



2017

Advanced Materials for Energy and Bioengineering Applications II



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DEC 4TH 2017

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**Advanced Materials for Energy and Bioengineering Applications (AMEBA)
Symposium Program
Dec 4th, 2017
Silver Maple Ballroom, Davis Center 401, University of Vermont**

8:30 AM - 8:55 AM **Healthy Start Continental Breakfast**

Morning Session I

Session Chair: Madalina Furis (Univ. of Vermont)

- 9:00 AM - 9:25 AM** **Tsukasa Yoshida** (Yamagata University, Chem Eng)
Solution-based organic and hybrid charge-transfer absorbers for solar cells
- 9:25 AM - 9:50 AM** **Ian Baker** (Dartmouth College, Engineering)
The Microstructure and Mechanical Properties of Alumina-Forming Austenitic Stainless Steels
- 9:50 AM - 10:15 AM** **Shawana Hollen** (University of New Hampshire, Physics)
Correlating atomic-scale structure with device-scale properties in 2D materials
- 10:15 AM - 10:40 AM** **Chengfeng Ke** (Dartmouth College, Chemistry)
Hierarchical Co-assembly Enhanced Direct Ink Writing
- 10:40 AM - 11:05 AM** **Coffee Break**

Morning Session II

Session Chair: Matthew White (Univ. of Vermont)

- 11:05 AM - 11:30 AM** **Martin Kaltenbrunner** (Johannes Kepler University)
Soft Electronics and Machines with Tough Hydrogels
- 11:30 AM - 11:55 AM** **Severin Schneebeli** (University of Vermont, Chem. & Mat. Sci)
Directing Electrophilic Aromatic Substitution Reactions from Above and Underneath Aromatic Rings
- 11:55AM - 12:20 PM** **Jenna Taft** (University of Vermont, Chemistry)
Heterogeneous catalysis using metal-doped porous nanoparticles
- 12:20 PM - 1:25 PM** **Lunch Break**

Afternoon Session I

Session Chair: Shawna Hollen (Univ. of New Hampshire)

- 1:25 PM - 1:50 PM** **Adrian Del Maestro** (University of Vermont, Physics)
Entanglement area law in superfluid 4He
- 1:50 PM - 2:15 PM** **Katherine A. Mirica** (Dartmouth College, Chemistry)
Ultra-thin van der Waals Materials
- 2:15 PM - 2:40 PM** **Jie-Xiang Yu** (University of New Hampshire, Physics)
Non-trivial topology in two-dimensional systems
- 2:40 PM - 3:05 PM** **Yang Li** (University of Vermont, Phy & Mat. Sci.)
Thermal-Expansion Effects on the Optical and Carrier-Transport Properties of Solution-Cast TIPS-Pentacene Thin Films

- 3:05 PM - 3:30 PM** **Coffee Break**
Afternoon Session II
Session Chair: Tsukasa Yoshida (Yamagata University)
- 3:30 PM - 3:55 PM** **Jianing Li** (University of Vermont, Chemistry)
Multiscale Simulations of Advanced Biomaterials
- 3:55 PM - 4:20 PM** **Juan Vanegas** (University of Vermont, Phys & MATS)
*Molecular and continuum models of elasticity in
coiled-coil filamentous proteins*
- 4:20 PM - 4:45 PM** **Kim-Ngan Hua** (Univ. of Vermont, Phys & Mat. Sci)
Exciton Coherence in 1D Crystalline Organic Semiconductors
- 4:45 PM - 5:00 PM** **Matthew White** (University of Vermont, Phys & Mat. Sci)
*Nonlinear Impedance Spectroscopy of Organic MIS Capacitors
and Planar Heterojunction Diodes*
- 5:00 PM - 6:00 PM** **Poster Session and Reception**

Morning Session I

9:00 AM – 9:25 AM

Solution-based organic and hybrid charge-transfer absorbers for solar cells

Tsukasa Yoshida, Yuki Tsuda, Taichi Yasuhara, Akito Masuhara, Jun Matsui, Shuji Okada, Hiroshi Katagiri, Ken-ichi Nakayama, Matthew White, Madalina Furis, Randall Headrick, Philipp Stadler, Niyazi Serdar Sariciftci

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Dye-sensitized (DSSC) and bulk-heterojunction (BHJ) organic solar cells suffer from inherently large voltage loss, as they rely on energy offsets of materials for carrier generation. Direct photogeneration of charge transfer (CT) exciton in organic and hybrid absorbers can overcome this problem to pave the avenue towards 20% efficiency with solution-based materials.

We have tested several intramolecular CT dyes in simple PEDOT:PSS/CT absorber/Ca:Al cells. The free carrier generation indeed became possible for intra-CT dyes, achieving 1 mA cm^{-2} short circuit current (J_{sc}) for DTDCPB together with a high open circuit voltage (V_{oc}) exceeding 1 V. Compared to that, J_{sc} is almost none for non-CT organic absorbers (e.g. $\text{H}_2\text{phthalocyanine}$). We find the reduced exciton binding energy (EBE) in CT compounds as the key to facilitate free carrier generation, i.e. as demonstrated in modified CT dyes using inserted thiophene linker (DTDCPB-T) to further reduce EBE reaching $J_{sc} = 2.64 \text{ mA cm}^{-2}$ in a single absorber architecture. Based on our breakthrough we pursue for alternative CT absorbers by solution-based methods. Novel bi-molecular organic CT salts are attractive candidates – they are obtained by combination of 1,3-bis(dicyanomethylidene)indan anin (TCNIH^-) and N,N'-alkyl-4,4'-bipyridinium cation such as methylviologen (MV^{2+}). The black shiny crystal exhibits an extended absorption up to 1,000 nm and shows a PL peaked at 1,030 nm (1.20 eV) from the CT state. Electrochemical self-assembly (ESA) of n-ZnO/dye and p-CuSCN/dye hybrid thin films is achieved by simply adding

organic dyes into the electrolytic baths for cathodic electrodeposition of ZnO and CuSCN, respectively. When there is a right chemistry between the constituents, interpenetrating and bi-continuous inorganic/organic network in nano-scale is effortlessly formed. These new materials may facilitate carrier generation and its transport, to become new candidates for solution-processed solar cells.

