

2013 George A. Jeffrey NanoExplorers Symposium

Tuesday, August 20, 10 a.m. – 5 p.m.

SLC 1.102, The University of Texas at Dallas

Schedule

10:00 **Opening Remarks**
Ray Baughman, Robert A. Welch Professor of Chemistry and Director, Alan G. MacDiarmid NanoTech Institute

Section A: Chair Austin Howard

- 10:10 (A1)** **Nitinol Films: Characterization Studies and Production of Free-standing Films**
Sophie Druffner, Monica Jung DeAndrade
- 10:22 (A2)** **SPIE: An Integrative RNA-seq Pipeline for Optimized Processing of RNA-seq Data**
Raahil Sha, William Su, Ashwinikumar Kulkarni, Yuxuan Liu, Yunfei Wang, Pradipta Ray, Michael Zhang
- 10:34 (A3)** **Exploring Mechanisms of VNS-Induced Enhancement of Conditioned Fear Extinction**
Catherine Jojo, Monica Lou, Amanda Alvarez, Shawn Willett, Bethany Dempsey, Kimberly Griffin, Lindsey Noble, Yousef Abdel-Raziq, Winson Chiu, Christa McIntyre
- 10:46 (A4)** **Stabilization of Immiscible Polymers with Structure Directing Metal Organic Frameworks (MOFs)**
Brianna Loomis, Nimanka P. Panapitiya, John P. Ferraris
- 10:58 (A5)** **Nitric Oxide Release from Electrospun Matrimid for Enhanced Wound Healing**
Taylor Trinh, Elise Cai, Alysia Lowe, Kenneth J. Balkus Jr.
- 11:10 (A6)** **Synthesis of Periodic Mesoporous Organosilica (PMO) for Enhanced Drug Delivery**
Jessica Hong, Alicia D'Souza, Imalka Munaweera, Kenneth J. Balkus Jr.
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Section B: Chair Na Li

- 11:22 (B1)** **Compatibilization of Macroscopically Phase Separated Immiscible Polymer Blends by Metal Organic Frameworks for Novel Gas Separation Membranes**
Rahim Noorani, Nimanka P. Panapitiya, John P. Ferraris
- 11:34 (B2)** **Preparing Mixed Matrix Membranes for Gas Separation**
Peter Nguyen, Edson Perez, John P. Ferraris, Kenneth J. Balkus, Jr. and Inga H. Musselman

- 11:46 (B3) **Fabrication of Porous Carbon Nanofibers for Supercapacitors Using Polybenzimidazole with Colloidal ZIF-8 Nanocrystals**
Shashwat Chaturvedi, Nimali Abeykoon, John P. Ferraris
- 11:58 (B4) **Dye-Sensitized Solar Cells: New Structures and Components for Greater Efficiency**
Mokshin Suri, Zharkynay Kuanyshbekova, Anvar Zakhidov
- 12:10 (B5) **Vertical Organic Field Effect Transistors with Carbon Nanotube Electrodes**
Jeffrey Chang, Jonathan Yuen, Alexander Cook, Joseph Micheli, Anvar Zakhidov
- 12:22–1:20 *Lunch Break*
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Section C: Chair Shaoli Fang

- 1:20 (C1) **Size Dependence of Magnetocaloric Materials and Potential Application as Energy Harvester**
James Bradford, Nathanael Mayo, Ali Aliev, Ray Baughman
- 1:32 (C2) **Harvest Waste Heat Through Electrochemical Thermocell**
Sneha Kurada, Na Li, Ray Baughman
- 1:44 (C3) **Energy Harvesting through Humanoid Robot**
Daniel Moore, Alec Burns, Yonas Tadesse
- 1:56 (C4) **Electroactive Shape Memory Composites: Synthesis and Characterization of A Novel Class of Smart Material**
Keith Chan, Cary Baur, Justin Sipes, Javier Fernandez-Han, Dennis W. Smith
- 2:08 (C5) **Upper Extremity Orthotic Powered By Artificial Muscle**
Piper Knudsen, Richard Rome
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Section D: Chair Marcio Dias Lima

- 2:20 (D1) **Synthesis and Characterization of Poly (acrylonitrile-co-N-vinylimidazole-co-styrene) terpolymer**
Sairaj Sajjath, Samsuddin Faisal Mahmood, Dennis W. Smith
- 2:32 (D2) **Testing Various Synthesis Conditions for Metal-Organic-Framework (MOF) Adsorption Optimization**
Ashwin Hari, Christina Thompson, Fei Li, Arosha Karunathilake, Ronald Smaldone
- 2:44 (D3) **Post-Polymerization Functionalization of Fluorinated Arylene Vinylene Ether (FAVE) Polymers**
Cara Santucci, Yash Patel, Remya Menon, Jingbo Wu, and Dennis W. Smith, Jr.
- 2:56 (D4) **Synthesis of Cyclic Diacetylenes by Topochemical Reaction**
Tony Jiang, Xiuru Xu, Ray Baughman
- 3:08 (D5) **Preparation and Application of PUA Aerogels**
C. Carter, L. Mamo, H. Churu, A. Lee, A. Hayes, M. Garci, and H. Lu
- 3:20–3:40 *Break*

Section E: Chair Carter Haines

- 3:40 (E1) Cryogenics and Applications to Characterization of Superconductivity**
Shailen Patel, Austin Howard, Jonathan Yuen, Anvar Zakhidov
- 3:52 (E2) Negative Differential Conductance (NDC) and Quantum Tunneling in Silicon CMOS Devices**
Sreekar Molakalapalli, Clint Naquin, Mark Lee
- 4:04 (E3) Effects of Processing Conditions on the Properties of SmMn₂O₅ Mullite Catalysts**
Vanessa Ibarra, Sampreetha Thampy, Alex Lee, Julia Hsu
- 4:16 (E4) Sound Generation Using Encapsulated Thermoacoustic Projectors**
Sachit Menon, Ali E. Aliev
- 4:28 (E5) Electroless Silver Deposition onto Polymeric Substrates**
Preethi Raju, Carter Haines, Ray H. Baughman
- 4:40 Closing Remarks and Certificate Ceremony**

2013 NanoExplorers Symposium Abstracts

(A1) Nitinol Films: Characterization Studies and Production of Free-standing Films

