UNIVERSITY of HOUSTON
TEXAS CENTER FOR SUPERCONDUCTIVITY

57th TcSUH Student Research Symposium

Thursday, April 28, 2022

Welcome & Student Presentations: 1:00 p.m. – 4:30 p.m.
University of Houston Science Center, Room 102

Outdoor Party/Southwest Fajitas Buffet: 4:30 p.m. – 6:30 p.m.

Agenda

Judges: Profs. Jiming Bao, Shuo Chen, Jarek Wosik
Chairs: Profs. Arnold Guloy, Di Chen, Lars Grabow
Prizes: 1 First Prize ($600); 2 Second Prizes ($300); 3 Third Prizes ($200). Winners eligible for TcSUH Travel Grants.

12:45 p.m. Soft Drinks, Juice, Water – 1st Floor Lobby

1:00 p.m. **Welcome, Introduction of Judges and Chairs, Guidelines for Review –** Zhifeng Ren, Director, TcSUH

1:10 p.m. **SESSION I** Chair: **Prof. Arnold Guloy, Chemistry**; Assistant Chair: **Fanghao Zhang**

1:10 – 1:25 **Mr. Congcong Xu**, Ph.D. student, Physics
(Prof. Zhifeng Ren, advisor)
Realizing high energy conversion efficiency in a segmented-$Mg_3(Sb, Bi)_2$/cubic-GeTe module for power generation

1:25 – 1:40 **Ms. Zhaoyang Chen**, Ph.D. student, Materials Science
(Prof. Yan Yao, advisor)
Constructing Favorable Microstructures in Solid-State Organic Cathodes via Mechanical Property Manipulation

1:40 – 1:55 **Mr. Mahesh Paidpilli**, Ph.D. student, Materials Engineering
(Prof. Venkat Selvamanickam, advisor)
Development of 50-meter Long High-Performance REBCO Tapes

1:55 – 2:10 **Mr. Trevor Bontke**, Ph.D. student, Physics
(Prof. Paul C.W. Chu, advisor)
Retaining Superconducting Phases Through Low-Temperature Pressure Quenching

2:10 – 2:20 Break / Drawing for Door Prizes

2:20 p.m.	**SESSION II**	Chair: **Prof. Di Chen, Physics**; Assistant Chair: **Fengjiao Pan**
	2:20 – 2:35	**Mr. Chenghao Wang**, Ph.D. student, Chemical and Biomolecular Engineering (Prof. Lars Grabow, advisor) **Revised activity descriptor for recombinative hydrogen desorption**
	2:35 – 2:50	**Ms. Ling-Hua Chang**, Ph.D. student, Physics (Prof. Chin-Sen Ting, advisor) **Phonon-mediated superconductivity in hole-doped hydrogenated monolayer-hexagonal boron nitride**
	2:50-3:05	**Mr. Zhongxin Liang**, Ph.D. student, Physics (Prof. Zhifeng Ren, advisor) **New insights into the effect of chemical bonding strength on thermoelectric performance and stability toward practical thermoelectric applications**
	3:05-3:20	**Mr. Nam-In Kim**, Ph.D. student, Materials Science and Engineering (Prof. Jae-Hyun Ryou, advisor) **Flexible Piezoelectric Sensor Made of Single-Crystalline III-N Thin Films for Personal-Healthcare and Extreme-Environment Applications**
	3:20 – 3:30	Break / Drawing for Door Prizes
3:30 p.m.	**SESSION III**	Chair: **Prof. Lars Grabow, Chemical and Biomolecular Engineering**; Assistant Chair: **Liqun Guo**
	3:30-3:45	**Ms. Ziyan Zhang**, Ph.D. student, Chemistry (Prof. Jakoah Brgoch, advisor) **Finding Superhard Materials Through Machine Learning**
	3:45-4:00	**Mr. Ken William Ssennyimba**, Ph.D. student, Physics (Prof. Di Chen and Prof. Wei-Kan Chu, advisors) **In-situ Thermal Property Measurement of Irradiated SiC/SiC Composites**
	4:00-4:15	**Mr. Nhất M. Ngo**, Ph.D. student, Chemistry (Prof. T. Randall Lee, advisor) **Stable Semi-Hollow Gold Silver Nanostar with New Optical Window and Superior Photothermal Performance**
	4:15–4:30	**Ms. Shruti Hariyani**, Ph.D. student, Chemistry (Prof. Jakoah Brgoch, advisor) **Advancing Human-Centric Lighting**
4:30 p.m.	**Closing Remarks** / Drawing for Door Prizes – Prof. Zhifeng Ren **Deliberation of Judges**	
4:35 p.m.	**Photo of all Presenters** *HSC 1st Floor Lobby, red wall*	