This work was supported by Program for Advancing Strategic International Networks to Accelerate the Circulation of Talented Researchers, “Advanced Next Generation Leadership (ANGEL, R2601) of Japan Society for the Promotion of Science (JSPS).

Morning Session I

9:25 AM – 9:50 AM

The Microstructure and Mechanical Properties of Alumina-Forming Austenitic Stainless Steels

I. Baker

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In order to achieve energy efficiencies of >50 % in power generation systems, materials are required that are both strong and corrosion-resistant at temperatures >700 °C, and economically viable. Austenitic steels strengthened with Laves phase, NiAl and Ni₃Al precipitates, and alloyed with aluminum to improve oxidation resistance, are potential candidate materials. The microstructure and microchemistry of the alumina-forming austenitic (AFA) stainless steels Fe-20Cr-30Ni-2Nb-5Al (in at.%) and of the more complex AFA stainless steels DAFA26 and DAFA29 that were recently-developed at Oak Ridge National Laboratory (ORNL) have been characterized using scanning electron microscopy, transmission electron microscopy, X-ray diffraction and atom probe tomography. Both the relationship between the crystallographic orientation of the precipitates and the f.c.c. parent matrix, and the increase of precipitate size and volume fraction after various thermo-mechanical treatments (TMTs) have been studied. Different TMTs were performed on these steels to improve their mechanical performance. Tensile tests were performed at both room temperature and elevated temperature on the materials at different aging conditions in order to understand the influence of the TMTs on the material’s mechanical properties. Appropriate TMTs were shown to reduce the grain size to the

nanoscale, raise the yield strength to >1000 MPa, and significantly increase the ductility. It was found that TMTs can also produce finer and more uniformly-distributed Fe_2Nb and NiAl precipitates. Both the nanoscale grains and a high volume fraction of Ni_3Al precipitates contribute to the high yield strength. Interestingly, even with Laves phase and NiAl precipitates almost completely covering the grain boundaries, significant room-temperature tensile ductility was observed. The results of preliminary creep studies will also be outlined.

Morning Session I

9:50 AM – 10:15 AM

Correlating atomic-scale structure with device-scale properties in 2D materials

Shawana Hollen (University of New Hampshire, Physics)

Two-dimensional materials are full of promise for applications in lightweight, flexible electronics, biomedical sensors, and even as new materials for batteries and catalysts. They also present a new opportunity to correlate changes in atomic-scale structure with device-scale transport through atomic-scale microscopy. In this talk, I will present projects that are beginning to take advantage of this link using scanned probe microscopy, including defect-induced disorder in graphene field-effect transistors, native defects in black phosphorus, and catalysis using MoS_2 .

Morning Session I

10:15 AM – 10:40 AM

Hierarchical Co-assembly Enhanced Direct Ink Writing

Chenfeng Ke

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Transforming nanoscopic molecular functions and motions into the macroscopic scale in a predictable manner is of great interest for the advancement of smart materials. By hierarchically controlling materials' nanoscale chemical structure, mesoscale assembly, and macroscale threedimensional (3D) features, actuators with shape-morphing and soft robotics with dynamic motions have been developed successfully. When these synthetic functional materials are

integrated with 3D printing technology, i.e. the extrusion-based direct ink writing, their micro- and macroscale properties are unleashed cooperatively as a result of the controlled assembly and complex 3D geometry. Herein, we present a hierarchical co-assembly approach to integrate a wide range of functional molecular monomer into 3D printing materials and transform their molecular functions through cooperative co-assembly. To realize this approach, co-assembled inks with suitable rheological properties formed through the hierarchical co-assembly of functional monomers and templates have been designed, synthesized and 3D printed. Subsequent chemical cross-linking of monomers afford hierarchically assembled monoliths. Our approach not only enables the incorporation of a variety functional molecules for direct ink writing, more importantly, it facilitates the precise organization of the small molecular assembly in macroscopic free-standing 3D objects in response to environmental stimuli, which is another example of 4D printing.

Reference:

Q. Lin, X. Hou, and C. Ke, *Angew. Chem. Int. Ed.*, 2017, 56, 4452 – 4457.

Morning Session II
11:05 AM – 11:30 AM

Soft Electronics and Machines with Tough Hydrogels

Martin Kaltenbrunner¹

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Introducing methods for instant strong bonding between hydrogels and antagonistic materials – from soft to hard – allows us to demonstrate elastic, yet tough biomimetic devices and machines with a high level of complexity. Tough hydrogels strongly attach, within seconds, to plastics, elastomers, leather, bone and metals reaching unprecedented interfacial toughness exceeding 2000 J/m². Healing of severed ionic hydrogel conductors becomes feasible and restores function instantly. Soft, transparent multi-layered hybrids of elastomers and ionic hydrogels endure biaxial strain with more than 2000 % increase in area, facilitating soft transducers, generators and adaptive lenses. We demonstrate soft electronic devices, from stretchable batteries, self-powered compliant circuits and autonomous electronic skin (Figure 1) for triggered drug delivery. Our approach is applicable in rapid prototyping and in delicate environments inaccessible for extended curing and cross-linking.

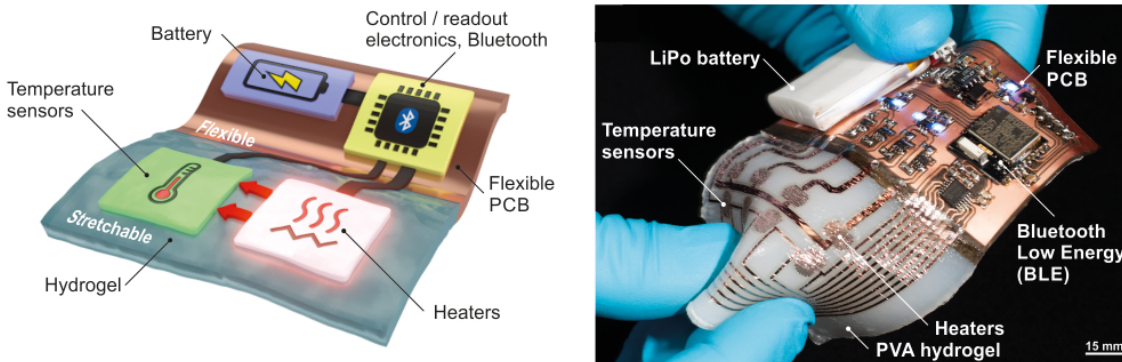


Figure 1: Hydrogel electronic skin. (left) Concept of a hydrogel smart skin, with a flexible unit bearing power supply, control, readout and communication units, and a stretchable transducer batch. (right) Photograph of an untethered electronic hydrogel with four stretchable heating elements and adjoined temperature sensors strongly bonded to a PVA hydrogel. Battery, control, readout and Bluetooth Low Energy communication electronics are hosted on a flexible circuit board.

