

# 2021 BECKMAN SYMPOSIUM

POSTER PRESENTATIONS FEATURING

**Beckman Young Investigators**

**Arnold O. Beckman Postdoctoral Fellows**

**Second-Year Beckman Scholars**

**Jeremy Baskin, PhD**

2017 Beckman Young Investigator  
Chemistry (Chemical Biology)  
Cornell University



**Chemical Tools that IMPACT Lipid Signaling**

The fidelity of intracellular signaling pathways requires that cells control the production of signaling agents in space and in time. Phosphatidic acid (PA) is both a central phospholipid biosynthetic intermediate and a multifunctional lipid second messenger produced at several discrete subcellular locations. The modes of action of PA differ based on upstream stimulus, biosynthetic source, and site of production. How cells regulate the local production of PA to direct diverse signaling outcomes remains elusive. To unravel these questions, we have significantly expanded the toolkit for visualizing and perturbing cellular PA production. These approaches have revealed new functions of spatiotemporally defined pools of PA in response to physiological and pathological stimuli. Our work highlights the power of combining bioorthogonal chemistries, chemoenzymatic tagging, directed evolution, and optogenetics to shed light on cell signaling pathways.

**DAY 1 PRESENTER – 8/5**

**Pamela Chang, PhD**

2017 Beckman Young Investigator  
Chemistry (Immunology, Virology &  
Infectious Disease)  
Cornell University

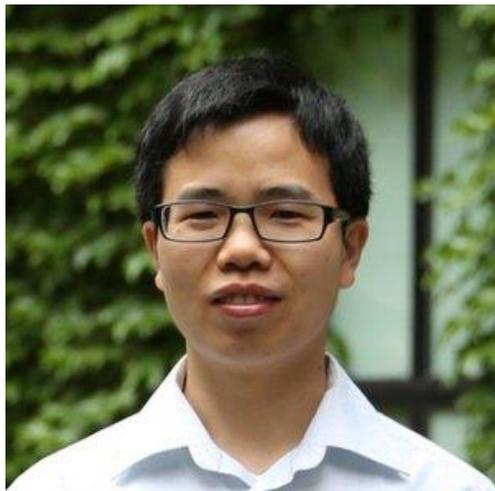


**Chang Lab: Research at the Interface of Chemistry, Immunology, and the Gut Microbiome**

Inflammation is a vital physiological process in infection and tissue repair after injury, but uncontrolled, chronic inflammation caused by overactivation of immune cells occurs in many diseases. Current anti-inflammatory drugs are delivered systemically and cause off-target effects in otherwise healthy tissues, and thus, there is a great demand for next-generation technologies to locally inhibit activation of the immune system to limit these side effects. We aim to develop precision chemical tools to inhibit local inflammation by modulating the functions of select target populations of immune cells and apply these tools to both study fundamental biological mechanisms of inflammatory pathways and control the immune response in therapeutic settings.

**Dan Fu, PhD**

2017 Beckman Young Investigator  
Chemistry (Biochemistry)  
University of Washington



**DAY 1 PRESENTER – 8/5**

**Quantitative Single Cell Phenotypical Imaging of Multicellular Systems**

Single-cell omics technologies have revolutionized our understanding of biological heterogeneity and its fundamental role in tissue functions. However, most single-cell technologies are limited to analyses of isolated cells instead of cells in their native environment. Connecting omics data to cell phenotypes is a significant challenge. Many cell phenotypes, such as mass, density, growth, and cell states, are also challenging to measure inside the tissue. For the BYI funded project, our focus is to develop new optical imaging instruments to address phenotype measurement problems. We demonstrate that we can image several essential phenotypic parameters, including shape, size, mass, density, and growth, using intrinsic vibrational contrasts of molecules. Importantly, these capabilities can be directly applied to tissues and live animals, allowing in situ characterization of cell phenotypes. In combination with machine learning and deep learning, we can further identify specific cell types and subcellular organelles. Together, these single-cell phenotypic imaging capabilities open new avenues of investigations into cell heterogeneity and its functional role in multicellular systems.

**Erik Grumstrup, PhD**

2017 Beckman Young Investigator  
Chemistry (Materials Spectroscopy)  
Montana State University



**Probing nanoscale materials with time-Resolved Vibrational Microscopy**

The past decade has witnessed remarkable advances applying the transformative insight of ultrafast spectroscopies to the nanoscale. By coupling femtosecond laser pulses into far-field microscopes, the spatial and energetic evolution of electrons can be correlated to specific micro- and nanoscale structural features, providing important insight into how anisotropic crystal structures, strongly interacting excited states, and structural and electronic defects influence the behavior of active (opto)electronic devices. We have developed excited state stimulated Raman microscopy, which provides a means to directly probe how electrons couple with vibrational degrees of freedom on the femtosecond time scale and on sub-200 nm length scales. By probing electronic excited states *via* perturbations to the Raman spectra, we overcome intrinsic limitations that are encountered when performing pump-probe type electronic spectroscopies.

**Jose Rodriguez, PhD**

2017 Beckman Young Investigator  
Chemistry (Biochemistry, Imaging &  
Spectroscopy)  
University of California, Los Angeles



**Ab initio fragment-based determination of protein structures by  
MicroED**

Structure determination of novel biological macromolecules by X-ray crystallography can be facilitated by the use of small structural fragments, some only a few residues long, as effective search models for molecular replacement to overcome the phase problem. We investigate the use of fragment-based methods to overcome the phase problem with the electron cryomicroscopy (cryoEM) method known as microcrystal electron diffraction (MicroED). Our approach provides phasing solutions for a structure of Proteinase K from 1.6Å data using model fragments derived from structures of proteins sharing sequence identity as low as 20%. The combined set of fragments was sufficient to arrive at a solution that resembled that determined by conventional molecular replacement using the known target structure as a search model. This approach obviates the need for a single, complete and highly accurate search model when phasing MicroED data and permits the evaluation of large fragment libraries for this purpose.

**DAY 1 PRESENTER – 8/5**

**A. Fatih Sarioglu, PhD**

2017 Beckman Young Investigator  
Biology (Bioengineering)  
Georgia Institute of Technology

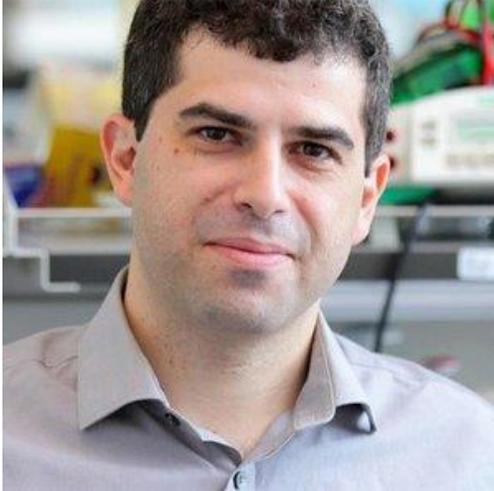


**All-Electronic Lab-on-a-Chip Platforms for High-Throughput Multi-Modal Cell Phenotyping**

Lab-on-a-chip devices are extremely attractive for cytometric analysis as they offer unique capabilities for deterministic cell manipulation under a variety of discriminating force fields. By spatially tracking cells as they are manipulated on lab-on-a-chip devices (e.g., determining the microfluidic channel they are sorted into or the location on the microfluidic device where they are captured), biophysical or biochemical assays can be performed. To obtain such spatial information, however, microfluidic devices require subsequent microscopic analysis negating the cost and portability benefits. Therefore, a simple integrated sensor that can track particles on a microfluidic chip can enable a new generation of devices with sample-to-answer capability in performing cell phenotyping based on different modalities. Such devices will be instrumental for the discovery of non-traditional biomarkers as well as point-of-care testing in resource-limited settings.

**Dmitriy Aronov, PhD**

2018 Beckman Young Investigator  
Biology (Neuroscience)  
Columbia University



**Flexible use of memory by food-caching birds in a laboratory behavioral paradigm**

A hallmark of human episodic memory is “flexibility” – the ability of a single memory to influence different behaviors in pursuit of different goals. It is unknown to what extent memory in other animals is similarly flexible. To address this question, we studied spatial behaviors of a specialist food-caching bird, the black-capped chickadee. These birds naturally pursue different goals at different moments in time as they explore an environment, cache food, and later retrieve caches. We designed a behavioral setup to engage these behaviors and track them automatically. We also used probabilistic modeling to disentangle the contributions of memory-guided and non-mnemonic strategies to the behavioral choices made by chickadees in this setup. We find that memories of the contents of individual cache sites are used by chickadees in a context-dependent manner. During caching, chickadees avoid sites that already contain food, resulting in an even distribution of caches throughout the environment. During retrieval, they instead efficiently navigate to such occupied sites to obtain food. Therefore, a single memory can be used by a chickadee to achieve at least two unrelated behavioral goals. These results demonstrate memory flexibility in an animal in a tractable spatial paradigm.

**DAY 1 PRESENTER – 8/5**

**Alistair Boettiger, PhD**

2018 Beckman Young Investigator  
Biology (Developmental Biology)  
Stanford University



**Deep learning connects DNA traces to transcription to reveal predictive features beyond enhancer–promoter contact**

Chromatin architecture plays an important role in gene regulation. Recent advances in super-resolution microscopy have made it possible to measure chromatin 3D structure and transcription in thousands of single cells. However, leveraging these complex datasets with a computationally unbiased method has been challenging. Here, we present a deep learning-based approach to better understand to what degree chromatin structure relates to transcriptional state of individual cells. Furthermore, we explore methods to “unpack the black box” to determine in an unbiased manner which structural features of chromatin regulation are most important for gene expression state. We apply this approach to an Optical Reconstruction of Chromatin Architecture dataset of the Bithorax gene cluster in *Drosophila* and show it outperforms previous contact-focused methods in predicting expression state from 3D structure. We find the structural information is distributed across the domain, overlapping and extending beyond domains identified by prior genetic analyses. Individual enhancer-promoter interactions are a minor contributor to predictions of activity.

**Henry 'Pete' LaPierre, PhD**  
2018 Beckman Young Investigator  
Chemistry (Inorganic Chemistry)  
Georgia Institute of Technology



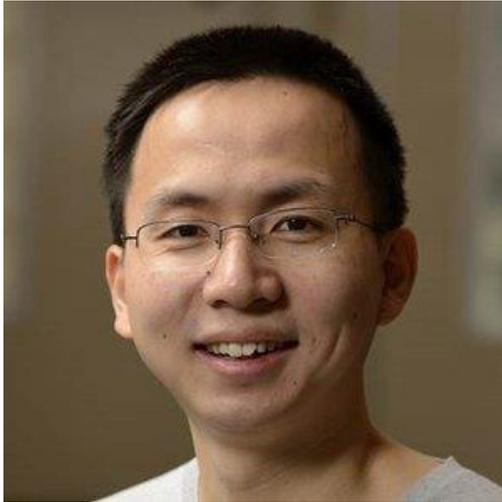
**Covalency and Magnetic Superexchange in Magnetic Materials Design**

Magnetic exchange phenomena are important for the design of novel functional magnetic materials such as single molecule magnets and the discovery of exotic phases including quantum spin liquid states. The magnetic exchange constants,  $J$ , link closely to the degree of bond covalency,  $\lambda$ . This program aims to find quantitative relationship between  $J$  and  $\lambda$  with the assist of ligand K-edge X-ray absorption spectroscopy (XAS) and the modern magnetic measurement techniques. Recent results in these fundamental physical and spectroscopic studies and their application in the development of molecular and extended solid magnetic materials are presented.

