56th TCSUH Student Symposium

ABSTRACTS

SESSION I

Dr. Elie Track, CEO, nVizix LLC; Treasurer, IEEE Council on Superconductivity (IEEE-CSC)

10:05-10:25 **Mr. Eric Buko** (Pei Hor, advisor)

Analytical Segmented T2 Correction Approach to Extract Intravoxel Incoherent Motion Perfusion Fraction

In Magnetic Resonance Imaging (MRI), functional information from the tissue can be derived using Diffusion-Weighted Imaging (DWI) performed with multiple weightings (b values) on the basis principle of intravoxel incoherent motion (IVIM) which allows both tissue microstructure and microcirculation (perfusion) to be investigated at once. Such information includes, Diffusion Coefficient (D_s), Perfusion Coefficient (D_f) (pseudo diffusion) and Perfusion Fraction (f) which have been used to detect disease, characterize lesions, evaluate organ functions, and assess treatment response of diseases. Despite this valuable insight, determination of IVIM model parameters remains a challenge. Several groups have reported that spin-spin relaxation (T_2 relaxation) rate differences between the tissue and flowing blood can introduce significant overestimation of f as a function of encoding time (TE) when using conventional fitting approaches. It was suggested in 2016 that f be estimated at different TE values and then extrapolated to TE=0 which greatly increases the scan time as the entire TE-b field needs to be acquired. In this work, we propose a new approach, called analytical segmented (AS-T_2) method, to extract f without the need to acquire the entire TE –b field; and compare it to the suggested one. Our proposed method reduces scan time.

10:25-10:45 **Mr. Devendra Khatiwada** (Venkat Selvamanickam, advisor)

Fabrication and Optimization of Single-Junction GaAs Thin Film Solar Cells on Epi-ready Flexible Metal Tapes for Low-cost Photovoltaics

Despite the high efficiency of III-V solar cells based on GaAs, their usage in large-scale terrestrial application is very limited due to the excessive cost of GaAs and Germanium (Ge) wafers. We have developed high-quality epitaxial semiconductor thin films on inexpensive flexible metal tapes to overcome the wafer cost as well as benefit from the lower manufacturing cost of roll-to-roll processing. Metal organic chemical vapor deposition (MOCVD) is used to grow high-quality epitaxial GaAs solar cell structure on 'single-crystalline-like' Ge film over an epi-ready buffer.

These grown thin films were further processed via photo-lithography, etching and contact deposition to fabricate 1J GaAs solar cell devices. Steps were taken to improve the quality of p/n junction by improving the quality of Ge template and incorporating an intrinsic layer with P-I-N solar cell structures. Solar cells fabricated with the improved processes showed a device efficiency of more than 13% at 1 sun with open circuit voltage (V_{OC}) of 650 mV, short circuit current density (J_{SC}) of 28 mA cm^{-2}, and fill factor (FF) of 72 %. These thin film GaAs photovoltaics, with further improvement in quality, can potentially lead to light-weight, inexpensive and scalable solar cell manufacturing.

This work is partially funded by the U.S. Department of Energy Sunshot Initiative award DE-EE0006711.

10:45-11:05 **Mr. Jie Chen** (Jae-Hyun Ryou, advisor)

Flexible Piezoelectric Generators and Pulse Sensors using Single-Crystalline III-N Thin Film

The flexible piezoelectric generator (F-PEG) and the flexible piezoelectric pulse sensor (F-PPS) were developed with single-crystalline group III-nitride (III-N) thin film, by transferring the as-grown thin film from the Si (111) substrate to a foreign flexible substrate. A large area and defect free flexible single-crystalline III-N thin film was obtained by this layer-transfer method. The III-N thin-film F-PEG can generate an open-circuit voltage of 50 V, a short-circuit current of 15 μA, and a maximum power of 167 μW with a corresponding optimum load resistance of 5 MΩ. The III-N thin-film F-PEG is able to directly power electronics such as light-emitting diodes and electric watches, and charge commercial capacitors and batteries. The III-N thin-film F-PPS is sensitive enough to convert the subtle deflection caused by the arterial pulse into electrical signal and detect the pulse waveform with detailed characteristic peaks from most arterial pulse sites. Both the F-PEG and the F-PPS showed high durability and stable outputs after being subjected to long-term tests. The flexible piezoelectric devices made from single-crystalline III-N thin films have great potential applications in future flexible wearable electronics, such as the energy harvesters and passive pulse sensors.