Morning Session II**11:30 AM – 11:55 AM****Directing Electrophilic Aromatic Substitution Reactions from
Above and Underneath Aromatic Rings****Severin T. Schneebeli, PhD****Abstract for the 2017 AMEBA Symposium at the University of Vermont**

Ortho-, *meta*-, and *para*-directing groups have been used for decades to control the selectivities of electrophilic aromatic substitution (SEAr) reactions. Enzymes, on the other hand, are able to control this class of reactions efficiently by positioning protein residues above and underneath aromatic substrates. Inspired by the enzymatic approach, this presentation will discuss how abiotic SEAr reactions can be controlled precisely with partially flexible ester arms, placed over specific positions on aromatic systems. We are able to access new chiral materials with this bioinspired, through-space-directed approach, which are now starting to be used as vertices for stable molecular cages.

Morning Session II**11:55 AM – 12:20 PM*****Structural characterization and sulfide oxidation of V-DTPA immobilized on mesoporous silica*****Jenna Taft**

Mustard gas, bis(2-chloroethyl)sulfide, is a vesicant whose chemical toxicity can be reduced by oxidation of the sulfur atom. We recently showed that V-doped mesoporous silica nanoparticles are active catalysts for the oxidation of 2-chloroethyl ethyl sulfide (CEES, an analogue of mustard gas) under ambient conditions, using O₂ from air as the oxidation source. In the present studies, we focused on using diethylenetriamine pentaacetate (DTPA) mounted to the nanoparticle surface to reduce leaching of V in aqueous solutions, which was confirmed with ICP-OES. TGA

and N₂ physisorption measurements indicated that the materials remained highly porous even after modification. Only one study has attempted to structurally characterize V-DTPA; here, we used ²⁹Si and ¹³C solid-state NMR and EPR to understand the V coordination geometry of the immobilized complex. Finally, GC-MS was used to show that the V complex was able to perform the same oxidative process as unchelated metal.

Afternoon Session I**1:25 PM – 1:50 PM*****Entanglement area law in superfluid 4He*****Adrian Del Maestro** (Department of Physics, University of Vermont)

Area laws were first discovered by Bekenstein and Hawking, who found that the entropy of a black hole grows proportional to its surface area, and not its volume. Entropy area laws have since become a fundamental part of modern physics, from the holographic principle in quantum gravity to ground state wavefunctions of quantum matter, where entanglement entropy is generically found to obey area law scaling. As no experiments are currently capable of directly probing the entanglement area law in naturally occurring many-body systems, evidence of its existence is based on studies of simplified theories. Using new exact microscopic path integral ground state Monte Carlo simulations of superfluid 4He, we demonstrate for the first time, area law scaling of Entanglement entropy in a real quantum liquid in three dimensions. We validate the fundamental principles underlying its physical origin, and present an "entanglement equation of state" showing how it depends on the density of the superfluid.

Afternoon Session I**1:50 PM – 2:15 PM*****Porous Scaffolds for Electrically-Transduced Gas Sensing and Capture*****Prof. Katherine A. Mirica** (Dartmouth College, Hanover, NH)

Electrochemically active and conductive metal-organic frameworks (MOFs) constitute an emerging class of multifunctional materials with remarkable properties that can help address global challenges in gas purification, sequestration, sensing, and catalysis. This presentation will describe several approaches for interfacing metal organic frameworks with electrodes to create devices with promising utility in gas detection and capture. First, I will present several approaches for direct self-assembly of conductive two-dimensional (2D) MOFs into portable device architecture, and demonstrate the utility of this approach in the context of gas sensing, capture, and filtration. Second, I will describe how the modular structure-property relationships within this class of 2D MOFs can be designed to achieve electrochemically-driven capture and release of gases (e.g., ethylene) directly at the solid-gas interface and in liquids. Taken together, the methods described herein may offer environmental protection from toxic chemicals and may lead to improvements in energy-efficient utilization of petroleum-based resources.

Afternoon Session I

2:15 PM – 2:40 PM

Non-trivial topology in two-dimensional systems

Jie-Xiang Yu and Jiadong Zang

Department of Physics, University of New Hampshire

Topology has revealed its beauty in condensed matter physics for about 35 years since the discovery of quantum Hall effect in two-dimensional (2D) electronic gas. Numerous fascinating physics, such as quantum spin Hall effect in 2D topological insulators and skyrmions in spin systems has non-trivial topological structures in both momentum and real spaces. There always exists a non-zero topological number laying behind each topology. In momentum spaces, Z_2 number is the topological number of topological insulators, of which non-trivial topology is originated from time-reversal symmetry, spin-orbit coupling and band inversion at Fermi level of the band structure. Here I would like to introduce a series of 2D topological insulators $A-C_{14}N_3$ with similar structures. The band inversion in this 2D system is complex and can be controlled. In real spaces, on the other hand, the topological charge is used to quantize magnetic skyrmions. Skyrmions appear in the inversion symmetry broken systems with Dzyaloshinskii-Moriya (DM) interaction. However, one skyrmion has one topological charge but one topological charge does not necessarily correspond to on skyrmion. Our recent study provides the first example that non-trivial topology can even been emerged in a spin-disordered random systems at high temperature. We expect such thermal driven topology can be detected by magnon Hall effect. Finally, I would like to introduce our prediction that giant DM interaction can be found in 2D Mn-Bi thin film system with various novel spin textures. Giant DM interaction with giant perpendicular magnetic anisotropy can lead to nano-scaled skyrmions, which can be used to design energy-saving ultra-dense data storages. This work was supported by by the grant DE-SC0016424 funded by the U.S. Department of Energy, Office of Science.

