Mini Symposium on 2D Materials Synthesis
Room 303 - Session MS-2DMS+2D+EM+NS-TuM

Direct Growth of 2D Materials, Including CVD and MBE

Moderators: Matthias Batzill, University of South Florida, **Erica Douglas**, Sandia National Laboratories, **Maryam Ebrahimi**, Lakehead University, Canada, **Kathleen McCreary**, Naval Research Laboratory

8:00am **MS-2DMS+2D+EM+NS-TuM-1 Efficient Control of 2D Magnetism**, ***Cheng Gong***, University of Maryland **INVITED**

The recently discovered magnetic two-dimensional (2D) van der Waals materials [1, 2] provide ideal platforms to enable the atomic-thin, flexible, lightweight magneto-optical and magnetoelectric devices. Though many have hoped that the ultra-thinness of 2D magnets should allow an efficient control of magnetism, the state-of-the-art has not achieved notable breakthroughs to this end, with only proof-of-concept reports. There appear to be some fundamental obstacles for efficient control. In this talk, I will analyze the challenges and present our recent theoretical and experimental progress on efficient electrical and optical control of 2D magnetism [3-7]. We envision the efficient control of 2D magnets could open new avenues for the low-power spintronics and photonics.

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4. S.-J. Gong, et al. PNAS 115, 8511-8516 (2018).
5. E.-W. Du, et al. Nano Letters 20, 7230-7236 (2020).
6. T. Xie, et al. under review (2022).
7. S. Liang, et al. under review (2022).

8:40am **MS-2DMS+2D+EM+NS-TuM-3 Epitaxial Growth of Transition Metal Dichalcogenide Monolayers for Large Area Device Applications**, *J. Redwing,* ***Thomas V. Mc Knight***, The Pennsylvania State University **INVITED**

Wafer-scale epitaxial growth of semiconducting transition metal dichalcogenide (TMD) monolayers such as MoS_2, WS_2 and WSe_2 is of significant interest for device applications to circumvent size limitations associated with the use of exfoliated flakes. Epitaxy is required to achieve single crystal films over large areas via coalescence of TMD domains. Our research has focused on epitaxial growth of 2D semiconducting TMDs on c-plane sapphire substrates using metalorganic chemical vapor deposition (MOCVD).Steps on the miscut sapphire surface serve as preferential sites for nucleation and can be used to induce a preferred crystallographic direction to the TMD domains which enables a reduction in twin boundaries in coalesced films. The step-directed growth is dependent on the surface termination of the sapphire which can be altered through pre-growth annealing in H_2 and chalcogen-rich environments. Uniform growth of TMD monolayers with significantly reduced inversion domains is demonstrated on 2" diameter c-plane sapphire substrates enabling large area transfer of monolayers for characterization and device fabrication and testing.Applications for wafer-scale TMD monolayers in nanoelectronics, sensing and photonics will be discussed.

9:20am **MS-2DMS+2D+EM+NS-TuM-5 Formation of Transition Metal Dichalcogenide Janus Monolayers and 2D Alloys Through Non-Equilibrium Synthesis and Processing Approaches**, ***Kai Xiao***, *S. Harris, Y. Lin, C. Liu,* Center for Nanophase Materials Sciences, Oak Ridge National Laboratory*; G. Duscher,* University of Tennessee Knoxville*; M. Yoon,* Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA*; L. Liang, C. Rouleau, A. Puretzky, D. Geohegan,* Center for Nanophase Materials Sciences, Oak Ridge National Laboratory

Doping and alloying in 2D materials are efficient ways to tune the optical and electronic properties, induce new crystal structures and phases, and add new functionalities. In this talk, I will introduce how to precisely tailor the doping of 2D TMDs using non-equilibrium synthesis and processing techniques including chemical vapor deposition and hydrothermal laser implantation. By tailoring isoelectronic doping of chalcogens and metals in 2D TMDs (e.g., $MoSe_2$, WS_2) during CVD synthesis, the uniform alloys, gradient alloys, and lateral heterostructures are controlled grown on substrates which exhibit many novel properties including tunable bandgaps, enhanced photoluminescence, modulated charge carriers, etc. I will also describe a novel PLD approach with in situ diagnostics such as Raman and photoluminescence to sensitively tune the kinetic energies of Se clusters (3-5 eV/atom) to selectively implant Se atoms within monolayer WS_2 and MoS_2 crystals to form novel Janus WSSe and MoSSe monolayers. Synthesis science was supported by the U.S. Dept. of Energy, Office of Science, Materials Science and Engineering Division. This work was performed at the Center for Nanophase Materials Sciences, which is a DOE Office of Science User Facility.