11:05-11:10 Break

11:10-11:30 **Mr. Geethal Gamage** (Zhifeng Ren, advisor)

Boron Arsenide Single Crystals with Unusually High Thermal Conductivity

Material with high thermal conductivity is beneficial to heat management and energy consumption of modern electronic devices. Most recent first principles calculations and our experimental efforts prove that zinc-blende boron arsenide (BAs) has unusually high thermal conductivity (exceeding 1100 W m^{-1} K^{-1} at room temperature), which breaks the long-held criteria that high thermal conductivity can only be observed in crystals consist of strongly bonded light elements. The basic mechanical, optical, electrical and thermal properties of this novel material are step-by-step investigated by proper methods. Though great progresses have been made, BAs single crystal growth is still extremely challenging. The uncontrollable growth rate, spontaneous nucleation, and unavoidable impurities lead to the formation of defects, which are embodied in the unneglectable variations of the measured properties and further inspire the optimizations of the growth process to obtain BAs single crystals with bigger size and better quality by series of trials to solve these problems. These findings not only arouse new insights into the physics of thermal transport, but also provide the fundamental information of BAs to play as an alternative in future upgrade industries due to its combination of favorable semiconductor performances and outstanding ability of heat dispersion for the first time.

11:30-11:50 **Ms. Sarah Aderyani** (Haleh Ardebili, advisor)

The Effect of Nanoscale Architecture on Ionic Diffusion in rGO/Aramid Nanofiber Structural Electrodes

Structural energy storage is a rapidly emerging area with tantalizing applications such as integrated devices in textiles, smart suits and uniforms. Due to several outstanding properties, graphene oxide (rGO)/ aramid nanofiber (ANF) composite material has emerged as a compelling choice as a structural electrode for supercapacitors and batteries. A key question of significant technological relevance pertains to what kind of nanoscale architecture motifs may lead to enhanced ionic diffusivity---the key characteristic dictating the overall performance of the electrode. In this study, we attempt to address this precise question, through multi-physics simulations, in the context of several *experimentally realizable* architectures. We investigate different arrangements for "layer-by-layer" and "house of cards" architectures, considering various degrees of waviness of the rGO nanosheets as well as various percentages of ANF polymer. Our results indicate that decreasing waviness of the rGO sheets can enhance the ion diffusivity in the staggered and aligned arrangements of the electrode

material, while this effect is stronger in staggered arrangement than aligned arrangement. Also, increasing the ANF percentage improves mechanical properties of the composite electrode, however it decreases the ionic diffusivity. The insights obtained from this study can lead to a more effective design of electrode architectures.

11:50-12:10 **Ms. Audrey Wang** (Yan Yao, advisor; undergraduate student)

An Ab Initio Investigation of Structure-Function Relationships in Solid-State Electrolytes

Solid-state electrolytes (SSEs), or superionic conductors, are a promising method of energy storage and a safer alternative to conventional Li-ion batteries. However, the ionic conductivities of most known SSEs, a characteristic integral to battery performance, are not yet commercially competitive. Ionic conductivity in SSEs is often achieved through the interstitial hopping of the mobile cation, so understanding the energetics of the crystal structure is important. The objective of this presentation is to use density function theory (DFT) to investigate the relationships between crystal structure and ionic conductivity of SSEs. Activation energies were calculated using DFT and nudged elastic band theory for sulfide and oxide frameworks with either lithium or sodium cations. The energy pathways generated in this study for the sulfur cases were consistent with previous findings that materials with body-centered cubic structures have the lowest energy barriers and thus have the highest ionic conductivities due to their homogenous tetrahedral sites.