Afternoon Session I**2:40 PM – 3:05 PM****Thermal-Expansion Effects on the Optical and Carrier-Transport Properties of Solution-Cast TIPS-Pentacene Thin Films****Yang Li¹**, Jing Wan¹, Detlef-M Smilgies², Matthew White¹, Randall. L. Headrick¹⁽¹⁾ *Department of Physics and Materials Science Program, University of Vermont, Burlington, VT 05405*⁽²⁾ *Cornel High Energy Synchrotron Source (CHESS), Ithaca, New York 14853*

Polarized absorption spectroscopy, polarized optical microscopy and wide angle X-ray diffraction were used to determine the direction of transition dipoles in TIPS-pentacene thin films. The results showing that a-axis of TIPS-pentacene unit cell is parallel to the writing direction at low writing speed and the lowest energy absorption peak results from transition dipole along the short axis of the molecule. A large and continuous blue shift of the lowest energy absorption peak has been observed when the sample is annealed from 25°C to 140°C, which is due to the thermal driven structure evolution. An increased mobility in the high temperature polymorph has been observed compared to the room temperature polymorph.

Afternoon Session II**3:30 PM – 3:55 PM*****Multiscale Simulations of Advanced Biomaterials*****Jianing Li** (Department of Chemistry, University of Vermont)

It is essential to develop modeling technology to explain and/or predict the structures and the resulting properties of biomaterials in complex environments. To achieve chemically relevant time and length scales, we have created a new mixed-resolution method and tested with peptides/proteins in biological membranes. The strength of this method and its current applications to multiscale simulations of peptide self-assembly will be discussed. In addition to the methodology, we will also describe our recent efforts to combine multiscale modeling with GPU-accelerated computing to investigate highly complex systems in DNA nanotechnology. At the end, our current focus to invent new multiscale models and methods will be briefly presented. With the current success in peptide/protein/DNA-based materials, we believe that multiscale simulations can provide useful tools for rational discovery of advanced biomaterials.

Afternoon Session II**3:55 PM – 4:20 PM*****Molecular and continuum models of elasticity in coiled-coil filamentous proteins*****Juan M. Vanegas** (Univ. of Vermont, Phys. & MATS)

Coiled-coils proteins form the basic building block of important mechanical transducers in cells and tissues, such as intermediate filaments or myosin motors. In addition to their biological importance, coiled-coil proteins are increasingly being employed in the design of new biomaterials including fibers, nanotubes, or hydrogels. Coiled-coils undergo a structural transition from an α -helical coil to an unfolded state upon extension, which allows them to sustain large strains and is critical for their biological function. By combining molecular dynamics and continuum mechanics, we show that a simple one-dimensional continuum model based on phase-transforming rods can describe the progressive unfolding of these molecules. Unlike two-state models based on Kramer or Bell's theories, our continuum model resolves the spatial distribution of force on the protein. We show that this feature is critical to understand the physics of unfolding at different pulling regimes. Thus, this work exemplifies the versatility of blending molecular and continuum models to understand the mechanics of biomolecules at the nanoscale

Afternoon Session II**4:20 PM – 4:45 PM*****Exciton Coherence in 1D Crystalline Organic Semiconductors***

Kim-Ngan Hua, Lane Manning, Naveen Rawat, Victoria Ainsworth, Libin Liang and Madalina Furis

Department of Physics and the Materials Science Program, University of Vermont

Organic electronic have been drawing a lot of attention over the past few decades with recent commercial applications such as organic photovoltaics, OLEDs, and flexible organic displays. One of the key components of creating organic molecules suitable for electronic devices is a fundamental understanding of excitonic behaviors.

To this end, we investigated the exciton coherence of small organic molecules. Specifically, the exciton coherence of phthalocyanine derivative (H_2OBPc) and their organic alloys systems were explored using temperature dependent time-resolved optical spectroscopy. Organic alloys of naphthalocyanine derivative (H_2OBNc) and H_2OBPc with H_2OBNc concentration (x) ranging from 0 to 1 were prepared using solution-processed deposition¹ that results in macroscopic long-range order even at the ratio of $x = 0.5$, which is unique and important for spectroscopic studies.¹ Our temporal- and polarization-resolved photoluminescence (PL) experiments on H_2OBPc reveal the existence of a delocalized singlet exciton polarized along the high mobility axis in this quasi-1D electronic system.² The temperature dependent PL spectroscopy of H_2OBPc is also consistent with that of a one-dimensional J-aggregate semiconductor with an excitonic band curvature of 240 meV as predicted by Spano et. al.³ and a coherence length of approximately 54 nm at low temperatures. Radiative lifetimes of H_2OBPc remains constant up to 50K and have a quadratic increase after this threshold temperature indicating the “activation” of exciton-phonon coupling. Furthermore, we demonstrate that this band gap exciton energy in thin films fabricated from metal-free H_2OBPc and octabutoxynaphthalocyanine (H_2OBNc) mixtures is tunable over a 30nm range as a function of mixing ratio.

References:

¹R. L. Headrick, et al., Applied Physics Letters., 2008, 92, 063302.

²Pan. Z., et. al, Nat. Comm., 2015, 6

³Yamagata, H., Spano, F., J. Phys. Chem. Lett. 2014, 5, 622–632

Afternoon Session II

4:30 PM – 4:45 PM

Nonlinear Impedance Spectroscopy of Organic MIS Capacitors and Planar Heterojunction Diodes

Matthew White (Univ. of Vermont, Phys. & Mat. Sci.)

Metal-Insulator-Semiconductor (MIS) capacitors and planar heterojunction diodes consisting of donor and acceptor organic semiconductor layers were characterized by nonlinear impedance spectroscopy. Frequency-domain analysis of nonlinear processes reveals the onset of recombination current and the transition to transport-limited Space-Charge Limited Current (SCLC). This technique opens pathways to fully characterize transport and recombination in thin film devices in the frequency domain.