4:45 p.m. **Party on the Patio: Southwest Fajitas Buffet** (with drawings for Door Prizes)

Announcement of Symposium Winners Zhifeng Ren

Award Presentations & Photo of Prize Winners

Awards: First Prize (one prize): $600; Second Prize (two prizes), $300; Third Prize (three prizes): $200. Judges are selected from TCSUH Faculty members. Prizes will be awarded based on originality of research (25%), quality of research (25%), quality of presentation (25%), and skillful use of visual aids (25%). For fairness, the judges' decisions will be normalized so that undergraduates and graduates can compete on an equal footing. Cash prizes will not be presented at the Symposium. The winners will receive their cash prize as a supplement to their paycheck. Winners will be interviewed for a press release.

Door Prizes: Great door prizes from local merchants and restaurants will be given throughout the Symposium and buffet! Each attendee will receive a special ticket at the door and must be present to win.

ABSTRACTS

Each presentation is allotted 15 minutes, including 4-5 minutes for Q&A.

1:10 – 1:25 **Mr. Congcong Xu**, Ph.D. student, Physics (Prof. Zhifeng Ren, advisor)

Realizing high energy conversion efficiency in a segmented-$Mg_3(Sb, Bi)_2$/cubic-GeTe module for power generation

The performance of thermoelectric materials has increased dramatically in recent decades, enabling the concept of generating energy from waste heat through a solid-state thermoelectric device to be more realistic. Theoretically, a high zT_{avg} and a significant temperature difference between two sides of the device are necessary to boost energy conversion efficiency. However, employing the same material over a wide temperature range results in lower zT_{avg} due to the temperature dependence of thermoelectric properties. Therefore, constructing a multi-segmented module based on complicated parameter optimization to maximize the efficiency of the thermoelectric legs in their optimum operating temperature range becomes the development direction of the device structure. Motivated by this idea, we first fabricated a multi-segmented n-type $Mg_3(Sb, Bi)_2$ with low contact resistance buffer layers. We then designed a phase-transition inhibited cubic p-type GeTe of excellent thermoelectric performance to match the segmented n-type legs. The prepared segmented-$Mg_3(Sb, Bi)_2$/cubic-GeTe module exhibited a high conversion efficiency of ~12.8% under a temperature difference of ~480 K with the hot-side temperature of 773 K, which is comparable to the advanced thermoelectric modules. This work enriches the matching combination of n/p-type thermoelectric materials and further broadens the pools of potential candidates for segmented thermoelectric devices.

1:25 – 1:40 **Ms. Zhaoyang Chen**, Ph.D. student, Material Science (Prof. Yan Yao, advisor)

Constructing Favorable Microstructures in Solid-State Organic Cathodes via Mechanical Property Manipulation

Due to low environmental footprint and high material-level specific capacities, organic electrode materials have become competitive alternatives to inorganic materials for solid-state batteries (SSB). Additionally, the soft nature of organic compounds ensures intimate contact with solid sulfide electrolytes during cycling, which is beneficial for battery longevity. However, upon mixing and compression, the low-modulus organic materials and high-modulus sulfide electrolytes would form an unfavorable composite microstructure where electrolytes cannot form efficient ion conduction paths. This mismatch in mechanical property prevents a high fraction of organic compounds from being used in a solid-state cathode, limiting the energy density of organic SSB. Here we report the formation of favorable microstructures of organic cathodes by "softening" the sulfide electrolytes. Solvent treatment of the sulfide electrolyte Li_6PS_5Cl more than halves its modulus. As a result, the utilization of an organic material, pyrene-4,5,9,10-tetraone (PTO), is increased by 133.6% and 90.8% compared with cells with a re-hardened and the pristine Li_6PS_5Cl, respectively. The mass fraction of PTO can be improved from 20 to 40wt% while maintaining high utilization (85.7%). Our exploration of softened electrolytes builds the correlation among structure, mechanical property, microstructure engineering and battery performance. The strategy is applicable to other active materials with low modulus.