**DAY 1 PRESENTER – 8/5**

**Chen Li, PhD**

2018 Beckman Young Investigator  
Biology (Engineering)  
Johns Hopkins University



**Neuromechanics of Locomotor Transitions on Energy Landscapes of Complex Terrain**

Effective locomotion in nature happens by transitioning between modes (e.g., walk, run, climb). However, mechanistic understanding of terrestrial locomotion has mainly been on how to generate and stabilize around near-steady-state movement in a single mode. Consequently, robots cannot robustly traverse complex terrain for critical applications like search and rescue. Our research focuses on using an energy landscape approach to elucidate how animals and how robot should make active adjustments to make locomotor transitions. Recently, we discovered that locomotor transitions can be modeled as barrier-crossing transitions on potential energy landscapes. We are developing tools to enable experiments and modeling of locomotor transitions: (1) experimental platforms and techniques to quantify locomotor transitions and active adjustments, (2) robots with animal-like motion as physical models, and (3) force sensors to measure physical interaction during adjustments. We highlight two discoveries enabled by these tools: (1) legged insects actively adjust head, body, and appendages to lower potential energy barriers; (2) besides vision, limbless snakes must use mechanical sensing to adjust body form and control terrain contact to maintain propulsion and stability.

**Jean-Hubert Olivier, PhD**  
2018 Beckman Young Investigator  
Chemistry (Organic Materials)  
University of Miami



**Molecular Strategies to Engineer 2D Nanoscale Objects: Towards Organic Piezoelectric Materials**

Having established the synthetic protocols for the covalent anchorage of molecular dipoles onto Si surfaces, we have delineated synthetic protocols to reticulate surface-anchored molecular dipoles using sequential hydrothiolation (i.e., thiol-yne and thiol-ene) “click” chemistry. The presented synthetic strategy exploits hydrothiolation “click” reaction of dithiol-based cross-linkers with the disubstituted 1,3-alkadiyne motifs that are structurally placed between a neutral phenyl ring and either the cationic or the anionic aromatic moiety of the molecular dipole precursors. To establish the viability of hydrothiolation “click” chemistry with such disubstituted aromatic 1,3-alkadiyne motifs that are anchored as part of the hybrid Si interfaces, we first validated the conditions by following three control strategies in a stepwise manner: 1) thiol-yne “click” reactions of Si interfaces terminated with aliphatic alkyne motifs, 2) sequential thiol-yne and thiol-ene “click” reactions of Si interfaces terminated with aliphatic alkyne motifs for dual functionalization, and 3) thiol-yne “click” reactions of Si interfaces terminated with aliphatic 1,3-alkadiyne motifs.

**DAY 1 PRESENTER – 8/5**

**Ian Seiple, PhD**

2018 Beckman Young Investigator  
Chemistry (Pharmaceutical Chemistry)  
University of California, San Francisco



**Platforms for the generation of new classes of antibiotics**

Our Beckman work focuses on antibiotics that bind to the bacterial ribosome but have not yet reached their therapeutic potential due to lack of chemistry to modify their structures. It comprises three aims: 1) modular synthesis, 2) synthesis of chimeric antibiotics, and 3) binding-induced hybridization. Each of these three aims centers around a structurally rich and unique class of antibiotics: the pleuromutilin antibiotics. During Year 1, our efforts resulted in two new routes that give access to the 5,6-bicyclic structure present in the pleuromutilin core. Year 2 has yielded extremely exciting results across all three of our aims. We have initiated a new route to the pleuromutilin core that will enable rapid functionalization of all three rings. We have conducted a screen for synergy among protein synthesis inhibitors, and found that, pleuromutilins exhibit synergistic antibacterial effects with streptogramin antibiotics, and have characterized their binding with CryoEM. Finally, we have synthesized unprecedented antibiotic hybrids of several classes that bind to the bacterial ribosome.

**Michaela TerAvest, PhD**  
2018 Beckman Young Investigator  
Biology (Synthetic Biology)  
Michigan State University



**A bacterial chassis to convert electricity and carbon dioxide into fuels**

My lab is developing a bacterial strain to catalyze the conversion of carbon dioxide to fuels and products using electrons from an electrode as the sole source of energy. This process would represent an exciting new biotechnology termed ‘microbial electrosynthesis’. Our platform for developing electrosynthesis is *Shewanella oneidensis*, a metal-reducing bacterium with the capacity to exchange electrons with extracellular electrodes. We previously demonstrated that *S. oneidensis* can take up electrons from a cathode and use them for intracellular reduction reactions. This is an important proof of concept for microbial electrosynthesis, but the initial electron transfer rates were orders of magnitude lower than would be required to make the process economically viable. To understand what factors contribute to enhanced electrosynthesis performance we compared the proteomes of high- and low-performing populations of bacteria and identified proteins that were associated with faster electron transfer rates. We observed that proteins related to respiratory electron transfer and biofilm formation were more abundant in the high-performing population. Our next goal is to further upregulate these proteins to further enhance electrosynthesis performance.

**DAY 1 PRESENTER – 8/5**

**Ashleigh Theberge, PhD**

2018 Beckman Young Investigator  
Chemistry (Biomaterials)  
University of Washington

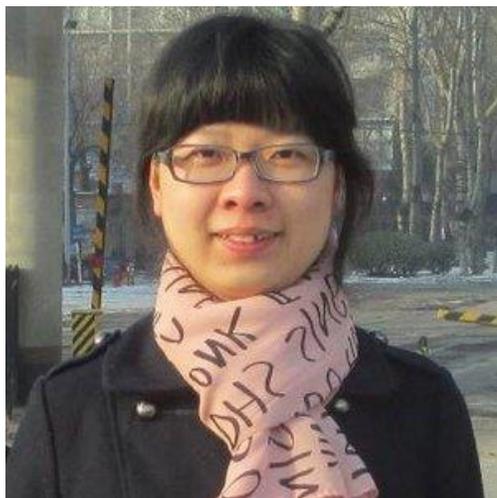


**Spatial Control over Logically Responsive Multi-Material Structures**

The ability to create structures comprising dynamic soft materials in a spatially resolved 3D pattern provides unprecedented control over an engineered material. The Theberge lab has developed an open microfluidic 3D patterning method, based on surface tension-driven flow, compatible with any material with a liquid-to-solid transition and is simple to implement without material modification. Our collaborators in the DeForest lab have pioneered a suite of dynamic hydrogels that can be chemically or physically modulated on demand in response to environmental inputs. Incompatibilities of these materials with existing 3D patterning technologies (e.g., stereolithography extrusion) had limited their ability to be assembled with spatial control. We combined our novel surface tension-based patterning strategy (Theberge lab) with DeForest's novel actuatable materials, enabling 3D spatial control of multicomponent structures that respond dynamically to stimulus, yielding a new breed of four-dimensional (4D) functional multi-materials.

**Weiwei Xie, PhD**

2018 Beckman Young Investigator  
Chemistry (Materials Science &  
Development)  
Rutgers University



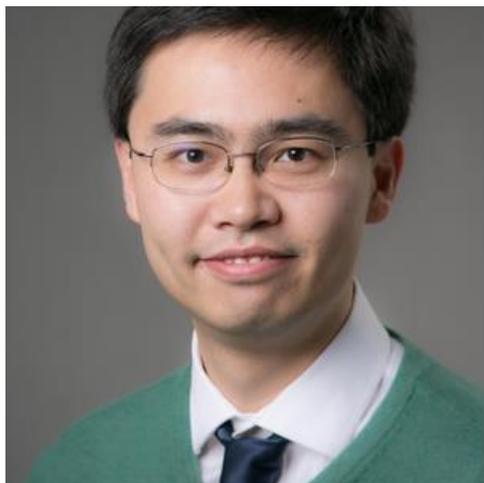
**Direct-learning Method to Find New Superconductors**

Machine-learning method is widely used in finding new materials recently. However, applying machine-learning method for finding new superconducting materials is not as productive as other classic quantum materials. In this poster, we will present our new method – Direct-learning method to find new superconductors. The highest  $T_c$  we can reach now is 7 K in sigma phase alloys.

**DAY 1 PRESENTER – 8/5**

**Xiaoji Xu, PhD**

2018 Beckman Young Investigator  
Chemistry (Physical/Analytical  
Chemistry)  
Lehigh University



**Peak Force Infrared Microscopy: Chemical Nanoscopy in Both Air and Liquid Phases**

This poster illustrates our approaches toward infrared nano-imaging and spectroscopy to bring the spatial resolution to sub 10 nm in both air and liquid phases. The method of peak force infrared (PFIR) microscopy utilizes temporal domain mechanical detection of the tip-enhanced infrared photothermal response of the sample with a nanoscopic atomic force microscope (AFM) tip. We have demonstrated the imaging capability of PFIR on a wide range of materials in chemistry, physics, and material sciences, from block copolymer, amyloid fibril, cellular structures to secondary organic aerosols, oil shale source rock, and two-dimensional polaritonic materials. A spatial resolution of 6 nm is demonstrated across samples. Recently, we have upgraded the PFIR microscopy to operate within the liquid phase in a method called the liquid phase peak force infrared (LiPFIR) microscopy. We probed the hyperbolic phonon polaritons of hexagonal boron nitride submerged in water to reveal modification of its dispersion relations. In addition, we demonstrated the *in situ* detection of product molecules of Click chemistry reactions at the liquid/solid interface.

**Keriann Backus, PhD**

2019 Beckman Young Investigator  
Chemistry (Chemical Biology)  
University of California, Los Angeles



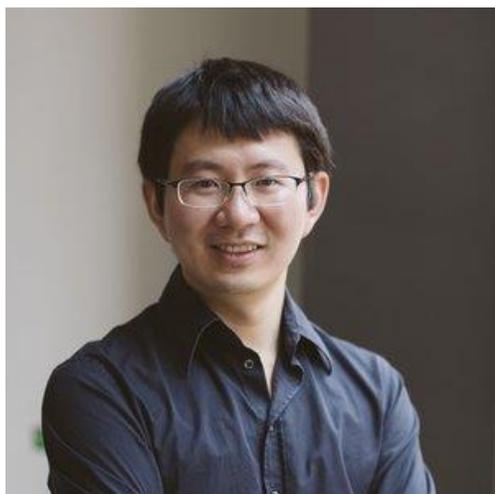
**Expanding the Druggable Proteome**

Chemical probes are powerful tools for characterizing protein function, which offer the advantages of producing graded effects (both agonism and antagonism) and acute application, features that are well suited to the study of essential genes and post translational processes. Despite their proven utility, most human proteins (>90%) lack selective chemical probes, and entire classes of proteins remain 'undruggable.' Prior chemoproteomics studies have demonstrated that the human proteome contains hundreds and quite possibly even thousands of small molecule-targetable, termed ligandable, cysteine residues. However, what remains unclear is whether and how the attached probes alter protein function. Combining proteomics, genomics, and covalent probes, our research aims to decipher the functions of these numerous ligandable cysteines, and by doing so we will generate a roadmap for the use of covalent probes to study and manipulate protein function. Here we report progress towards a proteogenomic platform to identify functional and druggable acquired cysteine residues as a new approach to develop precision therapies.