Sophie Druffner, Monica Jung DeAndrade

Nitinol (NiTi) is a metallic shape memory alloy of nickel and titanium at about 1:1 atomic ratio. Films of NiTi were prepared by bilayer depositions of nickel and titanium either on a silicon or polymeric (polymethylmetacrylate and polyvinyl alcohol films) substrate by sputtering followed by thermal treatments between 500-600°C in vacuum or argon. Samples were subsequently characterized by X-ray diffraction (XRD) to ascertain the presence of NiTi crystalline phases. The samples that showed martensite in their XRD diffractograms were then selected to measurements of electrical resistance versus temperature. For these experiments, samples were heated on a hot plate from room temperature to around 100°C. A thermocouple was placed tangent to the sample in order to monitor the temperature at the film, while a multimeter was used to monitor the electrical resistance change through the films with increasing temperature. Additionally, tests to obtain free-standing films were performed by dissolving the polymeric substrates formerly tested. The selected films showed during heating that the alloy began to crystallize to austenite at about 74°C and finished crystallization at around 79.5°C. During cooling, martensite started at about 48.5°C and finished crystallization at approximately 44°C. These transformation temperatures can slightly shift by 5-10°C higher temperatures when thermally treated at 550°C. In conclusion, the presence of martensite phase was successfully confirmed for samples thermally treated between 500-550°C by XRD analyses and temperature-dependent electrical resistance measurements of the films. Free-standing films were also effectively produced.

(A2) SPIE: An Integrative RNA-seq Pipeline for Optimized Processing of RNA-seq Data

Raahil Sha, William Su, Ashwinikumar Kulkarni, Yuxuan Liu, Yunfei Wang, Pradipta Ray, Michael Zhang

With the rapid development of next generation RNA sequencing algorithms, various tools have been created to allow users to analyze such RNA-seq data for read mapping, transcriptome assembly, expression quantification, and comparison of transcriptomes. Most of these tools rely on the UNIX command line for input and have clearly defined input and output formats, which makes them ideally suited for building computational pipelines. We present SPIE (next generation Sequence Processing using an Integrative Environment), a GUI-based tool for generating a pipeline from the various RNA-seq tools, scheduling the computation on multiprocessor systems, and automatically delivering an integrated report of the in-silico experiments to the user.

As the first goal of the project, we aim to create a robust graphical user interface to assist biologists in pipelining a sequence of RNA-seq tools, by choosing the tool of their choice for mapping, assembly, and downstream analysis. SPIE can be used to specify the parameters, load and save pipeline configurations, and automatically monitor pipeline errors. Written in Java, SPIE is multiplatform and can be run both as a standalone application or can be used as a part of a client-server infrastructure, allowing users on non-UNIX based operating systems access to tools that are native to UNIX.

Second, while most RNA-seq tools have multithreading capabilities, they are not inherently optimized for multiprocessor environments. To allow for a faster turnaround while running these pipelines, a framework was built to utilize parallel multiprocessor cluster infrastructure to decrease runtime. We present a map-reduce like environment for splitting input jobs into smaller pieces, simultaneously processing many small jobs on the cluster using the CONDOR job scheduling environment, and merging the results back together. This allows for a multi-fold speedup over traditional serial processing using these tools.

In the future, analysis will be performed on public datasets to discover strengths and weaknesses of similar tools using probabilistic framework. We plan to compare Tophat and OLEGO amongst mapping tools, MISO and Splicetrans amongst Splicing analysis tools, MISO and Cufflinks for isoform level analysis tools, and DESeq and Cufflinks for differential expression analysis. Careful analysis of the differences in the outputs of these tools could lead to characterization of pipelines which can automatically pick the best performing tools based on our dataset and genes of interest. Such ensemble-based RNA-seq analysis can lead to future biological discoveries.

With special thanks to: Kotamari, Aaron; Wang, Yu; Zhao, Xiaoping; Churu, Gitogo; Wu, Jie; and the rest of the Zhang Lab

(A3) Exploring Mechanisms of VNS-Induced Enhancement of Conditioned Fear Extinction

Catherine Jojo, Monica Lou, Amanda Alvarez, Shawn Willett, Bethany Dempsey, Kimberly Griffin, Lindsey Noble, Yousef Abdel-Raziq, Winson Chiu, Christa McIntyre

Emotionally arousing events often enhance long-term memory consolidation. In stressful events, the adrenal glands release epinephrine, which activates the release of norepinephrine in the brain. The norepinephrine attaches to receptors in the amygdala, which modulates memory storage and synaptic plasticity in other regions of the brain, including the hippocampus. Understanding the circuitry and molecular mechanisms underlying memory storage could potentially lead to the development of a cure for pathological anxiety disorders. Post-traumatic stress disorder is a pathological anxiety disorder in which patients associate a trigger with an aversive memory. Many psychologists treat this disorder with exposure therapy where patients are taught, through repeated exposure, that this trigger will not lead to immediate harm. Unfortunately, anxiety is only reduced temporarily. The present study used a rat model of exposure therapy to test a potential adjunct therapy aimed at enhancing the efficacy of exposure therapy. Rats were fear conditioned to associate a conditioned neutral stimulus (tone) with an aversive unconditioned stimulus (foot shock). After fear conditioning, rats were given fear extinction training paired with vagus nerve stimulation (VNS). Stimulation of the vagus nerve causes the release of norepinephrine in the brain, resulting in amygdala activation and further leading to enhancement consolidation of new long-term memories. As in exposure therapy, rats were exposed to the conditioned stimulus without any unconditioned stimulus. During exposure to the conditioned stimulus, rats create a new memory, in which the cue is associated with safety. When vagus nerve stimulation was paired with fear extinction, the effectiveness of fear extinction was enhanced. To investigate what proteins are involved in these biological mechanisms, brain tissue was removed from rats, synapses were isolated from the brain tissue, and then western blot analysis was performed. Through imaging of western blots, the types of proteins and their densities were analyzed and have allowed for a better understanding of the specific proteins that change in the brain, supporting the exposure-induced change in behavior. Understanding the proteins involved in long-term memory consolidation may lead to the development of more effective treatments for stress-related memory disorders.

