PCSI

Room Ballroom South - Session PCSI-SuE

Energy & Van der Waals Heterostructures I

Moderators: Leonard Brillson, Ohio State University, Arend van der Zande, University of Illinois at Urbana Champaign

7:30pm **PCSI-SuE-1 Understanding Surface Chemistry of Atomic Layer Deposition: Toward Renewable Energy Applications*, Stacey Bent,*** Stanford University **INVITED**

With the intensifying interest in functional nanoscale materials for applications in electronics and energy conversion, methods for fabricating materials with atomic-level control are becoming increasingly important. Atomic layer deposition (ALD) is a method that provides excellent capabilities for depositing thin films, nanoparticles, and other nanoscale materials. This talk will describe research into the surface chemistry occurring during ALD, focusing on the ALD of metal oxides of interest for renewable energy applications. Deposition of binary, ternary, and doped metal oxides at a range of important interfaces has already been demonstrated using ALD. However, a fundamental understanding of the growth process for metal oxides is still lacking. Moreover, it is often difficult to correlate the material properties and growth characteristics with the process parameters due to the limited understanding of the underlying surface chemistry. In this talk, we will describe the results of both *in situ* and *ex situ* studies investigating nucleation in metal oxide deposition, using zinc tin oxide (ZTO) as a model system. Based on a combination of quadrupole mass spectrometry, infrared spectroscopy, low energy ion scattering, and density functional theory, we propose mechanisms explaining the presence of a nucleation delay that occurs when the metal oxide processes are mixed. The application of ALD metal oxides to renewable energy applications will also be presented. We will examine both a photovoltaics application, in which ALD is used to deposit layers in thin film solar cells, and an application in clean fuel synthesis for which ALD produces active electrocatalysts.

8:00pm **PCSI-SuE-7 Li-ion Synaptic Transistor for Low Power Analogue Computing (LISTA)*, Alec Talin,*** Sandia

Neuromorphic networks that emulate brain plasticity and adaptive learning will revolutionize artificial intelligence and computing. The key element for neuromorphic networks is the artificial synapse, which emulates the function of its biological counterpart using strictly solid-state components. Necessary attributes of an artificial synapse are non-volatile memory and history-dependent analogue states. These synapse characteristics can be realized using two-terminal memristive devices. However, two-terminal memristors cannot readily utilize existing computational algorithms designed for CMOS circuits, thus requiring development of new algorithms. Recently, three-terminal, transistor-like memristive devices utilizing an ionic liquid gate to control source-drain resistance by injection or extraction of oxygen vacancies have been demonstrated at Harvard and IBM. This functionality enables the implementation of spike time dependent plasticity (STDP) by converting the time difference between source (pre-neuron) and drain (post-neuron) spikes into a gate voltage. The exact channel conductance state achieved through a set of voltage pulses determines the synapse weight. The Harvard and IBM approach, however, has two principal drawbacks: 1) it requires a liquid gate to effectively inject or withdraw oxygen vacancies 2) switching is slow (~seconds) even at 160 ^{o}C due to the sluggish motion of oxygen ions in solid lattices at or near room temperature. To address these shortcomings, we describe an alternative synaptic transistor based on insertion/extraction of Li-ions from a Li_xCoO_2 channel. Similarly to oxygen vacancies, Li-ions act as dopants, contributing a mobile electron or hole every Li-ion insertion or extraction, depending on the specific material. Compared to O-vacancies, however, Li-ions move as interstitials with much lower activation energy. Since Li diffusivity at room temperature is relatively high, the ionic liquid gate is replaced in our device by a solid Li electrolyte to realize all-solid state synaptic transistors.

8:15pm **PCSI-SuE-10 The World of 2D: It's All About Interfaces*, Joshua Robinson,*** Penn State **INVITED**

The last decade has seen nearly 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. Furthermore, heterogeneous stacking of 2D materials also allows for additional "dimensionality" for band structure engineering. In this talk, I will discuss recent breakthroughs in two-dimensional atomic layer synthesis and properties, including novel 2D heterostructures and novel 2D nitrides. Our recent works demonstrate that the properties of 2D materials, especially those grown via CVD, are extremely sensitive to the substrate choice. I will discuss substrate impact on 2D layer growth and properties, doping of 2D materials with magentic elements, selective area synthesis of 2D materials, and the first demonstration of 2D gallium nitride (2D-GaN). Our work and the work of our collaborators has lead to a better understanding of how substrate not only impacts 2D crystal quality, but also doping efficiency in 2D materials, and stabalization of nitrides at their quantum limit.

8:45pm **PCSI-SuE-16 One-dimensional Metals in Twin Grain Boundaries of $MoSe_2$*, Y Ma, H Coy Diaz, S Kolekar,*** University of South Florida*; J Avila, M Asensio,* Synchrotron SOLEIL*; J Carmelo,* University of Minho*; **Matthias Batzill,*** University of South Florida

Electrons confined in one-dimension (1D) behave fundamentally different from the Fermi-liquid in higher dimensions. Material line defects are one dimensional but the search and proof of 1D electron behavior in such defects has been so far unsuccessful. In this presentation we show that a line defect in the 2D semiconductor MoSe2 is metallic and hosts 1D electrons. Scanning tunneling microscopy of monolayer MoSe2 films grown by MBE on other van der Waals materials reveal a high density of these line defects (figure). Furthermore, low temperatures STM shows the formation of a charge density wave (Peierl's transition) as is expected for any 1D-metal. Importantly, the high density of these crystallographically aligned defects enables the characterization of the electronic properties by angle resolved photoemission spectroscopy (ARPES) and thus, for the first time, a direct k-space resolved measurement of the electronic structure of a material's line defect. The measured Fermi-wave vector agrees with the measured periodicity of the charge density wave in STM. Further important verification of 1D behavior of these metallic states comes from the Tomonaga Luttinger liquid behavior of the density of states at the Fermi-level. The most 'exotic' property of 1D quantum liquids is, however, the separation of spin- and charge- excitations. Our ARPES measurements (figure) clearly exhibit the splitting of the spectral line into 'spinon' and 'holon' excitations. To understand these distinctive k-dispersion lines one has to go beyond the traditional Tomonaga Luttinger formalism for 1D electrons. Using a 1D Hubbard model with finite-range interactions enables to exactly reproduce our experimental data, demonstrating the observation of spin-charge separation in these line defects. Our results also imply that isolated quantum wires can be formed in twin boundaries of 2D transition metal dichalcogenides, which should enable quantum transport on these individual quantum line defects in the future.

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