**DAY 1 PRESENTER – 8/5**

**Chenfeng Ke, PhD**

2019 Beckman Young Investigator  
Chemistry (Materials Chemistry)  
Dartmouth College



**Kinetic Trapping of 3D-Printable Cyclodextrin-based Poly(pseudo)rotaxane Networks**

Synthetically trapping kinetically varied (super)structures of molecular assemblies and amplifying them to the macroscale is a promising, yet challenging approach for the advancement of meta-stable materials. Here, we demonstrated a concerted kinetic trapping design to timely resolve a set of transient polypseudorotaxanes in solution and harnessed a crop of them via micro-crystallization. By installing stopper or speed bump moieties on the polymer axles, meta-stable polypseudorotaxanes with segmented cyclodextrin blocks were hierarchically amplified into crystalline networks of different crosslinking densities at mesoscale, and viscoelastic hydrogels with 3D-printability at bulk. We demonstrated simultaneous 3D-printing of two polypseudorotaxane networks from one reactive ensemble, and their conversion to heterogeneous polyrotaxane monoliths. Spatially programming the macroscale shapes of these heterogeneous polyrotaxanes enabled the construction of moisture-responsive actuators, in which the shape morphing is originated from the different numbers of cyclodextrins interlocked in these polyrotaxane networks.

**Wesley Legant, PhD**

2019 Beckman Young Investigator  
Biology (Microscopy)  
University of North Carolina, Chapel  
Hill



**DAY 1 PRESENTER – 8/5**

**Intelligent Microscopes to Observe and Interact with Dynamic Specimens**

Modern microscopes produce terabytes of complex data in a single experiment. However, these instruments are still operated in the same point-and-shoot manner as their counterparts from over 100 years ago. Real-time image analysis and artificial intelligence could fundamentally change how we use these instruments in our work, allowing us to capture rare cellular events, at statistically significant numbers, and at high spatiotemporal resolution. Finally, these tools could be combined with targeted photomanipulation to dynamically interact with biological specimens as they change over time. We aim to benchmark these tools by imaging chromosome motion during cell division with the ultimate goal to quantify and control chromosome segregation errors in living cells. Errors in the mitotic process impact nearly all living organisms, ranging from fungi to humans, with immense implications for human health. However, because they require capturing the same cell at multiple stages of the division process, many longstanding and fundamental questions about normal and abnormal cell division can only be answered via high resolution live-cell imaging.

**Frank Leibfarth, PhD**

2019 Beckman Young Investigator  
Chemistry (Materials Science &  
Development)  
University of North Carolina, Chapel  
Hill



**Stereoselective Ionic Polymerizations**

The physical properties exhibited by synthetic materials are directly linked to their microstructures. We have recently designed chiral counterions that systematically bias the reactivity and chain-end stereochemical environment during cationic polymerization. In this Beckman Project, we aim to translate this unique concept to create new classes of stereo-defined plastics that are derived from naturally occurring resources and have a drastically reduced environmental footprint.

**Jarad Mason, PhD**

2019 Beckman Young Investigator  
Chemistry (Inorganic Chemistry)  
Harvard University



**Increasing the Intrinsic Porosity of Liquids Through Coordination Chemistry**

Porosity and fluidity are two extremely useful properties of matter that are rarely encountered together in conventional materials. Guided by coordination chemistry and thermodynamics, this research proposes the design, synthesis, and characterization of a new class of liquids that feature unprecedented intrinsic porosity. Such porous liquids will push the boundaries of the properties that can be achieved in porous materials and in liquids, affording new opportunities for the transport, storage, separation, and conversion of small molecules important to energy and health.

**DAY 1 PRESENTER – 8/5**

**Jia Niu, PhD**

2019 Beckman Young Investigator  
 Chemistry (Synthetic Chemistry)  
 Boston College



**Made to Degrade: Cascade Reaction-Driven Polymerization and Depolymerization**

Degradable polymers represent a promising solution to the environmental challenges posed by petroleum-based plastics. Herein, we describe two projects funded by the Beckman Young Investigator Award focused on developing novel degradable polymers that rely on energetically favored cascade reactions to achieve favorable reactivities in polymerization and depolymerization. In the first project, we uncovered a photocatalytic approach to degradable vinyl polymers with tunable main-chain composition via radical ring-opening cascade polymerization (rROCP). Radical copolymerization of the macrocyclic monomers and acrylates or acrylamides mediated by visible light at mild temperatures afforded vinyl copolymers with tunable degradable units evenly distributed in the polymer backbone. In the second project, we developed a novel class of enyne self-immolative polymers (SIPs) capable of metathesis cascade-triggered depolymerization. These SIPs demonstrated excellent stability in strong acid, base, and nucleophiles, and can undergo efficient and complete depolymerization once triggered by a metathesis catalyst. Together, these works established platform technologies for the synthesis of novel degradable polymeric materials for a broad array of applications ranging from packaging and construction materials to biosensing and drug delivery.

**Kimberly See, PhD**

2019 Beckman Young Investigator  
Chemistry (Inorganic Chemistry)  
California Institute of Technology



**Divalent Ion Conductivity in the Solid State**

Li-ion batteries revolutionized portable electronics and changed the way we live, but their cost and energy density are insufficient to target new applications like renewable energy storage. We aim to develop new battery chemistries that meet the cost and energy targets using more abundant and less expensive resources compared to Li. Of specific interest are divalent ions, like  $Mg^{2+}$ ,  $Ca^{2+}$ , and  $Zn^{2+}$ , that enable the use of metal anodes of high volumetric and gravimetric capacity while using Earth abundant metals. The electrochemistry associated with divalent ions is more complicated than their monovalent counterparts. Here, we address a specific component of divalent ion electrochemistry: ionic conductivity in the solid-state. We aim to develop a fundamental understanding of and the associated structure-property relationships for divalent ion conductivity. To study ionic conductivity in an electronic insulator, a model system based on the  $MPS_3$  family of materials is developed that supports  $Zn^{2+}$  conductivity. After installing a redox active metal, V, into the structure, we can leverage the combination of redox activity and ionic conductivity to create a reversible cathode.

**DAY 1 PRESENTER – 8/5**

**Kirk Wangenstein, MD/PhD**  
2019 Beckman Young Investigator  
Biology (Medicine, Cancer)  
University of Pennsylvania



**An *in vivo* MYC partner-gene screen identifies IQGAP3 as a synthetic-lethal target in hepatocellular carcinoma**

Hepatocellular carcinoma (HCC) results from chronic liver injury, is a leading cause of cancer-related death and has limited treatment options. Drugs used to treat HCC must be safe to use in injured livers undergoing repair and regeneration. MYC is one of the most prominent oncogenes driving cancer. Unfortunately, no effective drugs can block MYC. Here, we have designed a strategy to identify MYC synthetic lethal targets in HCC. Methods: We designed an *in vivo* CRISPR inhibition (CRISPRi) system to target 531 putative MYC partner genes in a synthetic lethal screen. We delivered plasmid libraries to the liver to target these genes in the context of MYC overexpression and hyperproliferation. We compared and validated gRNAs depleted to the condition of no overexpression of MYC. Results: gRNAs targeting the gene *Iqgap3* were depleted only in the setting of MYC overexpression. Targeting *Iqgap3* in individual mice blocked HCC development. IQGAP3 appears to be expressed in human HCC. Conclusion: *Iqgap3* is a promising target for drug development because it is predicted to have few side effects.

**Brad Zuchero, PhD**  
2019 Beckman Young Investigator  
Biology (Neuroscience)  
Stanford University



**IMAGeNs: genetically encoded tools for determining the role of myelin in brain circuits**

Human thought and memory is made possible by the activity and connections between the 100 billion neurons in the brain. These complex functions arise from a combination of the strength of synapses that connect neurons together, the ability of individual neurons to fire electrically, and the speed at which electrical signals propagate through neuronal axons. Neuroscientists have long focused on understanding how synapses and electrical excitability contribute to higher-order brain functions. However, far less is known about whether the speed of electrical signals through axons is also dynamically tuned to regulate brain function. We aim to determine how myelin—the electrical insulator around neuronal axons that speeds nerve signaling—contributes to the plasticity of neuronal circuits. We are building novel tools for perturbing myelin in the brain that we call IMAGeNs (Inhibitors of Myelination Around Genetically-defined Neurons). IMAGeNs will enable us to dissect how myelin contributes to specific brain circuits and types of neurons, bringing us closer to a holistic understanding of how cells in the brain collaborate to build a functional nervous system.

**DAY 1 PRESENTER – 8/5**

**John Blazeck, PhD**

2020 Beckman Young Investigator  
Biology (Immunology, Virology &  
Infectious Disease)  
Georgia Institute of Technology



**Synthetic antibody repertoires: Progress towards making new tool for antibody and vaccine development in yeast**

The immune system's failure to fight disease results in illness, morbidity, or even mortality, demanding the development of novel vaccines and therapeutics that effectively augment immune responses. To this end, our project's goal is to create synthetic microbial immune systems that can accelerate the development of these therapies and vaccines. We are seeking to import the ability to make antibodies 'from scratch' in yeast, mimicking what is done in human B cells, by enabling the immune-diversifying V(D)J recombination and somatic hypermutation (SHM) processes in yeast. By employing millions of yeast in a culture that can all generate different 'of human-origin' antibodies from scratch, we want to recapitulate human antibody repertoire generation – a vital aspect of immune response to disease. In this poster, we will detail our prior and planned attempts to engineer yeast to perform VDJ recombination and somatic hypermutation.