(A4) Stabilization of Immiscible Polymers with Structure Directing Metal Organic Frameworks (MOFs)

Brianna Loomis, Nimanka P. Panapitiya, John P. Ferraris

Global energy demand and environmental pollution have become major concerns of modern society. H₂ has become an alternative source of energy and during industrial H₂ manufacturing a mixture of gasses is generated including greenhouse gasses like CO₂. For the separation of these gasses currently used

methods are energy intensive and costly. Therefore membrane-based gas separation has become an attractive alternative. Mixed-matrix membranes (MMMs) have evolved as a superior membrane material over the conventional membranes but has reached a performance plateau. We believe a novel membrane microstructure can improve gas separation performances and in this work two high performance immiscible polymers were blended with colloidal ZIF-8 to obtain the targeted membrane microstructure. Colloidal ZIF-8 was synthesized and characterized with XRD, TGA and ATR-FTIR spectroscopy. For the component polymers both a commercially available and a synthesized polymer were used. Then the membranes with and without colloidal ZIF-8 were fabricated using an automatic membrane applicator. Fabricated membranes were characterized with SEM imaging and ATR-FTIR spectroscopy. The MMMs with colloidal ZIF-8 had a more uniform microstructure compared to the membranes without ZIF-8, suggesting an enhanced compatibility between the polymers. The gas separation properties of the fabricated membranes were determined with a custom built gas permeameter. Considering the superior gas separation properties and unique pore apertures of MOFs, this work may open up opportunities to produce novel materials for membrane based separations.

(A5) Nitric Oxide Release from Electrospun Matrimid for Enhanced Wound Healing

Taylor Trinh, Elise Cai, Alysia Lowe, Kenneth J. Balkus Jr.

In the body, nitric oxide (NO) functions as a physiological enhancer of diastolic blood flow and plays a significant role in the regulation of blood flow, aggregation of platelets, and transmission of neurological pathways. NO is naturally synthesized in the body by the enzyme nitric oxide synthase (NOS). In addition, NO plays a role as a bioregulatory agent in healing infected wounds and regulating antimicrobial activity. Due to its ability to regulate physiological functions, there is growing interest in NO drug delivery for a wide range of biomedical applications, such as the synthesis of bandages that are capable of the controlled release of NO to enhance wound healing.

Electrospun fibers of Matrimid/Dimethylformamide (DMF) were crosslinked with Diethylenetriamine (DETA). The electrospun Matrimid with DETA was loaded with NO. During this loading process, diazeniumdiolates, or NONOates, the donor group, was bound to the secondary amine of Matrimid/DETA. Nitrogen gas was flowed with a relative humidity of 85% into the sample chamber containing the Matrimid/DETA NONOate, which flowed into a water bath of 37°C to simulate human body temperature conditions. As the humidified air reacted with the sample, 2 molar equivalents of NO per NONOate were released. The gaseous NO was converted into dissolved NO₂⁻ (nitrites) and Griess Reagent was used to detect nitrite concentrations. Pink Azo Dye formed and allowed for the quantification of NO using UV Visible Spectroscopy.

From our current results, it can be seen that upon exposure to humidity, the Matrimid fibers gradually released an average of about 80 μmol/g of NO over a period of seven days. With these results, it can be concluded that bandages that are capable of the controlled release of NO to enhance wound healing can be synthesized.

(A6) Synthesis of Periodic Mesoporous Organosilica (PMO) for Enhanced Drug Delivery

Jessica Hong, Alicia D'Souza, Imalka Munaweera, Kenneth J. Balkus Jr.

Many therapeutic agents today often have problems dealing with low solubility and physiological obstacles, preventing usage of the preferred route or at all. To help prevent unwanted side effects, a drug delivery vehicle could be applied to deliver a payload to the targeted site.

Therefore, our project aimed to synthesize periodic mesoporous organosilica (PMO) to use as a delivery system. PMOs are silica based mesoporous materials with both organic and inorganic materials contained in the channel walls. Benefits of such a structure include high surface area, tunable pore size, easily modified surface, and biocompatibility. The incorporation of the organic groups into the walls versus hanging groups in the channels allows maximum loading capacity. Additionally, the use of organic groups creates hydrophobicity within the channel walls, compatible to many drugs found today.

To create the PMOs, we utilized surfactant mediated synthesis. After testing different surfactants and precursors, we selected cetylpyridinium bromide as the surfactant and 1,4-bis(triethoxysilyl)benzene as the precursor. This formed periodicity and a pore structure suitable for drug delivery. Using FT-IR and SEM, we determined the proper formation of silica and a uniform sphere size of approximately 40 to 50 nm in diameter, appropriate for drug storage. Furthermore, an ideal pore structure was seen in the TEM images. In conclusion, we have successfully synthesized PMOs capable of drug storage and delivery, beneficial to current treatments in the medical field.

(B1) Compatibilization of Macroscopically Phase Separated Immiscible Polymer Blends by Metal Organic Frameworks for Novel Gas Separation Membranes

Rahim Noorani, Nimanka P. Panapitiya, John P. Ferraris

Mixed-matrix membranes (MMMs) have been used as an efficient and cost-effective method to separate gas mixtures. To further improve the gas permeability properties of MMMs, the use of an immiscible polymer blend as the matrix has been investigated as a novel approach. The premise is that by blending a highly gas selective polymer with a highly gas permeable polymer, the performance of the MMMs can be enhanced. The highly permeable 6FDA based polyimide (P1), was synthesized and characterized with ¹H NMR spectroscopy, ATR-FTIR spectroscopy, and TGA and GPC techniques. With the commercially available highly selective polymer (P2) the blend membranes were fabricated using an automatic membrane applicator. In the preliminary investigation, it was found that in pure polymer blend membranes the two polymers macroscopically phase separate. In order to increase the miscibility between these polymers, a metal organic framework (MOF) was used as a nanoparticle. In this study synthesized colloidal ZIF-8 was used as the MOF. Not only does ZIF-8 increase the miscibility between the polymers, but it can increase the gas separation properties of the MMMs. Fabricated flat membranes were characterized with SEM imaging and ATR-FTIR spectroscopy. Gas separation properties of the membranes were determined with a custom built gas permeameter. The MOF-filled immiscible blend membranes had more uniform microstructure compared to the pure polymer blend. In this project, the ability of MOFs to function as a compatibilizer was demonstrated, and this discovery will lead to novel materials for membrane based separations.