1:40 – 1:55 **Mr. Mahesh Paidpilli**, Ph.D. student, Materials Engineering (Prof. Venkat Selvamanickam, advisor)

Development of 50-meter Long High-Performance REBCO Tapes

A high engineering critical density (J_e) REBCO [(Gd, Y)$Ba_2Cu_3O_{7-\delta}$)] coated conductor has an immense potential to increase the magnetic field and reduce the cost of the ultra-high-field magnets. We have demonstrated short REBCO samples with J_e in high magnetic fields 5.2x times that of commercial tapes. The imminent goal was to scale up these high-performance samples to 50-meter lengths. This work addresses the engineering challenges associated with the scale-up of 4+ µm thick REBCO films in a single pass using Advanced metal organic chemical vapor deposition (A-MOCVD). Dropouts or variations in the critical current along the length of long tapes have been correlated with process parameters of Advanced MOCVD. After the desired modification of the tool based on the correlation, we produced uniform, long REBCO tapes in our R&D A-MOCVD tool. Later, we transferred this knowledge to a pilot-scale A-MOCVD manufacturing tool to make 50-meter long REBCO tapes with film thickness over 4 µm in a single pass. A compositional map was constructed to fabricate 50-meter tapes with uniform critical current (I_c) over 1,750 A/12 mm at 65 K, 0.25 T, and 3000 A/12 mm at 4.2 K, 20 T, respectively.

This work is supported by the U.S. Department of Energy Advanced Manufacturing Office award DE-EE0007869 and the U.S. Department of Energy Office of High Energy Physics award DE-SC0016220

1:55 – 2:10 **Mr. Trevor Bontke**, Ph.D. student, Physics (Prof. Paul C.W. Chu, advisor)

Retaining Superconducting Phases Through Low-Temperature Pressure Quenching

In the past six years, the discovery of superhydride systems with critical temperatures (T_cs) that approach and exceed room temperature has pushed the field to new heights. Unfortunately, this novel room-temperature superconductivity (RTS) requires pressures in excess of 260 GPa, inhibiting its application outside academia. One of the greatest challenges remaining in the field of superconductivity is inducing and retaining RTS while lowering or removing the pressure. As a potential solution, we developed a low-temperature, pressure-quenching technique which we successfully used to retain superconducting phases in Bi and also FeSe and $Cu_xFe_{1-x}Se$. Quenching at 77 K and 4.2 K from pressures up to 26.6 GPa, we retained Bi phases with varying T_cs corresponding to Bi-II, -III, and -V, as well as some ambiguous and novel phases, including a new record T_c of 9.07 K. Similarly, we successfully retained superconducting phases with T_cs up to 37 K in FeSe and 27 K in $Cu_xFe_{1-x}Se$. Furthermore, the retained superconducting phases of these materials exhibited good stability at low temperature. In particular, $Cu_xFe_{1-x}Se$ exhibited perfect stability for at least seven days when quenched and kept at 77 K, retaining a T_c of ~25 K.

SESSION II Chair: **Prof. Di Chen, Physics**

2:20 – 2:35 **Mr. Chenghao Wang**, Ph.D. student, Chemical & Biomolecular Engineering (Prof. Lars Grabow, advisor)

Revised activity descriptor for recombinative hydrogen desorption

The widespread adoption of water electrolysis using renewable energy for the sustainable production of H_2 is hindered by the scarcity and high price of Pt, the catalyst of choice for the hydrogen evolution reaction (HER). The high catalytic activity of Pt for HER has been attributed to its optimal binding strength of hydrogen. The empirical correlation between the metal-hydrogen binding strength and HER activity was first reported by Parsons and later popularized by Nørskov. Despite its widespread adoption, however, the optimal activity requirement of $\Delta G=0$ has shortcomings. Zero coverage values are often unrealistic and attempts to estimate ΔG near saturation coverage are futile because thermodynamics dictate $\Delta G=0$ at equilibrium. We observed that the two H* atoms involved in the Tafel step on equilibrated surfaces typically bind in two different types of sites. When using the binding energy difference ($\Delta\Delta G$) between the weaker and stronger binding sites as descriptor instead. Notably, we identified several SAAs which have significantly lower E_a than expected and could be interesting candidates for further investigations. Overall, the kinetics of the Tafel step are rigorously captured by $\Delta\Delta G$ as alternative descriptor, as it conforms to thermodynamic principles and removes ambiguity in choosing surface coverages for DFT calculations.