POSTER SESSION

Poster Number: P001

Ultrasound as a vehicle to deliver drug inside the cells

Alina Karki, Jun-ru Wu

Department of Physics and Materials Science Program, University of Vermont

Emily Giddings, Mercedes Rincon

Department of Medicine, Division of Immunobiology

A sound wave with frequency between 1 megahertz to 10 megahertz can excite specially prepared gas encapsulated micrometer size bubbles to oscillate. The bubble oscillations may generate the shear stress to the cell membranes of the nearby cells; form the nanometer size holes on the cells' membrane temporarily, the specific drug in the same solution where ultrasound propagates can be delivered into the cells by the radiation force of the ultrasound. Shortly after that, the nanometer holes are patched by the cells themselves. This process is called sonoporation. The objective of this study is to establish sonoporation as a delivery vehicle for delivering siRNA (Small interfering RNA) drug into mice and human liver CD8 cells to silence the expression of MCJ protein. Methylation control-J (MCJ) protein is developed as a therapeutic target for the Non- Alcoholic Fatty liver disease (NAFLD), which occurs by the presence of the fat accumulation in the liver and is emerging as an epidemic disease. Blocking MCJ expression in the liver could be a strategy to increase lipid metabolism in the liver using siRNA drug. The preliminary experimental results will be presented.

Poster Number: P002

Organic thin films printed at high speed with controlled nucleation and bandlike temperature dependence of mobility

Jing Wan,¹ Yang Li,¹ Jeffrey G. Ulbrandt¹, Detlef-M. Smilgies³, Jonathan Hollin,² Adam C. Whalley,² Randall L. Headrick¹

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² Department of Chemistry, University of Vermont, Burlington VT 05405, USA

³ Cornell High Energy Synchrotron Source, Cornell University, Ithaca

Solution deposition of organic semiconductor thin films has great potential in large-area manufacturing of flexible electronics such as solar cells and displays. However, the control over morphology towards high performance devices, especially at high-speed processing has been a key challenge. In this study, the hollow pen writing method is used to deposit 2,7-dioctyl[1]benzothieno[3,2-b][1]benzothiophene (C₈-BTBT) organic semiconductor thin film from solution. Millimeter-scale grains and carrier mobility up to 3.0 cm²/V·s were achieved under very high writing speed (25 mm/s). In-situ synchrotron X-ray scattering experiments show that very large grain size at high speed is related to the formation of transient liquid crystalline(LC) and crystalline phases during the writing process. The control over morphology is achieved by adjusting the nucleation rate during the transformation between LC and solid phases. In addition, we measured the temperature dependence of OFETs to investigate the charge transport properties. It was observed that the “band-like” transport depends on the lateral electric field between source and drain, which suggests that de-trapping of charge carrier occurs at higher lateral fields.

Poster Number: P003

Copper Segregation Affected Yielding in Nanotwinned Silver

Xing Ke and Frederic Sansoz

Department of Mechanical Engineering and Materials Science Program, University of Vermont

Abstract

Recent studies have shown that small incoherent kink-like step defects in coherent twin boundaries play major roles on the strength and plasticity of nanotwinned face-centered-cubic metals and alloys. Understanding the small-scale mechanics of twin boundary defects under stress is critical for controlling their overall mechanical behavior; yet, the intrinsic yielding mechanisms associated with twin boundary defects remained unexplored. This poster will present large-scale hybrid Monte Carlo - molecular dynamic simulations used to investigate the effects of solute Cu segregation on the small-scale mechanics of nanotwinned Ag containing defective twin boundaries. Each simulated sample was segregated by annealing at 500 K with trace concentrations of 0.2 at%, 0.4 at%, 0.6 at% and 0.8 at% Cu, and subsequently deformed in pure tension up to 10% strain. Segregation simulations show that Cu atoms are strongly segregated to grain boundaries and kink-like twin boundary defects. Tensile simulations show that both twin stability and yield strength increase dramatically as the Cu content increases. Smaller bicrystal models made of only one kink defect were also segregated and sheared along three different directions. We find strong Cu segregation dependence of yield strength and underlying plastic deformation behavior in bicrystals with a kink-like twin boundary defect. The yielding mechanism is observed to change from kink-step migration to kink-step splitting after segregation. The results offer new clues to further push the strength limit in nanotwinned alloys.

Poster Number: P004

In-situ Visualization of Crystal Nucleation and Growth Behaviors of PLA under High Pressure CO₂

Sandra Romero, Taylor Ducharme, and Patrick C. Lee

The crystallization kinetics of polylactic acid (PLA) treated by compressed CO₂ under an easily adjustable and uniform shear flow was investigated. PLA is a bio-derived biodegradable thermoplastic that has been considered as one of the most promising sustainable alternatives to petroleum-based plastics in medical fields, such as tissue engineering, drugs delivery, wound management, and orthopedic devices. In foam processes, a controlled melt strength and service temperature can be achieved by improving the PLA's crystallization kinetics. The isothermal crystallization test indicated that while PLA exhibited very low crystallization kinetics under atmospheric pressure, gas exposure significantly increased PLA's crystallization growth rate due to the plasticization effect from the dissolved CO₂. Furthermore, the crystallization growth of PLA under dynamic conditions was investigated by in-situ observation with a specially designed high-pressure visualization system. From the in-situ crystallization study, it was observed that crystal nucleation rate and maximum crystal density of PLA increased with the applied shear stress due to the decreased local system pressure. One peak on the spherulite growth could be found under both shear stress and static conditions, and this exhibited a great dependency on treatment pressure and applied shear stress.

Poster Number: P005

Hydrogen-bonded Cross-linked Organic Frameworks (H_cOFs)

Xuanfeng Jiang, Yunxiao Lin, Xunzhe Cui, Chenfeng Ke*

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Covalent organic framework (COF) is a class of promising porous materials, yet its practical applications in gas storage/separation, catalysis, and energy-related applications are limited by the delicate balance between its stability and crystallinity. Compared to COFs, highly crystalline porous molecular materials, such as hydrogen-bonded organic frameworks^[1] (HOFs) and porous (supra)molecular frameworks^[2,3] stabilized by weak interactions, are often too labile for their wide adoption. In this presentation, we report the design and synthesis of microporous hydrogen bonded crosslinked organic framework **H_cOF-1**, which was developed through single crystal to single crystal transformation of molecular monomer **1** via photo-irradiated thiol-yne reactions. The flexible crosslinkers offer elasticity to the framework, which expands its void space to adsorb iodine rapidly with a high uptake capacity in an aqueous media. The adsorbed iodine interrupts the crystallinity of **H_cOF-1** by breaking hydrogen bonds, which accommodates iodine beyond its theoretical capacity. In addition, the crystallinity of **H_cOF-1** is recovered after the desorption of iodine, suggesting the elastic and recyclable properties of **H_cOF-1** and its potential in practical application for the active enrichment and removal of radioactive iodine isotopes (¹²⁹I and ¹³¹I) that are produced in the nuclear power plants.