(B2) Preparing Mixed Matrix Membranes for Gas Separation

Peter Nguyen, Edson Perez, Kenneth J. Balkus Jr.

Abstract

Objective: The objective was to synthesize NH₂-MIL-53 and ZIF-8 nanocrystal for the preparation of NH₂-MIL-53/VTEC and 35% ZIF-8/PBI mixed matrix membranes for gas separation. Second objective was to prepare Matrimid to test the High Pressure High Temperature permeability at different pressure.

Procedure:

Matrimid

Matrimid was prepared by mixing Matrimid in chloroform and stirred for 1d. Then the solution was casted at 150micron using automatic sheen applicator. The membrane was then dried at RT for 3hrs and at 150°C for 1d in the vacuum oven.

NH₂-MIL-53

The NH₂-MIL-53 was prepared by mixing 1.74g Al(NO₃)₃•9H₂O and 1.02g of aminoterephthalic acid together. The mixture was refluxed in water at 100°C for 9hr. After 9hr, the NH₂-MIL-53 was filtered and reflux in dimethylformamide(DMF) at 100 °C for 1d. The solid was then retrieved by using a soxhlet extraction and activated in the vacuum oven at 150°C for 1d.

Preparing NH₂-MIL-53 in VTEC:

The NH₂-MIL-53 was then dispersed in VTEC and casted using an automatic sheen applicator. Then the membrane was dried under nitrogen at 70°C for 3hrs and then in the vacuum oven at 150°C for 1d.

ZIF-8/PBI

Zeolitic imidazolate framework-8(ZIF-8) was activated at 100°C for 1d in a vacuum oven. Then, .14g of ZIF-8 was then mixed with 2.5g of dimethylacetamide. The solution was then stirred at 80°C and bath sonicated alternatively for 4hrs. The ZIF-8 was precoated with 20% of PBI and stirred and bat sonicated for another 4hrs. Then the rest of PBI was added and further mixed for 10min using the Resodyn LabRam Acoustic Mixer. The extra solvent was then removed from the final mixture at 80°C with nitrogen purge. The membrane was casted at 150 microns using an automatic sheen applicator and dried under nitrogen at 80°C for 2.5 hrs. The membrane was further dried at 50°C for 5 hrs, 80°C for 12hrs, 140°C for 12hrs, followed by 180°C for 12hrs, and 240°C for 1d.

Result: Still Pending

Significance: Result will prove that mixed matrix membranes could be alternative to inorganic membranes for gas separation.

(B3) Fabrication of Porous Carbon Nanofibers for Supercapacitors Using Polybenzimidazole with Colloidal ZIF-8 Nanocrystals

Shashwat Chaturvedi, Nimali Abeykoon, John P. Ferraris

Supercapacitors are among the most promising electrochemical energy devices of today, as they are able to charge incredibly fast and last for a long time. However, supercapacitors currently are not able to replace batteries because of their lower energy storage capability. A supercapacitor derives its name from the fact that it is similar to a conventional capacitor, but it has two porous electrodes immersed in the electrolyte and can also store much more energy. The primary reason for this difference is because of the porous carbon electrodes; supercapacitors rely on the interactions between these electrodes and ions dissociated in a electrolyte to store energy and release it. Much of the research on supercapacitors is concentrated around increasing their energy density by using high surface area electrodes. The primary focus of this research is fabricating porous carbon nanofibers from electrospun polybenzimidazole (PBI) and zeolitic imidazolate framework 8 (ZIF-8) with varying weight loadings of colloidal ZIF-8 (10%, 20%, and 50% wt). The electrospun mats were stabilized at 450°C to prevent premature decomposition. Afterwards, the mats were carbonized at varying temperatures for one hour and then placed under CO₂ activation for an additional hour. Coin cell devices using the porous carbon electrodes aforementioned were fabricated, and cyclic voltammetry and charge-discharge tests were conducted. A specific capacitance of 65.5 F/g was observed at a high scan rate of 100 mV s⁻¹, and an energy density of approximately 27.0 Wh kg⁻¹ was observed at a current density of 1 A g⁻¹ for the 20% ZIF-8/PBI. These results indicate

the growing potential of supercapacitors; as more research is conducted, the observed energy densities of supercapacitors should inevitably increase, bringing about a profound change in our energy storage capabilities.

(B4) Dye-Sensitized Solar Cells: New Structures and Components for Greater Efficiency

Mokshin Suri, Zharkynay Kuanyshbekova, Anvar Zakhidov

Dye-Sensitized Solar Cells (DSSCs) can transform the solar energy industry by providing a potentially cost effective and practical alternative to conventional silicon based solar cells. The DSSC is a relatively new technology that uses abundantly available material thus making it cost effective. This research analyzes different structures and components of DSSCs with the goal of increasing photo-electric conversion efficiency.

The basic DSSC incorporates a transparent conductive oxide layer as the working electrode, multiple layers of TiO₂ particles, a layer of dye, an electrolyte layer, a catalyst layer, and a counter electrode. Using this framework, multiple types of the DSSC are created, including: a conventional FTO glass based DSSC, a photonic crystal based DSSC, and a fiber-based DSSC. These different types of DSSCs differ in their basic structure and components. For example, the FTO glass based DSSC uses two pieces of FTO glass as the electrodes with layers of TiO₂, dye, and catalyst between the glass pieces. The DSSC is sealed with a plastic gasket and the electrolyte is injected through a hole in the counter electrode. These conventional DSSCs are up to 7.1% efficient. The photonic crystal based DSSCs is created by similar processes except that a photonic crystal thread was used as the counter electrode. These DSSCs are around 2% efficient, and prove that photonic crystals are a promising new component of solar energy. Finally the fiber based DSSC uses CNT yarn as the working electrode and a photonic crystal thread based counter electrode. These fiber based DSSCs are up to 4.58% efficient and have promising future applications.

This research shows that the DSSC can be fabricated in various structures; thus proving the DSSC to be a highly versatile invention in the solar energy industry. While there are several challenges with the efficiency and life span of DSSCs, the initial results of this research are quite promising. However, it is recommended that further research be conducted to refine the fabrication process and to evaluate other structure and component options for DSSCs. The applications of the DSSC are highly impactful, promising, and endless. The FTO glass based DSSCs can be used in solar panels, fiber based DSSCs can be integrated into the textile industry, and flexible DSSCs can be used in thin films and plastic goods. Furthermore, by using more economical electrodes and catalysts, the DSSC has the potential to become more cost effective than conventional silicon based solar cells. In the future, when this new technology is implemented at the commercial level, it will positively affect the economy, aid the ailing environment, and benefit global energy relations.