**Jennifer Bridwell-Rabb, PhD**  
2020 Beckman Young Investigator  
Chemistry (Biochemistry)  
University of Michigan



**An O<sub>2</sub>-dependent Strategy for C-H bond functionalization in Photosynthetic Pigment biosynthesis**

The ability of photosynthetic organisms to harness sunlight and transform CO<sub>2</sub> into fuel, biomass, chemicals, and/or produce hydrogen makes them attractive for industrial processes. However, several obstacles remain towards harnessing the potential of these organisms, including the oxygen-sensitivity of hydrogen-producing enzymes and an uneven distribution of light in bioreactors. To overcome these limitations, my laboratory studies the mechanisms that photosynthetic organisms use to inhabit nearly every environment on Earth. One aspect of this work involves engineering photosynthetic pigment modification enzymes to build a library of custom-tuned natural and non-natural pigments. Here, we studied chlorophyllide a oxygenase (CAO), an O<sub>2</sub>-dependent metalloenzyme, that is involved in installing the formyl group of chlorophyll b. We accomplished the first purification and in vitro demonstration that CAO is involved in chlorophyll b production. We also identified a key intermediate that shows CAO works by catalyzing two hydroxylation reactions. This work thus adds to our fundamental understanding of chlorophyll biosynthesis and provides an enzyme platform that can be engineered to formylate other tetrapyrroles or to produce other formylated chlorophyll pigments.

**DAY 1 PRESENTER – 8/5**

**Laura Duvall, PhD**

2020 Beckman Young Investigator  
Biology (Neuroscience)  
Columbia University



**Peptide signals that control mosquito mating behaviors**

*Ae. aegypti* mosquitoes are vectors for pathogens that cause Zika, dengue fever, and chikungunya. A single mating event provides a female with sperm to fertilize all of the offspring she will produce for the rest of her life. During mating, male mosquitoes transfer peptide signals that act on receptors expressed in the female that block her from mating with other males. This enforces his paternity and ensures that he is the father of all of her offspring. These signals can also be used in a form of competition between two species termed “satyrization” when males of one species inappropriately “mate” with females of another species and block females from mating with males of their own species. This prevents the females from successfully reproducing, effectively sterilizing them. We aim to identify peptides transferred from the male to the female, determine which receptors they activate in the female, and ask how interspecies competition may affect these receptors. The molecules that we discover could be used to develop new ways to control mosquito populations by blocking female reproduction.

**Andrea Giovannucci, PhD**

2020 Beckman Young Investigator  
Biology (Neuroscience)  
University of North Carolina, Chapel  
Hill



**DAY 1 PRESENTER – 8/5**

**FIOLA: An accelerated pipeline for Fluorescence Imaging Online Analysis**

Optical microscopy methods, calcium and voltage fluorescence indicators of brain activity already enable fast (200-1000Hz) readout of large neuronal populations using light. However, the lack of corresponding advances in online algorithms has slowed progress in gathering information about ongoing experiments. This technological gap not only prevents the execution of novel real-time closed-loop experiments, but also hampers a fast experiment-analysis-theory turnover for high-throughput imaging modalities. The fundamental challenge is to reliably extract neural activity from fluorescence imaging frames at speeds compatible with new indicator dynamics and imaging modalities. To meet these challenges and requirements, we propose a framework for Fluorescence Imaging OnLine Analysis, named FIOLA. FIOLA exploits computational graphs and accelerated hardware to provide optimized motion correction, source extraction and spike detection routines that, for the first time, operate at speeds in excess of 300Hz on standard fields of view for calcium imaging and at over 400Hz for voltage imaging movies. We evaluate these algorithms on ground truth data and large datasets, demonstrating reliable and scalable performance. Our method provides the computational substrate required to interface precisely large neuronal populations and machines in real-time, enabling new applications in neuroprosthetics, brain-machine interfaces, and experimental neuroscience. Moreover, this new set of tools is poised to dramatically shorten the experiment-data-theory cycle by providing immediate feedback on the activity of large neuronal populations at experimental time.

**Stavroula Hatzios, PhD**

2020 Beckman Young Investigator  
Chemistry (Biochemistry/Chemical  
Biology/Microbiology)  
Yale University



**Precision Tools for the Selective Detection of Bacterial Pathogens in Complex Microbial Communities**

The rapid diagnosis and treatment of bacterial infections is critical for controlling the spread of disease. However, selectively targeting disease-causing bacteria in complex microbial communities, such as the human microbiota, remains a significant challenge. We are harnessing the native enzymatic machinery of pathogenic bacteria to develop biosensors that can detect disease-causing microbes in the gut. Our approach draws on the fundamental principles of protease biochemistry for the design of these precision tools. Through the chemical modification of a native, autoinhibitory protease domain, we have engineered a prototype biosensor that can selectively detect the cholera pathogen *Vibrio cholerae* in mixed microbial cultures. In the long term, our technology could form the basis of new point-of-care diagnostics to improve infection outcomes in resource-limited settings.

**Sarah King, PhD**

2020 Beckman Young Investigator  
Chemistry (Imaging & Spectroscopy)  
University of Chicago



**DAY 1 PRESENTER – 8/5**

**A new spectroscopic method to probe the “unreachable”**

Ultrafast charge transfer across the interface between two different materials underpins performance and energy storage in solar cells and batteries, catalysis, and medical devices. The mechanism of this interfacial charge transfer step, and whether it’s efficient, fast, and free of deleterious side reactions, is dictated by the electronic states and ultrafast processes at the buried interface. However, the electronic structure and dynamics at buried interfaces have proven notoriously difficult to selectively probe with the current spectroscopic methods. I will describe progress on our research project aimed at solving this problem – the innovation of a new all-optical, actively-stabilized, time-resolved heterodyned sum-frequency-generation spectrometer. We have successfully obtained interferograms of SFG with our spectrometer design and extensive simulations show how the new design will improve spectral fidelity even in the presence of phase instability.

**James McKone, PhD**

2020 Beckman Young Investigator  
Chemistry (Electrochemical  
Engineering)  
University of Pittsburgh



**Electrifying Chemical Manufacturing**

My lab is developing electrochemical tools and technologies that will transform chemical manufacturing into an environmentally sustainable enterprise. Our BYI-supported research program is focused on recycling environmental pollutants like CO<sub>2</sub> and plastic waste back into useful chemical feedstocks by using a coordinated network of catalysts that can extract hydrogen from water and activate it toward further reactions, just as molecules like NADH do in biology. This poster will discuss progress over the past year, during which we have developed a thermodynamic framework to design these types of multi-component catalysts. We have also demonstrated the ability to activate hydrogen by injecting it into an inorganic metal oxide compound and then releasing the hydrogen on demand to selectively hydrogenate gaseous hydrocarbons.

**Dipti Nayak, PhD**

2020 Beckman Young Investigator  
Biology (Microbiology)  
University of California, Berkeley



**Post-translational thioamidation of methyl-coenzyme M reductase:  
a key enzyme in methanogenic and methanotrophic Archaea**

Methyl-coenzyme M reductase (MCR), found in strictly anaerobic methanogenic and methanotrophic archaea, catalyzes the reversible production and consumption of the potent greenhouse gas methane. The  $\alpha$  subunit of MCR (McrA) contains several unusual post-translational modifications, including a rare thioamidation of glycine. Based on the presumed function of homologous genes involved in the biosynthesis of a thioamide-containing natural product, we hypothesized that the archaeal *tfuA* and *ycaO* genes would be responsible for post-translational installation of thioglycine into McrA. Mass spectrometric characterization of McrA from the methanogenic archaeon *Methanosarcina acetivorans* lacking *tfuA* and/or *ycaO* revealed the presence of glycine, rather than thioglycine, supporting this hypothesis. Phenotypic characterization of the  $\Delta ycaO$ -*tfuA* mutant revealed a severe growth rate defect on substrates with low free energy yields and at elevated temperatures (39 °C - 45 °C). Our analyses support a role for thioglycine in stabilizing the protein secondary structure near the active site.

**DAY 1 PRESENTER – 8/5**

**Maxwell Robb, PhD**

2020 Beckman Young Investigator  
Chemistry (Materials Science)  
California Institute of Technology



**A Universal Molecular Design Platform for Mechanically Triggered Release**

Polymer mechanochemistry is a nascent field of research at the intersection of polymer chemistry, organic chemistry, and materials science that uses mechanical force as a stimulus to promote chemical reactions of unique stress-responsive molecules called mechanophores. Our research aims to develop a modular and general mechanophore design platform to enable the mechanically triggered release of functional molecules from stimuli responsive polymers. Polymers that release molecular cargo in response to mechanical force are exciting targets for a diverse range of applications including drug delivery, sensing, self-healing materials, and catalysis.

**Yue (Jessica) Wang, PhD**

2020 Beckman Young Investigator  
Chemistry (Materials Science &  
Engineering)  
University of California, Merced



**Architected Conducting Polymer Hydrogels**

Conducting polymer hydrogels combine electrical conductivity and tunable water content, rendering them strong candidates for a range of applications including biosensors, cell culture platforms, and energy storage devices. However, these hydrogels are mechanically brittle and prone to damage, prohibiting their use in emerging applications involving dynamic movement and large mechanical deformation. Here, we demonstrate that applying the concept of architecture to conducting polymer hydrogels can circumvent these impediments. A stereolithography 3D printing method is developed to successfully fabricate such hydrogels in complex lattice structures. The resulting hydrogels exhibit elastic compressibility, high fracture strain, enhanced cycling stability, and damage-tolerant properties despite their chemical composition being identical to their brittle, solid counterparts. Furthermore, concentrating the deformation in the 3D geometry, rather than polymer microstructure, effectively decouples the mechanical and electrical properties of the hydrogel lattices from their intrinsic properties associated with their chemical composition. The confluence of these new physical properties for conducting polymer hydrogels opens broad opportunities for a myriad of dynamic applications.

**DAY 1 PRESENTER – 8/5**

**Roxanne Beltran, PhD**

2021 Beckman Young Investigator  
Biology (Ecology and Evolutionary  
Biology/Marine Biology)  
University of California, Santa Cruz



**A novel acoustic recorder for eavesdropping on the ocean soundscape**

Man-made sounds disrupt and, in extreme cases, kill marine mammals around the world. However, the ocean soundscape remains poorly understood, especially in offshore regions. To characterize the natural and human-generated sounds that marine vertebrates experience, and to measure the detrimental impacts of anthropogenic noise, I will develop and implement groundbreaking new technology - a miniature, self-contained acoustic recorder designed for underwater applications. By attaching this new technology to wild elephant seals that migrate ~10,000-kilometers each year, we will provide the first large-scale recordings of the open ocean and the twilight zone (200-1000 meters below the ocean surface). Each new tag will provide ~70 days of audio recordings for only \$5,000, approximately 115 times cheaper and infinitely less noisy than the vessels used for traditional acoustic surveys. This project would represent the first long-term application of animals as platforms for recording sound. By enabling more comprehensive monitoring of ocean noise and revealing the most prevalent and harmful sound sources, we will provide valuable recommendations for marine mammal conservation, including the designation of future Marine Protected Areas.

**Tania Lupoli, PhD**

2021 Beckman Young Investigator  
Chemistry (Chemical Biology)  
New York University



**Designing Synthetic Bacterial Cell Surfaces**

This poster provides an overview of our proposal to design synthetic bacterial cell surfaces by tuning the activity of dedicated enzymes called glycosyltransferases.