References:

1. He, Y., Xiang, S., Chen, B. *J. Am. Chem. Soc.*, 2011, **133**, 14570-14573.
2. Zhang, G., Presly, O., White, F., Oppel, I. M., Mastalerz, M. A *Angew. Chem. Int. Ed.*, 2014, **53**, 1516-1520.
3. Hasell, T., Cooper, A. I. *Nat. Rev. Mater.*, 2016, **1**, 16053.
4. Lin, Y., Jiang, X., Kim, S. T., Alahakoon, S. B., Hou, X., Zhang, Z., Thompson, C. M., Smaldone, R. A., Ke, C. *J. Am. Chem. Soc.*, 2017, **139**, 7172-7175.

Poster Number: P006

Hierarchical Co-assembly Enhanced Direct Ink Writing

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The development of smart materials and devices has attracted increasing attention as a result of the demonstrated capability of altering their macroscale properties in a controlled manner.¹ Integrating these synthetic functional materials with 3D printing technology, *i.e.* the extrusion-based direct ink writing²⁻⁴ (DIW) will allow us to amplify their nanoscale properties to the macroscale by taking advantage of the hierarchical nature of the controlled assembly and pre-designed complex 3D geometry. In this presentation, we report a general method based on *hierarchical co-assembly* by using supramolecular templates to facilitate shear-thinning and self-healing properties to overcome the obstacle of integrating functional small molecules into DIW-printable materials.⁵ The co-assembled supramolecular template and functional small molecules rapidly deform and reform during the DIW extrusion process. After extrusion, the molecular monomers and templates in the 3D printed monolith re-assemble dynamically upon external stimulus, *e.g.* controlled evaporation, affording functional monolith with enhanced printing resolution. After post-printing crosslinking and template removal, monoliths with predesigned macroscale architecture and molecular functions were obtained, which respond to external stimuli with dynamic fluorescent color changing and shape morphing.

References:

1. Urban, M. W., Stimuli-Responsive Materials: From Molecules to Nature Mimicking Materials Design. Royal Society of Chemistry: 2016.
2. Gladman, S. A.; Matsumoto, E. A.; Nuzzo, R. G.; Mahadevan, L.; Lewis, J. A. *Nat. Mater.* 2016, **15**, 413-418.
3. Lin, Q. M.; Hou, X. S.; Ke, C. F. *Angew Chem Int Edit* 2017, **56**, 4452-4457.
4. Ouyang, L.; Highley, C. B.; Sun, W.; Burdick, J. A. *Adv. Mater.* 2017, **29**, 1604983.
5. Jungst, T.; Smolan, W.; Schacht, K.; Scheibel, T.; Groll, J. *Chem. Rev.* 2016, **116**, 1496-1539.

Poster Number: P007

Imaging atomic vacancies in commercially available black phosphorus

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Black phosphorus (BP) is receiving significant attention because of its direct 0.4-1.5 eV layer-dependent band gap and high mobility. Because BP devices rely on exfoliation from bulk crystals, there is a need to understand native impurities and defects in the source material. In particular, samples are typically p-doped, but the source of the doping is not well understood. Here, we use scanning tunneling microscopy and spectroscopy to compare atomic defects of BP samples from two commercial sources. Even though the sources produced crystals with an order of magnitude difference in impurity atoms, we observed a similar defect density and level of p-doping. We attribute these defects to phosphorus vacancies and provide evidence that they are the source of the p-doping. We also compare these native defects to those induced by air exposure and show they are distinct and likely more important for control of electronic structure. These results indicate that impurities in BP play a minor role compared to vacancies, which are prevalent in commercially-available materials, and call for better control of vacancy defects.

Poster Number: P008

A multi-mode ultrahigh vacuum system for investigating 2D Materials

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Two-dimensional materials are only one or two atoms thick and exhibit properties unique from their bulk counterparts. Some of these properties include outstanding carrier mobility, exceptional strength. They are also lightweight and flexible. By tuning these materials, they can be used in a wide range of applications, for example flexible electronics, solar cells, transistors, etc. In the Hollen lab at University of New Hampshire, we designed an ultra-high vacuum system to correlate atomic-scale imaging with device-scale transport and *in situ* surface functionalization. The preparatory chamber houses an evaporator, ion gun, and a fixed-geometry four-point probe for transport measurements and sample functionalization. An attached imaging chamber houses a closed-cycle 9 K scanning tunneling microscopy (STM), and atomic force microscopy (AFM) with transport feedthroughs for atomic-scale imaging and transport measurements. Current projects that use this suite of tools include: 1) Studying of native and induced defects in black phosphorus (BP) with STM, with a focus on their impact on the local band structure, probed using scanning tunneling spectroscopy, to better understand BP device quality; 2) Measuring transport in black phosphorus with a fixed-geometry four-point probe, which allows us to study how light exposure affects the degradation of black phosphorus when exposed to oxygen; 3) Studying the catalytic properties of MoS₂ with AFM to find new ways to improve the desulfurization reactions currently used in the petroleum industry. Using this combination of UHV tools, we aim to provide insight into emerging two-dimensional science and technology.

Poster number: P009

Electrochemical self-assembly of CuSCN-DAST hybrid thin films

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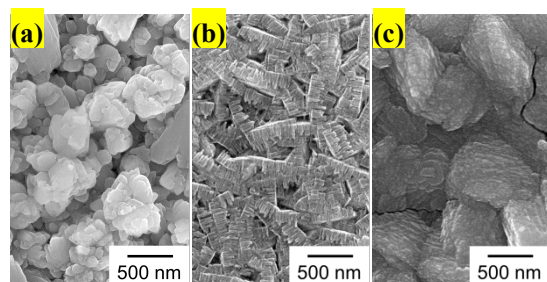


Fig.1 SEM photographs of the films,

DAST = (a)0, (b)500, (c)1100 μM

4-N,N-dimethylamino-4'-N'-methylstilbazolium tosylate (abbreviated as DAST) and its derivatives are known to give one of the most promising organic second-order nonlinear optical crystals, and their applications for terahertz emitters and electro-optic devices have been extensively investigated.