(B5) Vertical Organic Field Effect Transistors with Carbon Nanotube Electrodes

Jeffrey Chang, Jonathan Yuen, Alexander Cook, Joseph Micheli, Anvar Zakhidov

In this project, the development of an improved organic field effect transistor was attempted, one that would allow precise control of device current. The creation of such a device would have a large advantage over the typical transistor structure in terms of current density. The device described is termed a vertical organic field effect transistor (VOFET), in which charge injection in a source-drain channel is controlled via modulation of the work function of the drain electrodes. This is done through capacitive gating of the electrode, which is a carbon nanotube (CNT) sheet. The large surface area to bulk volume ratio of the CNTs enable enough charges to be induced in the CNTs to modify its work function. In our device

configuration, we have utilized a CNT-based ionic liquid supercapacitor for gating. We have successfully implemented an "Always-On" transistor, but an "Always-Off" device was sought after in order to provide a default of near zero current passing through the transistor, with current passing through only when desired.

To carry out this objective, a variety of devices using different of organic semiconductors and thicknesses were created and tested. This was done to determine their efficacy and adherence to normal transistor current voltage (IV) characteristics, i.e. a starting linear region abruptly transitioning into a saturation region after a few volts. Devices were created on an ITO (Indium Tin Oxide) glass substrate, with either a PEDOT:PSS or a ZnO/TiOx blend deposited on top using spin coating. Next, a variety of organic semiconductors (P3HT, PCBM, or Si PCPDTBT) were spun-coated. With all of the polymers deposited, carbon nanotubes were laid on the substrate to create drain and gate electrodes. Ionic liquid was deposited on the CNT electrodes and sealed with a glass cover slide. The finished device was then tested with a Keithley 4200 Semiconductor Characterization System, which applied gradual amounts of gate voltage to the device in order to measure the resulting source-drain current. The tests provided large amounts of data that were then processed and plotted to understand the details of the device performance.

The tests revealed a definite transistor trend; however, the devices' performance was not ideal, as the transitions from linear to saturation were gradual, or not present. It was seen that an "n-type" organic semiconductor, such as PCBM performed better than a "p-type" one, such as P3HT, but still did not fully exhibit transistor properties. Thicker coats of the polymer, achieved with slower spin speeds, were also found to enhance performance, due to decreased potential for leakage current. While some tests showed promise, more research is needed to find out the reasons for this difference. By optimizing current polymers and testing new ones, better data will be gathered that could eventually lead to the development of an optimal "Always-Off" field effect transistor.

(C1) Size Dependence of Magnetocaloric Materials and Potential Application as Energy Harvester

James Bradford, Nathanael Mayo, Ali Aliev, Ray Baughman

Magnetocaloric materials are substances that exhibit a strong change in entropy upon heating and cooling, and conversely an adiabatic temperature by introducing an external magnetic field. We explored the size dependence of magnetocaloric materials on the change in entropy as a function of temperature. Increasing the surface area per volume of the particles by decreasing their size enables a more efficient heat exchange between the particles and an external fluid, which could be advantageous in a refrigeration device. Through hand grinding on an agate block and a sedimentation process, we created particles of a Gd₅Si₂Ge₂ alloy between 1 and 50um. We measured samples of a certain particle size range in the Magnetic Property Measuring System (MPMS). Our results indicate that, as a general rule, as the particle size decreases, so does the peak of the isothermal entropy change ($-\Delta S$). Our bisrolled samples and powder only samples, though, both exhibited roughly the same Curie temperature (270K) regardless of particle size.

We also explored an energy-harvesting device using magnetocaloric materials. By placing a magnetocaloric material near an induction coil and varying the temperature of the magnetocaloric material, we can create a varying magnetic field that generates a potential difference across the inductor via electromagnetic induction. We modeled a testing device after a transformer and created it by coiling a copper wire into a planar spiral inductor and running an AC current through a second coil hanging directly above to induce a magnetic field. In preliminary testing, the potential difference in the planar solenoid depended on the frequency of the applied voltage, as expected, but we observed only a significant po-

tential difference in frequencies above 4 kHz. We also performed crude calculations on the maximum efficiency of a transformer to estimate the secondary coil efficiency, and the efficiency of the magnetocaloric material responsible for creating a varying magnetic field. For the transformer at high frequencies, we calculated the power efficiency as roughly 98%, however, for our magnetocaloric material, we used the DSC to calculate an ideal efficiency of roughly 37%. Further research into this device would include fabricating a sheet with hundreds of coils using photolithography and testing its efficiency, as well as determining an optimal temperature range and frequency that a magnetocaloric can respond to.

(C2) Harvest Waste Heat Through Electrochemical Thermocell

Sneha Kurada, Na Li, Ray Baughman

Waste heat is a type of renewable energy source. Multiple ways were developed in order to harvest waste heat. An electrochemical thermocell utilizes the potential difference made by a redox couple with a temperature difference, and eventually converts heat directly to electricity. Seebeck coefficient describes how much potential difference can be achieved when there is 1 K of temperature difference. In order to attain a high efficiency of the thermocell, a redox couple with a higher Seebeck coefficient is demanded. Usually Potassium Ferrocyanide and Potassium

Ferricyanide are used in this application where there is a Seebeck coefficient of 1.4 mV/K. In this work, we studied the effect of different chelation groups to the Seebeck coefficient of Fe II/Fe III redox couple, and discovered that it changed from 1.0 mV/K to 2.0 mV/K. This may give an insight of how to design redox couples with a high Seebeck coefficient. Another important question is to how to maintain a sufficient temperature difference in the thermocell. For this purpose, a salt bridge was developed and the performance of thermocell was studied.

(C3) Energy Harvesting through Humanoid Robot

Daniel Moore, Alec Burns, Yonas Tadesse

Humanoid Robots have capabilities ranging from rehabilitation to entertainment. As the human race advances, robots are becoming more pragmatic and feasible. One unexpected, yet useful function is the capacity to harvest energy through mechanical movement. The aim of this project is to expand upon the energy harvesting potential of humanoid robots. Work was also conducted to test the limitations of 3D printers. The purpose of this additional work was to evaluate the effect of noise and vibration on 3D printed products.