**DAY 1 PRESENTER – 8/5**

**Quinn Burlingame, PhD**

2019 Arnold O. Beckman Postdoctoral Fellow

Chemistry (Chemical Engineering)  
Princeton University



**Molecular Design of UV-Absorbing Organic Semiconductors for Transparent Solar Cells**

Transparent photovoltaic cells are an emerging technology that can provide point-of-use electricity generation for building-integrated applications. While most transparent solar cells to-date target absorption of the photon-rich near-infrared portion of the solar spectrum, these devices compromise color neutrality and transparency due to the parasitic absorption of long wavelength visible light. One solution to eliminate this parasitic absorption is to instead employ materials that absorb near-ultraviolet light with sharper absorption cutoffs. While their power output is lower, their theoretical transparency and color neutrality can be much higher, making them a potential match for low-power applications that benefit from maximum optical clarity. Here, we synthesize a series of five UV-absorbing organic donor molecules, and integrate them into organic solar cells with an indium tin oxide top electrode and an organic optical outcoupling layer. The two best performing solar cells exhibit average photopic-response-weighted transmittances of 80.3 – 81.8% and color-rendering indices of 95.0 – 97.1, both of which are records, while maintaining output power densities of 6.1 – 7.0 W/m<sup>2</sup> under simulated solar illumination.

**Kangway Chuang, PhD**

2019 Arnold O. Beckman Postdoctoral  
Fellow

Chemistry

University of California, San Francisco



**Attention-Based Learning on Molecular Ensembles**

The three-dimensional shape and conformation of small-molecule ligands are critical for biomolecular recognition, yet encoding 3D geometry has not improved ligand-based virtual screening approaches. We describe an end-to-end deep learning approach that operates directly on small-molecule conformational ensembles and identifies key conformational poses of small-molecules. Our networks leverage two levels of representation learning: 1) individual conformers are first encoded as spatial graphs using a graph neural network, and 2) sampled conformational ensembles are represented as sets using an attention mechanism to aggregate over individual instances. We demonstrate the feasibility of this approach on a simple task based on bidentate coordination of biaryl ligands, and show how attention-based pooling can elucidate key conformational poses in tasks based on molecular geometry. This work illustrates how set-based learning approaches may be further developed for small molecule-based virtual screening.

**Julie Fenton, PhD**

2019 Arnold O. Beckman Postdoctoral  
Fellow

Chemistry (Materials Chemistry)  
Northwestern University



**Re-evaluating and improving covalent organic framework  
membranes for molecular separations**

Covalent organic framework (COF) materials are a class of crystalline, permanently porous polymers with a regular reticular architecture. The stable covalent bonds and tunable pore sizes seem to optimally position COFs as functional membranes for energy-efficient separations, with intuitive structure-property relationships. Thick, polycrystalline COF films have been reported to separate dyes, salts, bacteria, and nanoparticles on the basis of size-selective transport through ordered pores. This talk will highlight a paired experimental and computational approach that identified adsorption as the primary mechanism driving molecular separations in these state-of-the-art films, rather than size-selective sieving. Our results suggest that separations based on differential transport through ordered COF pores remain an important yet unrealized frontier. Efforts to improve the routine materials quality of COF films, critical towards the goal of realizing a size-sieving membrane, are ongoing.

**Miguel Gonzalez, PhD**

2019 Arnold O. Beckman Postdoctoral  
Fellow

Chemistry (Inorganic Chemistry)  
Harvard University



**Taming the Chlorine Radical: Observation and Control of Chlorine Radical-Mediated C–H Activation**

The activation of C–H bonds requires the generation and control of high-energy intermediates. In particular, chlorine radicals readily cleave strong C(sp<sup>3</sup>)–H bonds, but their inherently high reactivity leads to nearly indiscriminate activation of molecules with different C–H bonds. We demonstrate that photochemical generation of chlorine radicals within the secondary coordination sphere of an iron(III) pyridinediimine complex enables the spectroscopic and photocrystallographic observation of the preferential activation of a C–H bond in the solid state. Furthermore, we designed a series of iron(III) pyridinediimine complexes that confine photoeliminated chlorine radicals within the secondary coordination sphere, thereby enforcing steric control over chlorine radical reactivity. As a result, these complexes exhibit selectivity for the activation of more accessible primary and secondary C–H bonds, overriding thermodynamic selectivity for weaker tertiary C–H bonds.

**DAY 1 PRESENTER – 8/5**

**Stewart Mallory, PhD**

2019 Arnold O. Beckman Postdoctoral  
Fellow

Chemistry (Materials Science &  
Development)

California Institute of Technology



**A mechanical theory of nonequilibrium phase coexistence and its application to motility-induced phase separation**

Here, we present a mechanical theory of phase coexistence broadly applicable to nonequilibrium and equilibrium systems. Our approach is motivated by ideas developed nearly a half-century ago to study the behavior of inhomogeneous classical fluids. We demonstrate the utility of our method by applying it to the important problem of motility-induced phase separation (MIPS) of active Brownian particles. In addition to quantitatively determining the phase diagram of MIPS in two and three dimensions, our theory predicts previously unreported anomalous interfacial phenomena, which we confirm by computer simulations. The self-consistent determination of bulk and interfacial phase behavior offered by this mechanical perspective provides a concrete path towards a general theory for nonequilibrium phase transitions.

**Alexander Schuppe, PhD**

2019 Arnold O. Beckman Postdoctoral  
Fellow

Chemistry (Organic Chemistry)  
Massachusetts Institute of Technology



**Enantioselective Hydrocyanation of Olefins without Cyanide**

Although hydrocyanation of feedstock olefins is conducted on a million-metric ton scale annually to produce nitrile polymers, these protocols employ gaseous hydrogen cyanide and form achiral products. Enantioenriched nitriles are found in numerous natural products, materials and pharmaceuticals, however, the currently available methods to access this substructure often necessitate the use of extremely hazardous chemical reagents and are limited to minimally functionalized substrates. Though strategies for the asymmetric olefin hydrocyanation have existed for decades, few synthetic advances been achieved. Herein, we report a cyanide-free dual Pd/CuH-catalyzed protocol for the asymmetric Markovnikov hydrocyanation of vinyl arenes and the anti-Markovnikov hydrocyanation of terminal olefins in which oxazoles function as nitrile equivalents. After an initial hydroarylation process, the oxazole substructure was deconstructed using a [4 + 2]/retro-[4 + 2] sequence to afford the enantioenriched nitrile product under mild reaction conditions. Using a related reaction manifold we have demonstrated that the intermediate alkyl oxazole can serve as a surrogate for additional important functional groups in organic synthesis, including highly substituted pyridines and imides.

**DAY 1 PRESENTER – 8/5**

**Adam Slavney, PhD**

2019 Arnold O. Beckman Postdoctoral  
Fellow

Chemistry (Materials Chemistry)  
Harvard University



**Low-temperature melting and recrystallization in a hydrogen-bonded framework and ionic liquid**

Molten phases of microporous framework materials may be able to adsorb large numbers of guest molecules directly from the liquid state. However, most framework materials do not melt and the few that do have melting point that are too high ( $> 200\text{ }^{\circ}\text{C}$ ) for appreciable physisorption to occur in the melt. My work is to lower the melting point of a framework material further and observe its sorption behavior. I will show that by using a hydrogen-bonded organic frameworks and lowering the symmetry of the framework molecules, the framework melting point can be lowered to the range of  $70 - 140\text{ }^{\circ}\text{C}$  depending on the framework guest. The framework is only stable in the presence of guests and forms an ionic liquid when guests are removed. Exposure of the neat ionic liquid to guest molecules reforms the crystalline framework. This phase behavior is similar to that observed in clathrate hydrates and may be general for frameworks with low melting points where the driving forces for melting and physisorption are of similar magnitude.

**Benjamin Snyder, PhD**

2019 Arnold O. Beckman Postdoctoral Fellow

Chemistry (Inorganic Materials Chemistry)  
University of California, Berkeley



**A Ligand Insertion Mechanism for Cooperative Adsorption in Metal-Organic Frameworks**

Porous materials have been explored extensively as solid adsorbents for gas storage and separation. However, it remains difficult to attain a high working capacity with high adsorbate selectivity. Here, we report a new mechanism for cooperative gas adsorption that addresses this challenge. For a large family of metal-dicarboxylate frameworks, adsorbates reversibly insert into structural metal-ligand bonds. Adsorbate insertion induces a transformation from a porous three-dimensional framework to a dense one-dimensional polymer in which each metal center binds four equivalents of adsorbate. Upon desorption, the polymer spontaneously re-assembles into the original porous framework. Focusing on the economically significant application of selective ammonia adsorption, we have found that metal-dicarboxylates are stable to adsorption/desorption cycling, with adsorption profiles that can be readily tuned based on the identities of the metal and organic linker. Framework modifications also enable cooperative uptake of other adsorbates such as atmospheric water. These results underscore the potential utility and generalizability of this unusual mechanism for high-capacity cooperative gas adsorption.

**DAY 1 PRESENTER – 8/5**

**Dayne Swearer, PhD**

2019 Arnold O. Beckman Postdoctoral Fellow

Chemistry (Materials Science & Development)

Stanford University



**Single Particle Cathodoluminescence Spectroscopy with sub-20 nm Electron-Stable Phosphors**

Lanthanide-doped nanophosphors have emerged as promising optical labels for high-resolution, “multicolor” electron microscopy. Here, we develop a library of eleven unique lanthanide-doped nanophosphors with average edge lengths of  $15.2 \pm 2.0$  nm ( $N = 4284$ ). These nanophosphors consist of an electron stable  $\text{BaYF}_5$  host lattice doped at 25% atomic concentration with the lanthanides  $\text{Pr}^{3+}$ ,  $\text{Nd}^{3+}$ ,  $\text{Sm}^{3+}$ ,  $\text{Eu}^{3+}$ ,  $\text{Tb}^{3+}$ ,  $\text{Dy}^{3+}$ ,  $\text{Ce}^{3+}$ ,  $\text{Ho}^{3+}$ ,  $\text{Er}^{3+}$ ,  $\text{Tm}^{3+}$ , and  $\text{Yb}^{3+}$ . Under  $\sim 100$  pA/nm<sup>2</sup> beam current in a transmission electron microscope, each nanophosphor species exhibits strong cathodoluminescence spectra with sharp characteristic emission lines for each lanthanide. The bright emission and stability of these nanoparticles enable not only ensemble, but also single-particle cathodoluminescence spectroscopy, which we demonstrate with  $\text{BaYF}_5:\text{Ln}^{3+}$  where  $\text{Ln}^{3+} = \text{Tb}^{3+}$ ,  $\text{Ho}^{3+}$ ,  $\text{Er}^{3+}$ ,  $\text{Sm}^{3+}$ ,  $\text{Eu}^{3+}$ , or  $\text{Pr}^{3+}$ . Single-particle cathodoluminescence corresponds directly with HAADF intensity across nanoparticles, confirming high spatial localization of the measured cathodoluminescence signal of lanthanide-doped nanophosphors. Our synthesis and characterization of sub-20nm electron-stable nanophosphors provides a robust material platform to achieve single-molecule labeled correlative cathodoluminescence electron microscopy, a critical foundation for high-resolution correlation of single-molecules within the context of cellular ultrastructure.