SESSION II

Chair: **Dr. Bruce P. Strauss**, President, IEEE Council on Superconductivity; Treasurer, CCAS; Ret. DOE Office of Science

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12:45-1:05 **Mr. Zhoulyu Rao** (Cunjiang Yu, advisor)

Soft, Stretchable, and Wearable Devices from Fully Rubbery Electronic Materials

Soft wearable electronics with similar mechanical properties to the human skin were recently developed to overcome the mechanical mismatch between the rigid electronics and the soft skin. Soft stretchable electronics which are typically made of non-intrinsically stretchable materials are mainly achieved by structural engineering. Another approach is to build soft stretchable electronics from intrinsically stretchable electronic materials, which is advantageous in terms of scalable manufacturing, high mechanical robustness, low cost, and high-density device distribution. Thus, we build electronics based upon elastic rubbery electronic materials, namely, rubbery electronics, which has skin-like softness and stretchability. Our group previously innovated the rubbery conductor and semiconductor by composite engineering and fully rubbery electronics including sensors and transistors were also demonstrated. However, these devices showed a relatively low carrier mobility (~1 $cm^2/V{\cdot}s$) and rubbery integrated electronics were not constructed. To enable feasible usage, the rubbery semiconductor with a high effective mobility (~9.76 $cm^2/V{\cdot}s$), scalable manufacturing, and uniformity in device performance was developed. Moreover, fully rubbery transistors array and logic gates were also realized. As an application of these high-performance rubbery integrated electronics, a fully rubbery tactile sensing skin was further demonstrated.

1:05-1:25 **Mr. Yixuan Huang** (C.-S. Ting, advisor)

Charge Density Wave in One Dimensional Kondo Lattice Model

We report the existence of the charge density wave (CDW) in the one-dimension Kondo lattice model at zero temperature. The Kondo Lattice model describes a lattice of localized magnetic moments interacting with the itinerant electrons, which is the simplest model for the Heavy Fermion system. The CDW state is an ordered quantum fluid of electrons in a standing wave pattern. Based on our numerical results, we show that the CDW is driven by the effective Coulomb repulsion induced by the localized magnetic moments. The emergence of this phase could be used to explain the CDW found in the organic salts, which contains effective quasi-1D electron chains and localized magnetic moments.

1:25-1:45 **Ms. Sladjana Maric** (John H. Miller, advisor)

Formation of Proton Translocating Water Channels in Atp Synthase

F_1F_0-ATP synthase is a motor that converts energy from a proton gradient across the mitochondrial inner membrane into rotary and ultimately chemical energy. The hydrogen bond network within the entry and exit water channels in the *a*-subunit of F_0 portion of the motor enable proton translocation to and from the rotating *c*-ring. This talk highlights our studies of channel formation using molecular dynamics simulations. Quantitative analysis of water buildup in the half channels, hypothesized to promote and mediate proton translocation, was performed to characterize the half-channel formation along the *a-c* interface. The results elucidate possible proton pathways and reveal adverse changes affected by specific mitochondrial mutations.

1:45-1:50 Break

1:50-2:10 **Ms. Monica Martinez** (James K. Meen, advisor)

A Study of Unusual Fines in the Lunar Soil

Lunar regolith is the product of meteorite impact on both the lunar mare and highlands. Micrometeorites continually impact the lunar surface, melt it, and overturn its contents – a process called impact gardening. Additionally, solar wind and cosmic rays impact the surface materials. Precursor rocks derive the mineral content of the regolith, and agglutinate glasses dominantly consist of material derived from the minerals. Examination of the regolith fines reveals the presence of various phases that did not originate within the precursor materials and potentially provides insight into the regolith gardening process.