(C4) Electroactive Shape Memory Composites: Synthesis and Characterization of A Novel Class of Smart Material

Keith Chan, Cary Baur, Justin Sipes, Javier Fernandez-Han, Dennis W. Smith

Thermally responsive shape-memory polymers (SMPs) are smart materials that change shape with the application of thermal stimulation. The shape memory process involves straining a material to a temporary, stressed state, followed by a recovery back to the original shape upon heating. These materials can be used in applications such as shape and position control, vibrational dampening, impact damage, ergonomic devices and biomedical implants. Other materials considered "smart" are those that change in dimension with the application of voltage, referred to as piezoelectric material. This phenomenon occurs through the induction of internal stress resulting from electron displacement when placed under a

field. These materials are commonly used in sensing and actuating applications such as pressure sensors, active acoustic and vibrational dampening, low-voltage switches, structural monitoring, and biomedical devices.

In this study, the piezoelectric effect and the shape memory phenomenon are combined to create a novel class of smart material, namely electro-active shape memory polymer composites. This novel composite was created in hopes that the material could be remotely controlled for different applications such as for use in medical instruments, knives to circumvent sensitive areas in the body. To create this polymer composite, a thiol-ene reaction between Tris[2-(3-mercaptopropionyloxy)ethyl] isocyanurate (TMICN) and 1,3,5-Triallyl-1,3,5-triazine-2,4,6(1H,3H,5H)-trione (TATATO) was used as the shape memory polymer system, and piezoelectric Na_{0.5}Bi_{0.5}TiO₃-BaTiO₃ (NBTBT) nano-whiskers were dispersed within the polymer. After the composite was fabricated without error, basic composite material testing was conducted. The composite was tested with differential scanning calorimetry (DSC) to determine the glass transition temperature, which is vital to future applications using the electro-active polymers. In our research, the ideal glass transition temperature was around thirty-two degrees Celsius. In addition, SEM (Scanning Electron Microscopy) was performed on the material to analyze homogeneity and aggregations of the nano-sized ceramic particles. Furthermore, shape memory performance testing was conducted to see the material's total strain recovery. Additionally, experimentation on the composite's temperature change in response to DC and AC currents at varying voltages and frequencies was conducted. Finally, a bimorph was created using the polymer composite to amplify the mechanical strain induced upon the system, and thus to better characterize movement and shape-memory phenomenon. This research is significant because a remotely controlled material can bypass "hands on" programming and thus enabling many currently unattainable microelectronic, microcontrol, or biological applications.

(C5) Upper Extremity Orthotic Powered By Artificial Muscle

Piper Knudsen, Richard Rome

The purpose of our project was to research and create a prototype of an upper extremity orthosis that enables the wearer to preform acts of daily life.

The orthosis was designed as a bi-layered glove. The over glove will be completely cosmetic and, therefore, was ignored for the initial prototype; while the under glove, necessary to tie down the tendon system, was prototyped with a leather-gardening glove. Flexor tendons run from fingertip to elbow with rubber guide channels to secure them to the under glove. Because the actuators have not been completed, the tendons are manually controlled. The orthosis will make everyday life much easier with pre-programmed macros activated by a push of a button, or a flick of the wrist.

Continued to completion, this orthosis could be incredibly useful for stroke patients and patients with degenerative nerve disease.

(D1) Synthesis and Characterization of Poly (acrylonitrile-co-N-vinylimidazole-co-styrene) terpolymer

Sairaj Sajjath, Samsuddin Faisal Mahmood, Dennis W. Smith

Styrene-acrylonitrile (SAN) copolymers have begun to find widespread commercial applications due to the combination of unique properties of polystyrene (low cost and optical clarity) and the excellent mechanical properties of polyacrylonitrile. The addition of acrylonitrile, however, significantly raises glass transition of the copolymer, and therefore production temperature. We aim to lower the glass transition temperature, and thus increase the melt processability, of the copolymer through the incorporation of

vinylimidazole. Previously, melt processable poly acrylonitrile(AN)-co-vinylimidazole(VIM) polymers of different compositions were successfully synthesized by free radical polymerization and showed applicability in carbon fiber, super capacitors and in nitric oxide (NO) releasing suture and bandages with enhanced wound healing properties. Here, we present the synthesis and characterizations of a new novel terpolymer, poly (acrylonitrile-co-N-vinylimidazole-co-styrene) AN-VIM-Sty, with molar feed ratio of 80:15:5 for AN: VIM: Sty. The polymer was characterized through NMR, ATR-FTIR, GPC, DSC, and TGA. The monomers successfully reacted in a ratio of 80.5:14.5:5; the polymer was stable up to 310°C in both N₂ and air and had a glass transition of approximately 114°C. These results demonstrate that the AN-VIM-Sty terpolymer exhibits both melt processability and high thermal stability.

(D2) Testing Various Synthesis Conditions for Metal-Organic-Framework (MOF) Adsorption Optimization

Ashwin Hari, Christina Thompson, Fei Li, Arosha Karunathilake, Ronald Smaldone

Metal Organic Frameworks (MOF) are hybrid inorganic-organic structures whose porosity and robustness may be used in industrial, gas storage applications. A series of synthesis conditions has been tested in order to discover the relationship between different synthesis factors and crystal development, as well as to optimize MOF synthesis for commercial applications.

Firstly, the metal precursor was varied among a set of samples and tested for MOF optimization. Secondly, a set of pre-existent as well as newly altered organic ligands were tested for possible effect on crystal quality. Thirdly, independent as well as solvent mixtures were tested for the development of an optimal synthesis site. Fourthly, variant amounts of air pressure as well as temperatures in an oven and microwave environment were applied during the synthesis process to discover any potential, thermodynamic correlation. Finally, the possibility of post-synthesis modification of the resulting MOF structures was tested under various solvent and heating environments. All of the above tests were performed under a solvothermal process: the organic ligand and metal precursor were integrated through a solvent mixture, heated under the various environments, filtered, and stored in a vacuum dessicator.