2:35 – 2:50 **Ms. Ling-Hua Chang**, Ph.D. student, Physics (Prof. Chin-Sen Ting, advisor)

Phonon-mediated superconductivity in hole-doped hydrogenated monolayer-hexagonal boron nitride

The two-dimensional electron system in a honeycomb lattice has attracted huge attention since its single-layered atomic structure was realized by experiment. Monolayer-hexagonal boron nitride (h-BN), which is such an electronic system, has been theoretically shown to be a phonon-mediated superconductor by applying tensile strain and injecting holes into the strained sample. In this work, using the first principle calculation, we studied the effect of hydrogenation on the pristine h-BN and predicted that the hole-doped H_2BN becomes a phonon-mediated superconductor with a transition temperature above the boiling point of liquid hydrogen at the carrier density of 1.0×10^{14} holes cm^{-2} and higher. Applying biaxial tensile strain stabilizes the atomic structure when the carrier density goes higher than 1.0×10^{14} holes cm^{-2}. The high T_C originated from the higher electron density of states at the Fermi level and the phonon frequency associated with in-plane motion of B, N, and H atoms.

2:50 – 3:05 **Mr. Zhongxin Liang**, Ph.D. student, Physics (Prof. Zhifeng Ren, advisor)

New insights into the effect of chemical bonding strength on thermoelectric performance and stability toward practical thermoelectric application

The current consensus is that the chemical bonding in a thermoelectric material should be weakened as much as possible to obtain a lower lattice thermal conductivity and thus a higher thermoelectric figure of merit, *zT*. However, the consequent reliability issues, such as inferior structural stability and mechanical brittleness, are rarely emphasized. Here, experimental studies on p-type $YbMg_2Bi_2$-based compounds demonstrate the advantageous effects of chemical bonding stiffening toward practical applications. Despite the stronger chemical bonding in Sb-alloyed $YbMg_2Bi_2$, the compound still exhibits lower lattice thermal conductivity than its parent $YbMg_2Bi_2$ compound, as well as a comparable average *zT*, due to rigorous point defect scattering. More importantly, chemical bonding toughening guarantees better maintenance of thermoelectric performance under high temperatures and improved mechanical hardness, both of which are essential for the durable operation of thermoelectric generators. This research provides a new way of thinking about chemical bonding engineering toward practical thermoelectric applications.

3:05 – 3:20 **Mr. Nam-In Kim**, Ph.D. student, Materials Science & Engineering (Jae-Hyun Ryou, advisor)

Flexible Piezoelectric Sensor Made of Single-Crystalline III-N Thin Films for Personal Healthcare and Extreme-Environment Applications

We recently demonstrated high electromechanical conversion efficiency and mechanical flexibility from single-crystalline Group-III-nitride (III-N) semiconductor thin films which already possess excellent properties of thermal and chemical stability, no harm to human body and environments, and radiation hardness. The properties make the film an ideal choice for piezoelectric devices that are flexible, biocompatible, efficient, and robust to overcome the limitations of the existing piezoelectric devices. In this study, we developed the flexible piezoelectric sensors (FPS) for the applications in personal healthcare monitoring systems and extreme environments. First, we describe the FPS as a pressure sensor in harsh conditions. The sensor is attached on a diaphragm at high temperatures, which is connected to high pressure. The output voltages are measured and analyzed with temperature using intrinsic carrier concentration and Young's modulus effects. Second, the arrayed FPSs are attached on the human face (temple area) and the response signals are collected for eye blinking and eyeball movements. Any abnormality is related to brain disorders. Third, the surface-functionalized FPS is described to measure the concentration of the human stress hormone. Cortisol from the sweat of the stressed human body is monitored by the change of resonant frequency. The sensor shows excellent sensitivity and selectivity.

SESSION III Chair: **Prof. Lars Grabow, Chemical and Biomolecular Engineering**

3:30-3:45 **Ms. Ziyan Zhang**, Ph.D. student, Chemistry (Prof. Jakoah Brgoch, advisor)

Finding Superhard Materials Through Machine Learning

The budding field of materials informatics has enabled a shift towards artificial intelligence to discover functional materials. Superhard materials are essential in applications ranging from manufacturing to energy production. Finding new superhard materials has traditionally been guided by empirical design rules derived from classically known materials like diamond, *c*-BN, and, more recently, ReB_2. In practice, the measured hardness decreases asymptotically as the load increases, and the origin of this effect is not well understood. To address this challenge, we constructed a supervised machine learning model capable of directly predicting load-dependent hardness based only on chemical composition. Ensemble learning algorithms, including Gradient Boosting (GB) and XGBoost (XGB) trees, are employed to maximize the sparse hardness data collected from the literature. The predictive power of our model was validated with experimental data and showed a remarkable reproduction of the Vickers hardness at various loads. The trained model was then used to screen the Pearson's Crystal Data (PCD) set and combined with our recently developed machine-learning phase diagram tool to identify unreported high hardness compounds. This directed discovery method is poised to modernize the search for new superhard materials benefiting from the efficient, scalable, and transferable nature of machine learning.