Fine-grained regolith collected by Apollo 17, from which glass spherules were removed, was sprinkled on mylar in a layer as near to one grain thick as possible. X-ray mapping was employed in a JEOL JSM-6330F SEM with an EDAX Octane Pro EDS and TEAM software.

Non-igneous species were observed throughout the characterization of the regolith. These species consist of calcium-rich sulfides, chlorides of inter-soluble potassium and sodium, native antimony, and calcium and titanium oxides. The nature of these species can be attributed to the temperatures reached upon impact of micrometeorites. These temperatures are high enough to achieve the volatilization of these elements, resulting in their eventual reaction and grain crystallization.

2:10-2:30 **Mr. Jonnalagadda Venu Sushir** (John C. Wolfe, advisor)

A Neutral Particle Lithography Tool for Resist Exposure and Direct Substrate Modification Below 10 nm

Neutral particle lithography (NPL) is a proximity printing technique where a broad-beam of energetic (30-50 keV) helium atoms illuminates a stencil mask and transmitted beamlets transfer the mask pattern to resist on a substrate. It has the advantages of ion beam proximity lithography including the possibility of direct modification of high temperature superconducting and magnetic thin films. Neutral atoms are immune to the charging artifacts that limit resolution and pattern fidelity in *ion*-based approaches. Ions are extracted from a multi-cusp ion source, accelerated and focused by a 2-electrode lens, and partially neutralized in a high pressure, charge transfer cell filled with thermal He gas. The critical design consideration is to minimize the bending of ion trajectories within the cell, as this increases the virtual source size to improve resolution.

Secondary electron diffusion begins to degrade resolution in thin resist for mask openings below ~5 nm and printing becomes impossible below ~4 nm. Thus, the domain for direct substrate modification begins with 5 nm feature sizes; Resist can be used for larger structures. The requirements of direct modification in the sub-10 nm range imply a very small source capable of producing the high flux density.

2:30-2:50 **Mr. Moein Adnani** (C. W. Chu, advisor)

Magnetoelectric Effect in New Type *II* Multiferroic $HoFeWO_6$

Multiferroic materials are a type of materials with at least two coexisting ferroic orders. As a result, they are a promising candidate to exhibit a strong linear magnetoelectric effect. This coupling of orders is important from technological point of view, since it has a potential for smaller and more efficient devices.

In this work, we investigated multiferroicity and magnetoelectric effect in $HoFeWO_6$ with a polar structure of $Pna2_1$. This compound shows an antiferromagnetic transition at T_N=17.8 K with an onset of ferroelectric transition at the same temperature. We found that the electric polarization starts to decrease by further lowering the temperature after the initial increase up to the temperature T*. We also observed that at lower temperatures it shows a magnetodielectric effect with double hysteresis behavior and an increase of ~3.5 % in dielectric constant where the effect disappears as temperature increases.

A proposed phase diagram was constructed from the measurements taken to date, however additional measurements are still needed to confirm as well as identify the order of the observed transitions and more importantly identify the underlying mechanism behind the observed ferroelectricity.

2:50-2:55 Break

SESSION III

Chair: **Prof. Anne Delcour**, Associate Dean for Graduate Studies, College of Natural Sciences & Mathematics; Professor, Department of Biology and Biochemistry

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2:55-3:15 **Mr. Fanghao Zhang** (Zhifeng Ren, advisor)

Electrostatic-Attraction-Induced High Internal Phase Emulsion for Large-Scale Synthesis of Amphiphilic Janus Nanosheets