9:40am **MS-2DMS+2D+EM+NS-TuM-6 Effects of Deposition Technique on Monolayer MoS_2 and WS_2**, ***Ama Agyapong***, *S. Mohney,* Pennsylvania State University

It is important to understand how the deposition of metal contacts affects two-dimensional transition metal dichalcogenides (TMDs) so that we can successfully integrate TMDs into next-generation electronic and optoelectronic devices. This study employs Raman spectroscopy as a non-destructive method to probe structural changes induced by depositing metals on monolayer MoS_2 and WS_2. Differences between electron-beam evaporated and DC magnetron sputtered metal/MoS_2 and metal/WS_2 samples were observed in Raman spectra obtained through a transparent substrate using a backside geometry. The disappearance of characteristic Raman modes of the TMDs indicates structural disorder, as observed for sputtered In, Pd, and Pt films on both monolayer MoS_2 and WS_2. This disorder is introduced even though the metals are not reactive with the TMDs. On the other hand, Raman modes remain if the metals are e-beam evaporated. The mass of the metal atoms appears to impact the structural disorder caused by sputtering, as characteristic MoS_2 and WS_2 modes are preserved (albeit with some changes to the spectra) when lighter metal atoms (Cu and Al) are sputtered. The results of this work provide insight on structural changes at the metal/TMD interface that may not be easily detectable in bulk TMDs, and we conclude that e-beam evaporation is a less destructive deposition technique for forming metal contacts on 1L TMDs than sputtering.

11:40am **MS-2DMS+2D+EM+NS-TuM-12 The Growth of $Nb_{1+x}Se_2$ by Molecular Beam Epitaxy**, ***Peter Litwin***, *S. Jaszewski, J. Ihlefeld, S. McDonnell,* University of Virginia

$NbSe_2$, a metallic transition metal dichalcogenide, has been the focus of numerous recent scientific studies due to the coexistence of superconductivity and charge density wave states it exhibits at low temperature. While less studied, this material also exists in a metal rich, Nb-intercalated (self-intercalated) phase in which additional Nb atoms populate the van der Waals gap. The self-intercalated phase, $Nb_{1+x}Se_2$, has been studied in the bulk form since the 1960's when it was synthesized by chemical vapor transport techniques; however, thin film synthesis of this material is rarely reported. Here we report on the growth of few layer $Nb_{1+x}Se_2$ by molecular beam epitaxy (MBE). We demonstrate that the degree of Nb-intercalation can be tuned through alteration of the Se to Nb flux ratio used during growth. Interestingly, we find that Nb-intercalation exists in all multilayer films, even under Se to Nb flux ratios as high as 45,000:1. The presence of Nb-intercalation results in an expansion of the material's c-axis lattice parameter which we measure using ex-situ x-ray diffraction (XRD). Chemical analysis of the grown thin films is carried out using in-situ x-ray photoelectron spectroscopy (XPS) and further confirms the Nb-rich nature of the grown thin films. The in-plane electrical conductivity is measured using a 4-point probe measurement tool and shows an inverse relationship with the Se to Nb flux ratio used during growth. Lastly, we also report on the thickness scaling of the material's electrical conductivity down to few-layer thick $Nb_{1+x}Se_2$ thin films.

12:00pm **MS-2DMS+2D+EM+NS-TuM-13 Formation of 1D and 2D Carbon-Based Nanomaterials on Surfaces**, ***Maryam Ebrahimi***, Lakehead University, Canada

On-surface reactions offer a platform to design molecular-based low-dimensional nanomaterials whose chemical and electronic properties can be tailored by their chemical structure. The molecules' functional groups and the reactivity of the substrates control the molecule-molecule and molecule-substrate interactions, which steer the design of the obtained molecular structures.We present various surface reactions for creating 1D and 2D polymers, metal-organic networks, and organometallic structures on Au(111), Ag(111) and Cu(111).To identify their topography and chemical nature, we employ scanning tunnelling microscopy and non-contact atomic force microscopy, and other surface characterization techniques, such as X-ray photoelectron spectroscopy, complemented with density functional theory calculations.

The chemical and thermal stability and structural design of these molecular-based low-dimensional nanomaterials make them promising

candidates for various applications. These materials are tailored to exhibit unique electronic properties, charge mobility and/or electron spin-based structure, suitable for carbon-based nanoelectronics, spintronics, and quantum technology applications.

References

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