T measurements of high-quality hBN/Wse₂/hBN structures that permit an unambiguous identification and quantification of excited 1s, 2s, 3s, and 4s Rydberg states of neutral excitons [3], which allows a direct measurement of exciton mass in 2D materials.

[1] A. V. Stier et al., *Nano Letters* 16, 7054 (2016).

[2] A. V. Stier et al., *Nature Communications* 7:10643 (2016).

[3] A. V. Stier et al., *submitted*; arXiv:1709.00123

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