**Amy Marie Bartholomew, PhD**

2020 Arnold O. Beckman Postdoctoral Fellow

Biology (Inorganic Chemistry)  
Columbia University



**Building 2D Materials from Superatoms**

Atomically precise nanoscale clusters (“superatoms”) are ideal candidates for the bottom-up synthesis of tunable 2D van der Waals materials since their properties can be controlled via their constituent atoms, oxidation state, and ligand periphery. Superatoms can form cyanometalate frameworks, and an equatorially cyanide-ligated octahedral superatom would allow for 2D materials synthesis. Towards this end, we synthesized *trans*-Co<sub>6</sub>Se<sub>8</sub>(CO)<sub>2</sub>(PPh<sub>3</sub>)<sub>4</sub> regioselectively and in high yield, which forms [*trans*-Co<sub>6</sub>Se<sub>8</sub>(CO)<sub>2</sub>(CN)<sub>4</sub>]<sup>n-</sup> (n = 3, 4) upon treatment with tetrabutylammonium cyanide. Combination of Fe(II) or Co(II) salts, pyridine, and [*trans*-Co<sub>6</sub>Se<sub>8</sub>(CO)<sub>2</sub>(CN)<sub>4</sub>]<sup>3-</sup> in water formed crystals of the 2D frameworks [Fe(py)(H<sub>2</sub>O)][*trans*-Co<sub>6</sub>Se<sub>8</sub>(CO)<sub>2</sub>(CN)<sub>4</sub>] and [Co(py)<sub>4</sub>]<sub>2</sub>[*trans*-Co<sub>6</sub>Se<sub>8</sub>(CO)<sub>2</sub>(CN)<sub>4</sub>], respectively. Crystals of [Co(py)<sub>4</sub>]<sub>2</sub>[*trans*-Co<sub>6</sub>Se<sub>8</sub>(CO)<sub>2</sub>(CN)<sub>4</sub>] were exfoliated down to a thickness of 1.8 nm, corresponding to the height of a bilayer. After exfoliation, the photolabile CO groups on the surface of the sheets were readily exchanged for isocyanide ligands as assessed via Raman spectroscopy. The construction of 2D materials from superatoms allows for the incorporation of desirable cluster-associated features such as photolabile ligands into ultrathin exfoliated materials, and the superatoms described herein offer numerous opportunities for the further synthesis of 2D materials.

**DAY 1 PRESENTER – 8/5**

**Joseph Derosa, PhD**

2020 Arnold O. Beckman Postdoctoral Fellow

Chemistry (Organometallic Chemistry)  
California Institute of Technology



**Electrocatalytic Concerted Proton-Electron Transfer (eCPET) using a Cobaltocene-Derived Mediator: New Synthetic Strategies for Electroreduction of C–C  $\pi$ -Bonds at Lower Overpotentials**

Reductive concerted proton-electron transfer (CPET) is poorly developed for the reduction of C–C  $\pi$ -bonds, including for activated alkenes that can succumb to deleterious pathways (i.e., a competing hydrogen evolution reaction (HER) or oligomerization) in a standard electrochemical reduction. We demonstrate herein that selective hydrogenation of the C–C  $\pi$ -bond of fumarate esters can be achieved *via* electrocatalytic CPET (eCPET) using a CPET mediator comprised of cobaltocene with a tethered Brønsted base. High selectivity for electrocatalytic hydrogenation is only observed when the mediator is present. Mechanistic analysis sheds light on two distinct kinetic regimes based on the substrate concentration; low fumarate concentrations operate *via* rate-limiting CPET followed by an electron-transfer/proton-transfer (ET/PT) step, whereas high concentrations operate *via* CPET followed by a rate-limiting ET/PT step.

**Myles Drance, PhD**

2020 Arnold O. Beckman Postdoctoral Fellow

Chemistry (Inorganic Chemistry)  
Massachusetts Institute of Technology



**DAY 1 PRESENTER – 8/5**

**Altering the Reactivity of Phosphorus Through Geometric Constraint**

The reactivity of geometrically constrained three-coordinate phosphorus ( $\sigma^3$ -P) compounds is presented. Relative to typical  $\sigma^3$ -P compounds (e.g., phosphines) that display local  $C_{3v}$  symmetry, distorted  $C_s$ -symmetric  $\sigma^3$ -P compounds possess a significantly lower energy lowest unoccupied molecular orbital (LUMO) and a highest occupied molecular orbital (HOMO) of comparable energy. This decreased HOMO/LUMO gap leads to a phosphorus center that is both nucleophilic and electrophilic (i.e., biphilic). A representative example of this biphilic reactivity is the previously reported formal oxidative addition of water to a constrained phosphoramidite. We now leverage the resulting hydrido-hydroxyphosphorane as a source of  $H^+$  and  $H^-$  equivalents for the reduction of imines and ketones to amines and alcohols, respectively. Separately, geometrically constrained phosphorus triamides with pyridyl and phosphine sidearms have been synthesized for their use as chelating ligands to transition metals. Unusual metal-ligand cooperativity is observed in which metal-bound substituents migrate to the phosphorus center in some cases, and in other instances, phosphorus assists in the oxidative addition of substrate.

**James Gaynor, PhD**

2020 Arnold O. Beckman Postdoctoral  
Fellow

Chemistry (Physical Chemistry)  
University of California, Berkeley



**Savory Electronic Correlations Occur Within a Few Millionths-of-a-Billionth of a Second**

Core-excitons are bound electron-hole pairs in which the hole resides in a core-level. Core-excitons can be highly localized, atom-like, excitations which can exist in solid-state materials. Despite decades of study, the electronic structure and dynamics of core-excitons in materials is not understood. The prototypical alkali halide, NaCl, is studied here. This work bridges the gap between gas phase atomic spectroscopy and condensed phase materials chemistry by demonstrating that attosecond four-wave mixing (FWM) spectroscopy can be used to directly measure core-exciton dynamics in solids. FWM was pioneered to study gas phase electronic and vibrational coherent dynamics using an experimental geometry yielding background free signal measurement of excited state lifetimes directly in the time-domain. The atom-like nature of the core-excitons lend FWM particularly sensitive to these dynamics. This nonlinear experiment allows us to deconvolve a heterogeneous distribution of core-excitons in NaCl by studying both optically allowed and forbidden state dynamics. At least five core-excitons are revealed in this study, all of which undergo <10 femtosecond dephasing dynamics driven by multi-electron correlation and exciton exchange interactions.

**Megan Jackson, PhD**

2020 Arnold O. Beckman Postdoctoral Fellow

Chemistry (Inorganic Chemistry)  
University of California, Berkeley



**Molecular Control of Crystal Morphology in Anisotropic Metal-Organic Frameworks**

Metal-organic frameworks (MOFs) hold promise across a wide range of applications, including gas storage and separations, targeted drug delivery, catalysis, and sensing. MOF crystal phase, size, and morphology, all results of the crystallization process, dictate the bulk properties of the MOF, including active surface area, separation efficiency, and overall performance. Despite this potential, there is currently little understanding of the synthetic principles behind MOF crystallization, and the synthesis of MOF crystals of a given phase or morphology typically relies on brute-force strategies, including trial-and-error and high-throughput screening rather than rational design. Here, we demonstrate that noncoordinating buffers coupled with judiciously chosen coordination modulators can control crystal aspect ratio and overall morphology in an anisotropic MOF,  $\text{Co}_2(\text{dobdc})$ . We demonstrate that these modulators incorporate into the crystals at very low ( $\sim 100$  ppm) concentrations, and that they incorporate throughout the crystals, suggesting that they may determine morphology by reversibly binding to the framework throughout crystal growth. Together, these results provide molecular-level insights into how modulators governing crystal morphology and how they incorporate as defects into the final product.

**DAY 1 PRESENTER – 8/5**

**Forrest Laskowski, PhD**

2020 Arnold O. Beckman Postdoctoral  
Fellow

Chemistry (Materials Chemistry)  
California Institute of Technology



**Unsupervised Machines Discover High-performing Electrolytes  
for All Solid-State Batteries**

Discovery of new all-solid-state battery chemistries could be expedited by machine learning approaches. Identification of new solid lattices that support ionic conduction at room temperature are needed. However, use of traditional machine learning algorithms is impeded by a lack of “labels” – relatively few structures have been experimentally characterized. Herein, we employ unsupervised learning techniques that group structures according to input features and do not rely on an abundance of labeled data. All known Li-containing structures from the Inorganic Crystal Structure Database (ICSD) and the Materials Project are analyzed. We discover that a common spatial machine learning featurizer, Smooth Overlap of Atomic Positions (SOAP), results in favorable clustering of the known high-conductivity structures. By examining the non-labeled structures in the high-conductivity clusters, we discover ~200 new structures that are promising candidates for experimental investigation.

**Charles Markus, PhD**

2020 Arnold O. Beckman Postdoctoral  
Fellow

Chemistry (Physical Chemistry)  
California Institute of Technology



**Fast and Sensitive Infrared Spectroscopy with Chip-Scale Optical Frequency Combs**

Unraveling reaction mechanisms in combustion and atmospheric processes often requires measuring transient intermediates, which is inherently challenging. Optical frequency combs, which combine the beneficial properties of continuous wave lasers with broadband sources, can be paired efficiently with enhancement cavities to provide sensitive, fast, and broadband infrared absorption measurements. Here, we demonstrate the use of chip-scale optical frequency combs for measurements in the CH stretching region. Optical frequency combs generated by interband cascade lasers are novel devices which can provide light from 3-6  $\mu\text{m}$  at room temperature. These devices are perfectly suited for Vernier spectroscopy, which is a simple and robust approach to cavity enhanced spectroscopy. Here, we demonstrate the millisecond time resolution by detecting difluoroethane. This clearly demonstrates the viability for this technique in transient experiments, and it will soon be applied to multispecies detection in hydrocarbon radical chemistry.