Janus particles with asymmetrical chemical or physical properties exhibiting unique potential in multiple applications, thus is significantly demanded in recent years. However, the challenge of large-scale synthesis of amphiphilic Janus nanosheets remains unsolved after several attempts including template masking, phase separation, and selective modification methods, *etc.*. A high internal phase emulsion (HIPE), which contains a minimum internal phase volume fraction of 0.74, could improve the yield of interfacial reactions due to a higher interfacial area than non-HIPE counterparts. Furthermore, for water in oil (w/o) HIPEs, the reducing content requirement for organic phase ameliorate environmental and economic costs. In this work, we successfully synthesize Janus nanosheets on large scale *via* interfacial conjugation of graphene oxide (GO) with alkylamine by forming a w/o HIPE with a water-phase volume fraction of 0.8. The water-insoluble property of alkylamine achieves single-side hydrophobization of GO, rendering its amphiphilicity and Janus structure. This method not only simplifies the synthesis but also greatly increases the yield, *i.e.*, 100 wt% of GO fed, comparing to previous masking methods.

3:15-3:35 **Ms. Xiaojing Ma** (Arnold Guloy, advisor)

$Ce_5Ge_3O_x$ (x = 0.0 – 1.0): An Oxygen Interstitial Compound with Kondo-like Behavior

The Mn_5Si_3 structure is an attractive structure type in which chemical versatilities through the incorporation of interstitials allow the subtle exploration of the composition-property-electronic structure relationships in intermetallic compounds. Our studies on the oxygen interstitial chemistry of Ce_5Ge_3, with the Mn_5Si_3-type, led to the interstitial phase, $Ce_5Ge_3O_x$ ($0 \le x \le 1$). $Ce_5Ge_3O_x$ were synthesized by arc-melting, under controlled dilute-oxygen gas flow. Phase relationships were analyzed by powder X-ray diffraction, and chemical analysis were done by ICP-MS. The crystal structures of Ce_5Ge_3 and Ce_5Ge_3O were determined by single

crystal X-ray diffraction. Fourier map analysis and Raman spectroscopy confirm the absence of any oxygen in the binary Ce_5Ge_3. Contrary to previously published results magnetic measurements on $Ce_5Ge_3O_x$ ($x = 0, 0.2, 0.5, 0.8, 1$) indicate that Ce_5Ge_3 exhibits Curie-Weiss paramagnetism with no anomalous behavior. However, upon incorporation of oxygen in $Ce_5Ge_3O_x$ ($x > 0$), a Kondo-like magnetic behavior arises at low temperatures (2K -10K). This is consistent with previous reports on Ce_5Ge_3. The Kondo-like effect appears to increase with oxygen content; an optimum effect is observed with $x = 0.8$; it is suppressed with increasing magnetic field. Details of our studies will be presented.

3:35-3:55 **Mr. Rabin Dahal** (C. W. Chu, advisor)

Pressure-Induced Superconductivity and Doping-Tunable Structural Transition in Weyl Semimetal $Mo_{1-x}W_xTe_2$

Transition metal dichalcogenides $Mo_{1-x}W_xTe_2$ have generated much interest due to their reported topological properties and because their parent compounds, $MoTe_2$ and WTe_2, are reported to exhibit the Weyl semimetal state, large unsaturated magnetoresistance, and superconductivity. In addition, $Mo_{0.25}W_{0.75}Te_2$ has been confirmed to be a Weyl semimetal and should be tunable across the phase diagram. High-quality single crystals of $MoTe_2$ and WTe_2 were grown by flux method and $Mo_{1-x}W_xTe_2$ ($x = 0.10, 0.30, 0.40, 0.50, 0.70, 0.75$, and 0.90) were grown via chemical vapor transport method. Resistivity measurements up to 650 K were conducted using a home-made high-temperature resistivity probe and high-pressure measurements up to 17 kbar were performed using a BeCu clamp cell for selected doping compositions. With increasing W concentration, the structural transition temperature increased and was also suppressed under pressure. No superconductivity was observed in $Mo_{0.25}W_{0.75}Te_2$ down to 1.3 K or under pressure up to 17 kbar. However, superconductivity was induced in $Mo_{0.60}W_{0.40}Te_2$ with an onset T_c of 1.7 K under 8.4 kbar and in $Mo_{0.90}W_{0.10}Te_2$ with an onset T_c of 1.4 K under 3.9 kbar. As the T_c continuously increased with pressure for all samples, additional diamond anvil cell measurements are planned to explore pressure effects further.