A layered inorganic-organic hybrid structure in a (DAS)(Cu₅I₆) composition and its second-harmonic generation has also been reported. CuI is known to be a p-type semiconductor and could potentially

enhance photocarrier generation and transport. Highly crystallized p- CuSCN thin films can be directly electrodeposited from solutions containing Cu²⁺ and SCN⁻ ions.

The cationic DAS⁺ is expected to find a favorable affinity with CuSCN during its electrochemical growth to self-assemble CuSCN-DAST hybrid thin films. [1]

CuSCN-DAST hybrid thin films were successfully obtained. Hybridization with DAS⁺ ions results in deep coloration of the films, alteration of crystallographic orientation of CuSCN, varied nano-morphology and a phase transition from β - to α -CuSCN when DAST concentration was high. The loading of DAS⁺ was linear to the DAST concentration in the bath but exhibits a remarkable change of the slope at DAST concentration around 100 $\mu\text{mol dm}^{-3}$. Assuming transport limited loading of DAS⁺ for its low concentration range, its diffusion coefficient could be determined as $1.25 \times 10^{-6} \text{ cm}^2 \text{ s}^{-1}$. The significant decrease of the slope therefore could be interpreted as a consequence of kinetic limitation for hybridization in definitive structures. Unique “hair comb” shape β -CuSCN hybrid and “scale-like” α -CuSCN hybrid were indeed obtained under such high DAST concentration range (Fig. 1), achieving near 20% volume occupancy by the organic component in the hybrid film. Most likely, the products we obtained here are nano-composites of crystalline inorganic CuSCN and organic (DAS)(SCN) solid, possibly in its definitive composition. Since both of them were found to be interconnected and bi-continuous, such materials can be promising for light-induced carrier separation between CuSCN and (DAS)(SCN) and carrier transport in them.

[1] Yuki Tsuda et al., *Monatshefte für Chemie*, **148**, 845-854 (2017).

Poster number: P010

Microwave-assisted hydrothermal synthesis of ZnO and Zn-Terephthalate hybrid nanoparticles employing benzene dicarboxylic acids

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Nano-/micro-sized particles of zinc oxide (ZnO) have versatile functions represented in their applications as white pigments, photocatalysts, light-emitting materials and electron transport materials (ETM) for photovoltaics.

Control of their structure and size is the key to maximize their functionalities.

In our precedent work, we have succeeded to synthesize differently structured ZnO nanoparticles with well-defined preferentially exposed facets through the microwave assisted hydrothermal reaction and employing structure directing agents (SDAs).

In this study, three isomers of benzene dicarboxylic acids, phthalic acid (PA), isophthalic acid (IPA) and terephthalic acid (TPA) were employed as SDAs. ZnO nanoparticles with a variety of shape and size were obtained to reveal their strength in the order of TPA > PA > IPA when the solution pH > 10.

However, TPA behaved differently from the others when pH of the precursor solution was reduced. ZnO was no longer formed but Zn-TPA metal-organic frameworks (MOFs) were formed, in which layered double hydroxide of Zn²⁺ (Zn LDH) was stabilized by the intercalation of TPA dianion. Zn-TPA MOFs in four different structures and compositions were depending on pH. Three of them could be isolated to identify their compositions as Zn₃(OH)₄(TPA) · 6H₂O, Zn₄(OH)₆(TPA) and Zn₂(OH)₂(TPA) · H₂O, with their interlayer distances of 14.4, 10.8 and 9.03 Å under pH 7.0, 5.9 and 5.3, respectively, as revealed by XRD, TG-DTA and FT-IR analyses. Although such discrete change of the composition and structure should usually result from the difference of their thermodynamic stability under different pH, these Zn-TPA MOFs are hitherto unknown in their synthesis by slow hydrothermal reaction. These unique structures could kinetically be chosen in the rapid crystallization under microwave radiation.

Poster number: P0011

Novel Organic CT Salts Employing 1,3-Bis(Dicyanomethylidene)Indan Anion as a Donor

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Organic charge transfer crystals (CTCs) can be interesting candidates in solar cells to eliminate large voltage loss inherent in dye-sensitized and bulk hetero junction types, in which carrier generation relies on the energy cascades. We aim high voltage organic solar cells employing CTCs as a single absorber. We have synthesized novel CTCs by forming salts between 1,3-bis(dicyanomethylidene)indan anion (TCNIH⁻) and viologen cations, namely, N,N'-alkyl substituted 4,4'-bipyridiniums (methyl = MV²⁺, ethyl = EV²⁺, heptyl = HV²⁺ and octyl = OV²⁺).

Mixed salts of TCNIH⁻ and viologens were obtained by slowly evaporating solvent at room temperature from their 2 : 1 mixed solution in ethanol. While their crystal structures were examined on powder samples and single crystals, their optical properties were studied by measuring UV-Vis and PL spectra. HOMO-LUMO levels for the CT were estimated by cyclic voltammetry (CV) and density function theory (DFT) calculation.