**DAY 1 PRESENTER – 8/5**

**Matthew Nichols, PhD**

2020 Arnold O. Beckman Postdoctoral Fellow

Chemistry (Ultracold Chemistry)  
Harvard University



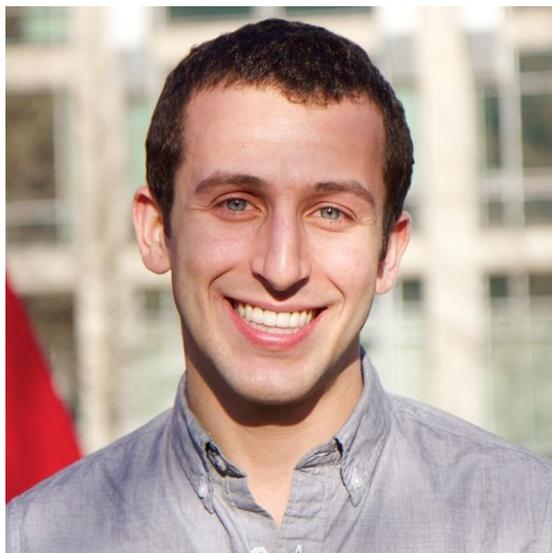
**Probing and Controlling Chemical Reactions Below One Microkelvin**

Poster Abstract (max. 175 words): Chemical reactions which occur at ultralow temperatures provide an ideal platform for studying quantum effects in chemistry, and for testing state-of-the-art quantum scattering calculations. In this poster, I will discuss our work on the exchange reaction,  $2\text{KRb} \rightarrow \text{K}_2 + \text{Rb}_2$ , where the reactants are prepared at a temperature of 500 nK in their rovibronic ground state. By combining state-selective photoionization with ion velocity-map imaging, we achieve state-resolved coincident detection of the products. This allows us to measure the full product state distribution, including the scattering probabilities for all rotational state-pairs allowed by the reaction exoergicity. In the second half of the poster, I will present a new study of collisions between KRb molecules and Rb atoms, where chemical reactions between the two species are energetically forbidden. Through direct detection of the  $\text{KRb}_2^*$  intermediates formed through such collisions, we measure their lifetime to be 0.39(6) ms, a result which is  $\sim 10^5$  times longer than recent estimates based on the RRKM statistical theory. Such a dramatic discrepancy calls for new theoretical insight to provide an explanation.

**Zachary Sherman, PhD**

2020 Arnold O. Beckman Postdoctoral  
Fellow

Chemistry (Chemical Engineering)  
University of Texas, Austin



**Plasmonic Coupling in Self-Assembled Nanoparticle Gels and Superlattices**

Certain nanoparticles, like inorganic nanocrystals, are plasmonic and interact strongly with particular resonant frequencies of light. Plasmonic coupling between nanoparticles results in structure-dependent effective properties, and experiments have shown that structures self-assembled from plasmonic nanoparticles are promising for switchable photovoltaics and electrocatalysts. However, a major challenge to realizing these possibilities is the enormous number of physical parameters and structures to screen. Computational methods can accelerate materials discovery, but probing the effective plasmonic properties remains a major bottleneck. The necessary optical calculations require expensive numerical solutions to many-bodied systems of equations and are therefore limited to configurations of only a handful of particles, which are not representative of large-scale structural features and heterogeneities. To address these shortcomings, we have developed computational tools to rapidly determine the optical response of nanoparticle materials, allowing for tens of thousands of particles to be probed at a time. We use these tools to investigate plasmonic coupling in two important classes of self-assembled materials, nanoparticle gels and superlattices, and establish design principles that connect target collective properties to experimental control knobs.

**DAY 1 PRESENTER – 8/5**

**Tyler Saint-Denis, PhD**

2020 Arnold O. Beckman Postdoctoral Fellow

Chemistry (Main-group chemistry)  
University of California, Berkeley



**Naked,' heavy main-group atoms in the transition metal coordination sphere**

The reaction of  $(\text{Me}^i\text{BDI}^{\text{Dipp}})\text{IrH}_4$  {BDI = ArNC(Me)CH(Me)CNAr, Ar = Dipp = 2,6-Pr<sub>2</sub>C<sub>6</sub>H<sub>3</sub>} with  $\text{E}[\text{N}(\text{SiMe}_3)_2]_2$  (E = Sn, Pb) affords the unusual dimeric metallotetrylylidyne,  $([\text{Me}^i\text{BDI}^{\text{Dipp}}]\text{IrH})_2(\mu_2\text{-E}^\bullet)_2$  in good yields.

Nonbonding orbital analysis of these compounds have revealed that each E atom possesses three non-bonding electrons (total of five electrons), two of which are confined to an orbital of >90% s-character, while the remaining is highly delocalized. Trimeric dimetallotetrylenes of Sn and Pb were also isolated under slightly modified reaction conditions. This reaction seems to be general for heavy main-group compounds with weak E-X (X = O,N) bonds:

The reaction of  $(\text{Me}^i\text{BDI}^{\text{Dipp}})\text{IrH}_4$  with  $\text{Bi}(\text{O}^t\text{Bu})_3$  led to isolation of the closed shell  $([\text{Me}^i\text{BDI}^{\text{Dipp}}]\text{IrH})_2(\mu_2\text{-Bi})_2$ . Attempts to expand syntheses to lighter congeners of the tetryls led to isolation of  $([\text{Me}^i\text{BDI}^{\text{Dipp}}]\text{H Ir}=\text{Ge}[\text{N}(\text{SiMe}_3)_2]_2)$ . The reactivity of these compounds as well as the electronic structure and magnetic properties are currently under exploration.

**James Utterback, PhD**

2020 Arnold O. Beckman Postdoctoral  
Fellow

Chemistry (Physical Chemistry)  
University of California, Berkeley



**DAY 1 PRESENTER – 8/5**

**Towards direct, label-free imaging of energy transport beyond charge carriers**

The nanoscale transport of energy is fundamental to nature and system functionality. At the nanoscale, heat must navigate material heterogeneities that can determine macroscopic properties. Relatedly, ion transport enables the diverse functionality of many electrochemical devices and photoelectrochemistry applications. Despite their immense importance, there are no demonstrations of direct, spatially and temporally resolved heat or ion imaging under complex *operando* conditions. We leverage the fact that refractive index generally increases with temperature and solute concentration. Optical scattering microscopy is sensitive to changes in refractive index, and thus can image heat and ion concentration gradient evolution without the need for an absorptive or emissive probe. In this presentation, I will present recent results visualizing nanoscale heat transport in disordered films of gold nanoparticles, and current progress towards imaging ion transport in solution.

**Stephen von Kugelgen, PhD**

2020 Arnold O. Beckman Postdoctoral  
Fellow

Chemistry

Northwestern University/ Massachusetts  
Institute of Technology



**One Qubit, Two Qubit, Red Qubit, Blue Qubit: Spectral  
Addressability in a Modular Two-Qubit System**

Quantum information science (QIS) leverages our burgeoning control over the quantum properties of light and matter to create transformative new technologies. The core unit of QIS is the quantum bit, or qubit. Molecular electron spin qubits are a promising platform for constructing qubits from the bottom-up, enabling atomically-precise customization of qubit structure and systematic study of fundamental structure-property relationships. One such relation is how the distance and interaction between two qubits dictate coherence properties. To answer this question, we designed a series of molecules containing two spectrally-distinct qubits 1.2 to 2.5 nm apart that we could manipulate independently: a Ti(III) complex and a Cu(II) complex. Using pulse electron paramagnetic resonance spectroscopy, we deconvolute the sources of decoherence to find that a qubit's ligand, not its electron spin, limits its partners' coherence. Quantum state tomography, however, shows that the coupling to the second qubit can still be felt in the coherent evolution of the qubit state. These results showcase chemistry's role in creating designer quantum systems and offer essential insights for future multifunctional, multi-qubit systems.

**Ren Wiscons, PhD**

2020 Arnold O. Beckman Postdoctoral Fellow

Chemistry (Materials Chemistry)  
Columbia University



**Single-Handed Chiral Absorption of the Full Visible Wavelength Range by a [6]Helicene**

The amplification of chiral absorbance and emission has long been perceived as the primary figure of merit for the design of competitive chiral chromophores; however, for dyes to be practically relevant in chiroptical applications, they must also absorb and/or emit chiral light over wide wavelength ranges. Here we investigate the interplay between molecular symmetry and broadband chiral absorbance in a series of [6]helicenes. We find that an asymmetric [6]helicene hosting two distinct chromophores absorbs a single polarity of chiral light across a wider wavelength range than either of the symmetric [6]helicenes investigated here. We propose that this is because the nondegeneracy between chromophores in the asymmetric helicene minimizes coupling between excited states, which generally inverts the handedness of absorbed and emitted light. Chemically reducing the helicenes shifts the absorption edge of the electronic circular dichroism spectra into the near-infrared wavelength range while preserving broad chiral absorption, yielding a [6]helicene that absorbs a single handedness of light across the entire visible spectral range.

**DAY 1 PRESENTER – 8/5**

**Abreanne Andlinger**  
2020 Beckman Scholar  
Biology (Genetics)  
West Virginia University



**Examining Essential Transcription Factor Networks for Neurodevelopment in Zebrafish**

70% of human genes have zebrafish orthologues, thus our findings in this model system might show how transcription factors genomic screen homeobox 1 and 2 (*Gsx1/2*) contribute to neurodevelopment in humans. We hypothesized that *Gsx1* and *Gsx2* regulate the expression of the genes *distal-less homeobox 5a* (*dlx5a*), *distal-less homeobox 6a* (*dlx6a*), *forkhead box P2* (*foxp2*), and *solute carrier family 6 member 3* (*slc6a3*). To test this hypothesis, zebrafish with a mutant allele for *gsx1/2* were used to elucidate the gene networks these transcription factors regulate. *In situ* hybridization was used to detect *dlx5a*, *dlx6a*, *foxp2*, and *slc6a3* mRNA expression in the embryonic zebrafish brain of *gsx1* and *gsx2* mutants. Results indicate *Gsx2* is necessary for the regulation of *dlx5a* and *dlx6a*, but *Gsx1* is not. Based on preliminary results it appears *Gsx2* regulates *foxp2* expression, but these have yet to be quantified. *slc6a3* was inconclusive due to the lack of a strong expression pattern. Future work could investigate other genes possibly regulated by *Gsx1/2* that are involved with neurodevelopmental disorders.

**Jordan Aucoin**  
 2020 Beckman Scholar  
 Chemistry (Physical Chemistry)  
 Amherst College



**The Microwave Spectrum and Molecular Structure of Trans-2-Fluoro-3-(Trifluoromethyl)Oxirane and its Complexes with the Argon Atom and a Chiral Analyte**

Chosen due to its structural similarity with previously characterized chiral tagging candidates, trans-2-fluoro-3-(trifluoromethyl)oxirane (tFTFO) is a small chiral molecule to be investigated, both theoretically and experimentally, as a potential chiral tagging molecule. With a strong, simple rotational spectrum, tFTFO shows promise for applications in chiral analysis through the conversion of enantiomers into spectroscopically distinct diastereomeric species through noncovalent attachment. The rotational spectrum of tFTFO and of Ar-tFTFO is obtained using Fourier transform microwave spectroscopy from 5.6 to 18.1 GHz. The spectrum is analyzed to determine the rotational constants for tFTFO and Ar-tFTFO which allow for the experimental equilibrium and zero-point average structures to be found via Kraitchman analysis and a structure fitting program, respectively. This work shows that the structure of the argon complex is distinct from the structures previously described for the 3,3,3-trifluoro-, 3,3-difluoro-, and 3-fluoro-1,2-epoxypropane species, suggesting that the addition of the lone fluorine atom alters bonding in the epoxy moiety. tFTFO's dimer with a chiral analyte is also studied to assess its effectiveness as a chiral tag.