The resultant samples were tested through Nuclear Magnetic Resonance Imaging, Fourier Transform Infrared Spectroscopy, and Porosity tests to determine chemical composition, porosity, and their potential for use in gas adsorption applications. Results confirm the existence of relationships between the above conditions and the final MOF precipitate; the data reveals possibilities in optimizing and targeting certain gas hosts through varying metal and organic constituents as well as the synthesis environment. Data also reveals the possibility in deliberate variation of synthesis conditions for a diverse set of crystalline structures.

(D3) Post-Polymerization Functionalization of Fluorinated Arylene Vinylene Ether (FAVE) Polymers

Cara Santucci, Yash Patel, Remya Menon, Jingbo Wu, and Dennis W. Smith, Jr.

Methyl ester pendant Fluorinated Arylene Vinylene Ether (FAVE) copolymers and terpolymers were prepared via step-growth polymerization from commercially available starting materials. Hydrolysis of the ester moieties to carboxylic acids was performed in quantitative yields post-polymerization. DCC coupling was employed to append a variety of functionalities to the polymer backbone including: a non-linear optical chromophore (DR-1), an alkene, an alkyne, an Anthracene moiety, and a POSS cage. All polymers were confirmed by ¹H and ¹⁹F Nuclear Magnetic Resonance (NMR) spectroscopy. Bulk polymeric properties were analyzed by differential scanning calorimetry (DSC), thermogravimetric analysis

(TGA), gel permeation chromatography (GPC), Fourier transform infrared spectroscopy (FTIR), and ultraviolet/visible spectroscopy (UV/Vis).

(D4) Synthesis of Cyclic Diacetylenes by Topochemical Reaction

Xiuru Xu, Tony Jiang, Ray Baughman

Despite the widespread interest in producing carbon nanotubes (CNTs) of one type, scientists have yet to come up with a synthetic route to specific targeted nanotubes. Here we propose a topochemical route to specific armchair SWNTs that uses solid state-polymerization of cyclic diacetylenes to form organic hydrocarbon nanotubes which can be transformed into carbon nanotubes of one type. For an armchair nanotube (n, n), the cyclic monomer must possess $8n$ carbon atoms. In our current work, An one-step synthesis of cyclic diacethlenes products has been developed that relies on the Eglinton Coupling reaction with 1,7-octadiyne. The crude was dissolved in chloroform and purified by silica gel column starting with hexanes/benzene (4:1) mixture. Columns were monitored by TLC using cerium molybdate stain. At least 8 products were isolated by gradient elution. The structures of the products are established by ^1H and ^{13}C NMR, raman spectroscopy, and mass spectroscopy. This synthetic route provides new opportunities for exploring armchair single wall carbon nanotubes.

(D5) Preparation and Application of PUA Aerogels

C. Carter, L. Mamo, H. Churu, A. Lee, A. Hayes, M. Garci, and H. Lu

Monolithic polyurea aerogels were synthesized by controlling the ratio of isocyanate/water/catalyst (Et3N) in acetone, and were dried using a low surface tension solvent (pentane). Multiple physical properties were tested: density, contact angle of water droplet, compressive strain, tensile strain, and sound impedance. Compressive and tensile strain of the 26/94 (N300A to Acetone) PUA was tested under quasi-static loading conditions. Both its compressive strength and tensile strength were relatively high for aerogels. The density of the aerogel varied between 0.016 and 0.7 g/cc, increasing with the concentration of isocyanate, which affects the nanomorphology of the material. The contact angle of water was also dependent upon the concentration of isocyanate with a correlation of low density to low hydrophobicity. Sound impedance was tested by passing frequencies ranging from 500Hz-20KHz through an aerogel box made with the ratio of 26 g of Desmodur N3300A to 94 mL of acetone and compared to that of multiple boxes made with other materials such as wood, Styrofoam, and acoustic foam. The sound impedance of the 26/94 aerogel is many times greater than the materials over the range of frequencies tested. These unique acoustic qualities of the 26/94 PUA aerogel combined with its mechanical properties allow it to be used as a versatile acoustic insulator.

(E1) Cryogenics and Applications to Characterization of Superconductivity

Shailen Patel, Austin Howard, Jonathan Yuen, Anvar Zakhidov

Characterization of superconductors (materials which exhibit no electrical resistance) require cooling them below their critical temperature. The highest recorded critical temperature of a superconductor is still only 150 K (-123 C). Most superconductors have much lower critical temperatures than that and reaching and maintaining these temperatures and lower (down to 4 K, or -270 C) is the goal of cryogenics, and in particular a device called a cryostat. In this presentation, we will discuss different cryogenic technologies, explain the installation and operation of a new cryostat that was installed, and give examples of the use of the cryostat in characterization of superconductors.

(E2) Negative Differential Conductance (NDC) and Quantum Tunneling in Silicon CMOS Devices

Sreekar Molakalapalli, Clint Naquin, Mark Lee

Transistors have revolutionized the world since their development in the early 1950's. Field-effect transistors in particular have become ubiquitous in modern electronics due to their high input resistance and low noise output. There has been much research conducted regarding Silicon CMOS devices as they form the cornerstone of integrated circuits and are built with specialized transistors (MOSFETS). However there is a dearth of knowledge regarding the explicit characterization of quantum tunnelling processes that can occur within these devices. The purpose of our research was to understand the conditions in which we can achieve negative differential conductance (NDC) and whether that NDC peak correlates to a quantum bound state.

We conducted our measurements using the Agilent 4156C Semiconductor Parameter Analyzer and a Lakeshore cryogenic probe station. We tested Silicon CMOS transistors that incorporate a double-barrier quantum well structure with gate lengths that varied from 35-45 nm. Quantum well structures exhibit a quantization of energy levels that can be experimentally observed as sharp changes in the current response to an applied potential. Current-voltage (IV) measurements were conducted in temperatures that varied from 4 K-298 K. Under these conditions we were able to see NDC peaks near room temperature by forward-biasing the substrate and sweeping the gate potential. Without this "body biasing" technique, NDC peaks would generally begin to appear around 150K. These peaks would become more defined at lower temperatures, which supports our current understanding of quantum well formation. We also tested for a response to high-magnetic fields by applying a field of 1-2 T. The field was produced by a superconducting magnetic coil housed beneath the probe station. We found no noticeable change in peaks using the magnet but more tests are required for a definitive conclusion. The NDC peaks observed on these devices can potentially be attributed to resonant tunneling, whereby electrons tunnel through the double barrier quantum well structure found in the NMOS region of the device. When the quantized energy levels inside the quantum well match the potential difference between the source and drain terminals, a large increase in current is observed. A smaller gate length also appears to increase the number of quantum well states that occur at higher temperatures.