3:55-4:00 Break

4:00-4:20 **Ms. Ya Zhuo** (Jakoah Brgoch, advisor)

Machine Learning Accelerates the Discovery of Efficient, Thermally Robust Inorganic Phosphors

Solid state light (SSL) is rapidly replacing incandescent and fluorescent lighting due to its high efficiency and long lifetime. The most common SSL combines a blue or near-UV LED with a rare-earth doped inorganic phosphor that down-converts the LED emission to longer wavelengths. The search for new phosphors has centered on host crystal structures that have a high Debye temperature (Θ_D), which indicates of a high photoluminescence quantum yield (PLQY). In addition, a large enough electronic band gap (E_g) of the host guarantees the rare-earth ion can down-convert light to the visible light region. This project is optimizing these two material parameters by using machine learning method to accelerate the discovery process of novel phosphors. Thousands of potential phosphor Θ_D are predicted using a support vector machine (SVM) model and their band gaps are obtained from density functional theory (DFT) calculation. Materials with the highest Θ_D and largest E_g are then selected for experimental analysis. Among those compounds, $NaBaB_9O_{15}$ shows outstanding $\Theta_{D,SVR}$ (729 K) and $E_{g,DFT}$ (5.5 eV). Substituting this material with Eu^{2+} yields UV excitation bands and a narrow violet emission. More importantly, $NaBaB_9O_{15}$:Eu^{2+} possesses a PLQY about 95% and excellent thermal stability.

4:20-4:40 **Mr. Jiahao Guo** (Kevin Bassler, advisor)

Reduced Network Extremal Ensemble Learning (RenEEL) Scheme for Community Detection in Complex Networks

Among the most basic and important problems in Network Science is to find the community, or modular structure within a network. This problem arises in many applications, including the analysis of gene network for targeting drug design. The most commonly used method of identifying this structure is to partition the nodes to maximize a metric known as Modularity. However, finding the particular partition that maximizes Modularity is a difficult NP-hard computational problem. We introduce a powerful

ensemble learning scheme for community detection. The scheme, an example of a Machine Learning algorithmic paradigm we call Extremal Ensemble Learning, uses iterative extremal updating of an ensemble of network partitions, found by a conventional base algorithm, to accurately find the node partition that maximizes modularity. At each iteration, core groups of nodes that are in the same community in every ensemble partition are identified and used to form a reduced network. Partitions of the reduced network are then found and used to update the ensemble. We use the method to analyze the community structure in a set of commonly studied benchmark networks and find that it outperforms all other known methods for finding the partition with maximum modularity.

4:40-5:00 **Mr. Hyunseok Sim (Shim)** (Cunjiang Yu, advisor)

Stretchable Elastic Synaptic Transistors and Neurologically Integrated Soft Engineering Systems

Synaptic devices that can be stretched like those appearing in soft bodied animals, such as earthworms, could be integrated onto soft machines towards enabled neurological functions. To date, stretchable synaptic transistors have never been reported. Here, we report for the first time a stretchable synaptic transistor fully based on elastomeric electronic materials, which exhibits a full set of synaptic characteristics. These characteristics were retained even when the artificial synapse is stretched by 50%. By implementing a stretchable synaptic transistor with a mechanoreceptor in an array format, we demonstrated a deformable neurologically integrated sensory skin, where the mechanoreceptors interface the external stimulations, generate presynaptic pulses and then the synaptic transistors render postsynaptic potentials. In addition, we developed a soft adaptive neurorobot which is able to perform adaptive locomotion based on synaptic memory in a programmable manner upon physically tapping the robotic skin. Our stretchable synaptic transistor and neurologically integrated soft engineering systems pave the way towards enabled neurological functions in soft machines and other soft applications.