Colorless TCNIH₂ turns into deep blue in ethanol due to deprotonation from its methylene carbon to become TCNIH⁻ anion. While its salt with Na⁺ was purplish black with its absorption onset around 800 nm, co-crystals with viologens were black with metallic shine to exhibit an extended CT absorption in NIR up to 850 (HV, OV) and 1,000 nm (MV, EV). Although all of them were mixed crystals as found in powder XRD, only MV and EV salts gave large enough single crystals. Stoichiometric composition of (TCNIH⁻)₂(MV²⁺ or EV²⁺) was found, in monoclinic and triclinic unit cell structures, respectively. The TCNIH⁻ and MV²⁺ ions are closely packed in distances shorter than the van der Waals radii of two carbon atoms, whereas longer for EV²⁺ due to steric hindrance caused by bulky ethyl group. Even bulkier HV²⁺ and OV²⁺ destabilized the crystal, thus making it difficult to obtain large single crystals. The close packing of the organic ions by coulombic attraction obviously contributes to the CT absorption in these salts. PL and PLE spectra were measured for the TCNIHNa and (TCNIH⁻)₂(MV²⁺) salts. TCNIHNa has a relationship of mirror symmetry between emission and excitation spectra. Whereas (TCNIH⁻)₂(MV²⁺) salt exhibits emission peaked around 1030 nm on excitation at 630 nm with its PLE spectrum closely matched with the absorption. Thus, it is obviously due to emission from the CT exciton with its energy of ca. 1.2 eV. DFT calculation indicated strong localization of HOMO and LUMO in TCNIH⁻ and MV²⁺ respectively with a slightly smaller energy gap of 1.06 eV. Thus, it is concluded that the (TCNIH⁻)₂(MV²⁺) salt exhibits CT absorption, in which TCNIH⁻ and MV²⁺ being donor and acceptor, respectively.

Poster number: P012

Linear Dichroism and Photoluminescence Imaging of Grain Boundary and Structure in Crystalline Organic thin Film

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Research on organic semiconductors has advanced tremendously for the past few decades as these materials have great potential for the development of novel electronic and photonic devices. Small molecules with well-defined chemical structure and π -conjugation, such as pentacene or phthalocyanine, exhibit very large charge carrier mobilities. They represent a cost-effective and flexible electronics alternative for certain traditional silicon-based semiconductor applications such as field-effect transistors and photovoltaic devices. However, fundamental studies on excitonic properties of organic crystals of small molecule organic thin films are not fully understood due to a high level of disorder in the polycrystalline samples inherent to standard fabrication methods. In this work, we report on the results of linear dichroism (LD)/ photoluminescence (PL) scanning microscopy experiments that simultaneously probe the excitonic radiative recombination and the molecular ordering in solution-processed phthalocyanine crystalline thin films with macroscopic grain sizes. LD images show that this technique could resolve the small-angle boundary and non-uniform triangular structure. With polarization-resolved PL, we could also explore the relative orientation of the singlet exciton transition dipoles at the grain boundary.

Poster number: P014

Optoelectrical characterizations of electrodeposited CuSCN / dye hybrid thin film

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Combination of inorganic and organic materials offers unlimited new opportunities. While “composites” stands for their physical mixtures, “hybrids” and “inorganic/organic compounds” are especially interesting for their new functionalities, as they are achieved by self-organization due to “chemistry” among the constituents. We have established electrochemical self-assembly (ESA) of inorganic/organic hybrid thin films from one pot containing all the ingredients. For example, hybrid thin films of highly porous yet highly crystallized zinc oxide (ZnO) and eosin Y can be effortlessly obtained by simply adding eosin Y into the bath for cathodic electrodeposition of ZnO.¹⁾ The two solids are totally segregated, so that the porous ZnO after removal of eosin Y exhibits a high performance as a photoelectrode in dye-sensitized solar cells. Properties of the dye aggregates in the film as well as the concerted functionalities of the hybrid materials are also interesting targets of the study.

In this work, we have employed cathodic electrodeposition of CuSCN as the test bed for ESA of CuSCN/dye hybrid thin films. CuSCN is a wide bandgap p-type semiconductor and its well crystallized thin film can be directly obtained from solutions, thus offers a good counterpart to the ESA of n-ZnO/dye hybrids. Chemical properties of dye molecules for successful ESA have been examined to understand the principle of self-assembly. The composition, nanostructure of the hybrid thin films as well as their functionalities are studied with the special interest in their optical properties. Photoluminescence (PL) and excitation (PLE) spectra were measured between 77 K and room temperature to elucidate the fate of the photogenerated exciton in the organic component of the hybrid thin films.

CuSCN / dye hybrid thin film was found that inorganic and organic have a “good chemistry” for successful ESA. CuSCN was good well zwitter ionic and cationic dyes and were loaded to yield colorful one. It was reasonable to happen partial replacement of Cu⁺ ions of CuSCN with cationic dyes. But FLNCS in anionic xanthene dyes group did hybridization. The hard and soft, acid and base (HSAB) principle nicely explains the successful ESA of FLNCS having a soft Lewis basic -NCS group for stable coordination to soft Lewis acidic Cu (I) sites of CuSCN. Loading dye color thin film change the morphology with specific hybrid nanostructures. In the case of 4-(N, N-dimethylamino)-4'-(N'-methyl) stilbazolium tosylate (DAST), this morphology and phase changed in accordance with dye concentration. Three type structure appeared β -CuSCN occluding DAS⁺ chromophore (“occl”), nano-phase separated interpenetrating β -CuSCN/DAS in a haircomb shape (“comb”), and nano-phase separated interpenetrating α -CuSCN/DAS in a scale-like shape (“scale”).²⁾ Absorption, PL and PLE spectra of CuSCN / DAST were between powder and solution like between single molecule and aggregate. In other words, Original compounds of inorganic and organic in molecular orbital generated and become to absorb light more than single molecule. In the 77 K, PL of DAST powder was blue shifted and was sharp. By cooling the sample, exciton-phonon interaction in powder was weaker, the excited state was stabilized and fluorescent from energy high level. Regarding hybrid film, “comb” and “scale” were red shifted compared with “occl” for making the complex compounds between CuSCN and DAST. It was found that those exciton changed fate by stability of structure or molecular orbital.

On the other hand, although both solution and powder of NB and RB exhibit PL whose PLE nicely matched with their absorption spectra, CuSCN / NB and CuSCN / RB that of the thin film was completely quenched. Due probably to charge transfer (CT) by hole transfer from the excited state of RB and DAST to the valence band of CuSCN. The present study already reveals some promising features of the “NB”, RB” especially in terms of their use as light absorbers in solar cells, since photoinduced CT between organic chromophore and inorganic CuSCN has been suggested.

1. T. Iwamoto et al., *J. Phys. Chem. C*, **118**, 16581-16590 (2014).
2. Y. Tsuda et al., *Microsys. Tech.*, DOI 10.1007/s00542-017-3394-9.