The application of these discoveries could greatly improve the performance of Silicon CMOS devices and in turn produce quicker and more efficient processors/logic gates. A way to optimize our devices is to assess their peak to valley ratio and determine the conditions required for implementation. Future research includes conducting more measurements with varying temperatures, gate lengths, body biases, etc. and numerically solving Schrodinger's equation for a realistic potential profile that will assist in designing the next generation of devices.

(E3) Effects of Processing Conditions on the Properties of SmMn₂O₅ Mullite Catalysts

Vanessa Ibarra, Sampreetha Thampy, Alex Lee, Julia Hsu

Complex metal oxides containing the rare earth Mn-mullite compound SmMn₂O₅ were recently shown to be effective catalysts for the oxidation of nitrogen oxides, a major pollutant in diesel exhaust. The SmMn₂O₅ compound is made through the co-precipitation synthesis method at a controlled basic pH range of 9.50 to 10.00 followed by calcination at high temperatures, which is a simple technique that is amenable for industrial scale production. However, there is currently limited knowledge about the correlation among the processing conditions for the mullite, its physical properties, and its catalytic activity. Higher crystalline states are preferable because a more pure SmMn₂O₅ compound with less amount of perovskite impurity phases is produced. The degree of crystallinity is determined using x-ray diffraction

by comparing the results to reference data of the mullite phase and various perovskite phases. High surface area is also preferable because it allows more area for the reaction to take place, increasing its catalytic activity. The specific surface area is measured using N₂ physisorption isotherms. We present a study aiming to better understand how varying processing conditions affect the crystallinity and catalytic activity of SmMn₂O₅. A sample of SmMn₂O₅ prepared at the normal pH range of 9.50 to 10.00 was divided and calcined to temperatures of 750°C, 800°C, and 1000°C. Four samples of SmMn₂O₅ were also prepared at varying pH ranges of 8.00 to 8.20, 8.90 to 9.20, 9.65 to 9.80, and 10.20 to 10.35. Analysis of the experimental data showed that a narrow range of processing conditions exist which yields crystalline mullite SmMn₂O₅ compound and high surface area, both of which should lead to an increase in catalytic activity. An improved understanding of the relationship between processing and properties of SmMn₂O₅ should pave the way toward the adoption of rare earth Mn-mullite catalysts for various real-world applications.

(E4) Sound Generation Using Encapsulated Thermoacoustic Projectors

Sachit Menon, Ali E. Aliev

The performance of thermoacoustic projectors using free-standing carbon nanotube sheet is extended for thin film, flexible and transparent loudspeaker applications. The protective encapsulation of free-standing CNT sheets in inert gases using different transparent and flexible polymer and inorganic films as vibrating membranes is studied. We provide an extensive experimental study of acoustic, thermal and electrical performance of such loudspeakers for different thermodynamic regimes. Various drawbacks exist to use of such loudspeakers; primarily, the nanoscale thickness of CNT sheets, their high sensitivity to the environment, and the high surface temperatures practical for thermoacoustic sound generation. We address these here by placement of two protective films around free-standing CNT sheets with the intent of creating small, nearly flat, transparent, flexible loudspeakers. Although use of protective films rectifies the previously mentioned problems, it significantly reduces both effective frequency range and efficiency. Thus, we studied a wide variety of experimental procedures in order to determine how films can be used and which films can be used to limit the drops in effective frequency range and efficiency. Factors tested include dependence on surface area of films, thickness of films, compliance (based on spacing between the two films), and number of layers of CNT sheets in film. Measurements were also taken varying with the distance of the sound generator from the microphone and with differing-band microphones. Polycarbonate, polyimide, and glass films were tested, with a control of an open CNT sheet. For all samples, sound pressure (Pa/W) was measured with regard to frequency of vibration (kHz) and sound pressure (Pa) was measured with regard to input power (W). Decrease in surface area corresponded to increase in efficiency due to decrease of flexural modes. Decreasing the film thickness led to increased efficiency in a much wider effective frequency range (~0.3-60 kHz) compared to thicker films' effective frequency range (~0.3-20 kHz). In general, increasing the number of CNT sheet layers decreased efficiency greatly. Finally, changing the spacing between the films did not seem to have much of an effect. Further research into changing the films to diminish the loss of efficiency and the narrowing of the effective frequency range could eventually lead to thermoacoustic nanotube-using loudspeakers replacing a number of current technology speakers, in applications such as cell phones and laptops.

(E5) Electroless Silver Deposition onto Polymeric Substrates

Preethi Raju, Carter Haines, Ray H. Baughman

Polymers are widely used because of their many important properties such as high strength, low cost, and long life. Building on these attributes, UT Dallas has recently pioneered polymer fiber artificial muscle re-

search. These polymer muscles can actuate repeatedly (contract and expand) when heated and cooled. However, polymers are naturally non-conductive, which restricts their use as electrically heated artificial muscles. Although commercially metal-plated polymer fibers exist, they increase cost and complexity, in addition to coming in limited forms. Therefore, we investigate a simple method to coat common polymers with silver using electroless deposition. Our process includes cleaning, etching/ sensitization, and plating. Using extremely dilute solutions based on Tollen's reagent reactions, we have successfully plated polymer substrates including nylon, polyethylene, and PVDF. In addition to testing different chemicals used in these solutions, we study how time, temperature, and agitation affect plating rate and silver deposition. Using our optimized method, we find resulting polymer fibers have rather uniform silver coatings. 2.4 mm diameter nylon monofilaments display resistances as low as 0.1 ohms per centimeter. Furthermore, plated polymer fibers can withstand coiling, heating, and bending. In addition to plating individual polymer fibers, molded or textile polymers can be silver plated and then electrically actuated, as we demonstrate with silver plated nylon fabric. Possible applications of conductive polymer fibers range from textile, medical, industrial, electronic, and decorative uses. In this study, we also briefly analyzed the ability of silver-plated polymer catheters to limit bacterial growth.