3:45 – 4:00 **Mr. Ken William Ssennyimba**, Ph.D. student, Physics (Prof. Di Chen, Prof. Wei-Kan Chu, advisors)

In-situ Thermal Property Measurement of Irradiated SiC/SiC Composites

Leveraging clean energy sources such as nuclear energy holds great potential for an emission-free future. For that reason, research on the commercialization of next-generation reactors is of high interest. These will be generation-IV reactors that will be safer, cost-efficient, and long-lasting. Examples include the gas-cooled fast neutron reactors, whose complex design poses various challenges to R&D regarding the development of materials, such as SiC/SiC composites which are a candidate for cladding and use as structural components in extremely hot, corrosive, and high irradiation environments. The development of such materials has been significantly stunted by slow and costly testing methods for their irradiation-dependent properties. In this study, we innovatively attempt to address this problem through an *in-situ* laser-assisted technique combined with multiphysics simulations. We predict the changes in thermal conductivity of carbon irradiated SiC/SiC composites at 300ºC. Our results not only depict thermal conductivity trends in agreement with those reported in other research but also shed light on the potential of our technique in the prediction of irradiation-induced properties of materials in a faster and more precise fashion.

4:00 – 4:15 **Nhất M. Ngo**, Ph.D. student, Chemistry (Prof. T. Randall Lee, advisor)

Stable Semi-Hollow Gold Silver Nanostar with New Optical Window and Superior Photothermal Performance

Semi-hollow gold-silver nanostars (hAuAgNSts), a new type of plasmonic nanostar, were fabricated via a facile method at mild conditions. The bimetallic nanostar opened a new operational window in the UV-visible region of the electromagnetic spectrum, providing a good complement to the active window of gold nanostars (AuNSts) in the near-infrared region. The active spectral band of hAuAgNSts can be tuned easily and reliably with a composition-based approach. This method makes it easier to control the activity of the new bimetallic nanostars compared to the complex size-based tuning method conventionally used for AuNSts. The new bimetallic nanostars also exhibited good stability compared to AuNSts, even at elevated temperatures and without the need for surface modification. Importantly, the hAuAgNSts demonstrated superior photothermal performance compared to AuNSts and other plasmonic nanoparticles, endowing them with great potential for applications in targeted non-invasive anticancer and antiviral treatments. The bimetallic nanostars, with their new operational window and inherently great enhancement property, also enable promising use in ultra-sensitive viral, bacterial, or toxin detection as well as in photovoltaics and photocatalysis.

4:15–4:30 **Ms. Shruti Hariyani**, Ph.D. student, Chemistry (Prof. Jakoah Brgoch, advisor)

Advancing Human-Centric Lighting

Lighting accounts for 22% of total US electrical energy use, which translates to a $50 billion/year industry. Replacing incandescent and fluorescent light bulbs with phosphor-converted LED-based technology is one of the most accessible opportunities to reduce electricity consumption worldwide. Current LED light bulbs down-convert blue LED emission using red- and green-emitting phosphors to create a broad-spectrum white light. However, LEDs are not problem-free. Long-term exposure to blue LED emission over-activates photoreceptors in the eye to continually suppress melatonin production, causing insomnia and mood disorders. This talk will investigate the production of 'human-centric' light that minimizes blue light exposure by using a violet LED and inorganic phosphors. This methodology, however, requires the discovery of new blue-emitting phosphors that are readily excited by violet light to produce a bright blue emission. We recently discovered a new blue-emitting phosphor, $Na_2MgPO_4F:Eu^{2+}$, which possesses nearly all the requirements for violet LED-based lighting, including excellent violet light absorption, a high quantum yield, and zero thermal quenching. Incorporating this material into a prototype LED light bulb demonstrates our ability to produce a warm-white light with a higher color rendering index than a commercially purchased LED light bulb while significantly reducing the intensity of blue light emitted.