**DAY 1 PRESENTER – 8/5**

**Allison Baker**

2020 Beckman Scholar  
Biology (Developmental Biology)  
Texas A & M University



**Exploring the Functions of Fgf Signaling on Otic Sensory Epithelia Through Its Downstream Target Gene Pou3f3b**

To better understand the role of Fgf signaling in the inner ear, we analyzed expression of downstream targets of Fgf. Of particular interest, we examined pou3f3b because it uniquely marks the auditory epithelium, it is required for hearing in mammals, and it is thought to be induced by low levels of Fgf signaling. However, treatment with the drug SU5402 to block all Fgf signaling, we unexpectedly saw that the domain of pou3f3b expands to cover the entire inner wall of the otic vesicle. We hypothesized altered expression of pou3f3b reflects residual low-level MAP Kinase activity induced by lactate, which we previously discovered is produced in the otic vesicle by “aerobic glycolysis” (akin to “The Warburg Effect” seen in metastatic tumors) to activate MAP Kinase independently of Fgf.

**Cristina Baker**

2020 Beckman Scholar  
Biology (Neuroscience)  
Georgia Institute of Technology



**Behavioral Gene Expression of the Cichlid Telencephalon**

We implement Spatial Transcriptomics to characterize the genetic profile of the teleost brain and preserve the spatial dimension and microenvironment of neural tissue in vivo. These experiments build upon our lab's single-nuclei RNA sequencing experiments, which explore the neuronal and genetic underpinnings of social behaviors. Through massively parallel sequencing, we multiplex mRNAs and construct information libraries of cell-type clustering based on gene similarity as well as anatomical location in 3D space. These experiments enable us to investigate the role of context-dependent immediate early genes (IEGs) active in intact brain tissue, facilitate the identification of neuronal populations involved in specific behaviors, and delineate evolutionary relationships through analysis of gene enrichment and semantic similarity to humans.

**DAY 1 PRESENTER – 8/5**

**Anton Barybin**

2020 Beckman Scholar  
Chemistry (Analytical Chemistry)  
University of Kansas



**Development of a Separation-Based Sensor for Monitoring Neurotransmitters**

Dysregulation of catecholamine neurotransmission has been linked with neurodegenerative pathologies (e.g., Parkinson's disease) as well as behavioral disorders. Development of highly sensitive and selective analytical tools for simultaneous in vivo monitoring of multiple neurotransmitters in the brain will yield a more comprehensive understanding of these disease states and provide a method for investigating the effects of potential therapeutic drugs. In this study, capillary electrophoresis (CE) with UV detection was used to separate a mixture of four neurotransmitters (dopamine, norepinephrine, epinephrine, serotonin), two metabolites (homovanillic acid, 3,4-dihydroxyphenylacetic acid), and an internal standard (hydroquinone). The optimized separation conditions were subsequently evaluated using microchip electrophoresis (ME) with electrochemical detection (EC). Electrochemical detection was performed at a pyrolyzed photoresist film electrode deposited on a quartz glass plate. The developed separation will ultimately be implemented in a hybrid glass/PDMS ME-EC device coupled to a microdialysis interface for continuous in vivo monitoring of neurotransmitters in rats or other animal model organisms.

**Camaryn Bennett**

2020 Beckman Scholar  
Chemistry (Organic Chemistry)  
Miami University



**DAY 1 PRESENTER – 8/5**

**Adding Transient Bonds to Hyperelastic Models**

Elastic materials have many applications. Dynamically bonded materials have many benefits that cannot be seen in static materials. They can dissipate stress, which is a useful property as it can allow more mechanical challenges to be applied to a system before it fails. Relaxation time of a system can depend on temporary bonds breaking, or the untangling of polymers within the system itself. We proposed a theory for highly elastic materials that included a time dependent element in the analysis of stress-strain curves of dynamic materials, thus accounting for the temporary bonds breaking in materials as opposed to just the stretching of bonds. This gives the ability to extract the modulus due to temporary and permanent bonds, strain hardening and the relaxation time of dynamic materials. This theory gives a more complete picture of the materials properties, and better characterization of the material before it is applied. The model was tested against a wide range of materials, experimental and taken from the literature, and found to be sensitive and applicable across these materials.

**Amber Birt**

2020 Beckman Scholar  
Chemistry (Analytical Chemistry)  
Union College



**Measuring Concentrations of Acrylamide in Brewed Coffee**

Amino acids, like asparagine, react with sugars via the Maillard reaction to form compounds that contribute to the color and flavor of roasted foods. However, some undesired products also form during this reaction, one of them being acrylamide. Acrylamide is a neurotoxin and a potential endocrine-disrupting chemical, and increased dietary amounts of acrylamide have been linked to different types of cancers, including ovary, renal and endometrial. In this study, acrylamide is extracted from the brewed coffee using simplified liquid extraction and analyzed alongside known standards using liquid chromatography-tandem mass spectrometry. The accuracy of the method has been validated using a standard reference material of fortified ground coffee. This method has been used to quantify acrylamide concentrations in various types of brewed coffee and investigate the effects of variables such as type of roast, decaffeination, and bean origin. Our results suggest that differences in roast or caffeination do not significantly affect acrylamide concentrations in brewed coffee. Ongoing studies include improving precision and accuracy using the established method and applying the method to investigate trends of acrylamide formation in various types of brewed coffee.

**Katharine Bowers**

2020 Beckman Scholar  
Biology (Developmental Biology)  
Tufts University



**DAY 1 PRESENTER – 8/5**

**Quantifying tadpole bullying behavior: Building an analytical pipeline to investigate how *Xenopus laevis* embryos identify deformities**

Many adult animals demonstrate an innate understanding of "correct" body shape and function through sexual selection, fitness-based competition, and limb regeneration. However, the mechanism by which these organisms identify abnormal morphology and function is unknown. From preliminary observations, we have characterized a new "tadpole bullying" phenomenon, in which morphologically normal *Xenopus laevis* tadpoles attack and kill deformed conspecifics over days when housed together.

We aim to quantify and analyze this bullying behavior. We hypothesize that tadpoles detect deformities and collide more frequently and violently with deformed conspecifics. How do they identify "normal" morphology and how do they decide which deformities warrant attack?

Here we report a system for positional tracking of deformed tadpoles and quantitative analysis of collisions between normal and deformed tadpoles. In future work, we will use this pipeline to analyze interactions involving tadpoles with deformities of different types, severities, and sources, to identify key bodily features and mechanisms with which tadpoles gauge deformity. Understanding how tadpoles identify and maintain correct morphology can open new possibilities in regenerative medicine including birth defect repair.

**Madison Britting**

2020 Beckman Scholar  
Biology (Neurobiology)  
University of Connecticut



**Investigating Sexual Dimorphisms in Thalamic Anatomy**

Two nuclei of the auditory thalamus, the medial division of the medial geniculate nucleus (MGm) and the posterior intralaminar nucleus (PIN), have a critical role of forming the primary path for auditory sensory information from the environment to the emotional behavioral center of the brain, the amygdala, forming the fear circuit that mediates fear responses in rats. The boundaries of these two nuclei have been inconsistently delineated, adding a degree of difficulty to studying fear circuitry. Qualitative analysis of the expression of the calcium binding protein, parvalbumin, following immunohistochemistry allowed the delineation of MGm and PIN. The expression of the transcription factor C-Fos, an indicator of learning, was quantified following standard fear conditioning protocol with tone-shock paired, unpaired, and tone-alone groups. Although no differences were found across behavior paradigms, the number of C-Fos positive cells in MGm and PIN were found to be sexually dimorphic. This is an important discovery due to the historically disproportionate use of male over female rats as experimental subjects and the disregard for sex differences in the field of physiology.

**Kelcie Britton**

2020 Beckman Scholar  
Biology (Plant, Ecology &  
Environmental Sciences)  
West Virginia University



**Functional and Genetic Analysis of Esterase Genes Involved in the Synthesis of Ergot Alkaloids**

Ergot alkaloids are lysergic acid containing compounds produced by fungi associated with human and animal toxicoses. Despite their toxicity, modified and appropriately dosed ergot alkaloid derivatives are effective pharmaceutical treatments for some neurodegenerative diseases. Pathways to some ergot alkaloids have been determined, but the final step in synthesis of lysergic acid amides remains elusive. This gap is significant because many of the pharmaceutically relevant ergot alkaloids are derived from lysergic acid amides. Lysergic acid  $\alpha$ -hydroxyethylamide (LAH) is the main ergot alkaloid produced by the fungus *Metarhizium brunneum*. We hypothesize two genes, *easP* and *estA*, encode esterases involved in the final step of LAH biosynthesis. To test this hypothesis, CRISPR mutants were engineered in *M. brunneum* with *easP* alone or both *estA* and *easP* mutated. Analysis of our mutant strains demonstrated the product of *easP* has a significant role in production of LAH; the *easP* mutant only accumulated half the LAH measured in non-mutant strains. Mutation of *estA* did not affect accumulation of lysergic acid amides, indicating the fungus has an alternate path to LAH.

**DAY 1 PRESENTER – 8/5**

**Luke Broughton**  
2020 Beckman Scholar  
Chemistry (Biochemistry)  
Clemson University



### **Probing the Kinetics of Metal-Catalyzed Thiol Oxidation**

Thiols are abundant throughout the body in molecules such as cysteine and the antioxidant glutathione (GSH). These thiols are biomarkers of cellular oxidative stress, with increasing amounts of oxidized thiol indicating higher amounts of stress.<sup>1</sup> Cellular oxidative stress and DNA damage is often caused by the Fenton and Fenton-like reactions where  $\text{Fe}^{3+}$  and  $\text{Cu}^{2+}$  react with hydrogen peroxide to produce damaging hydroxyl radical.<sup>2</sup> In its reduced form (GSH), glutathione scavenges reactive oxygen species such as hydroxyl radical and can oxidize to form the oxidized glutathione disulfide (GSSG). Neurodegenerative diseases, aging, and other chronic conditions are marked by a decrease in cellular GSH concentrations, and disease prognosis and progression is associated with GSH/GSSG ratios. Similarly, many of these diseases have been linked to the cellular misregulation of copper and iron.<sup>3,4</sup> In this study, we examined the kinetics of metal-catalyzed thiol oxidation in the presence of both  $\text{Cu}^{2+}$  and  $\text{Zn}^{2+}$ . These studies demonstrate the importance of considering the presence of metals in traditional assays.

**Henry Cardwell**  
2020 Beckman Scholar  
Chemistry  
College of William and Mary



**Determination of Experimental and Computational Proton Affinities of Proline Containing Dipeptides**

Peptide fragmentation via the mobile proton model depends on the specific residues of the peptide. One notable example of this can be seen in the “proline effect” which is the tendency of proline-containing peptides to selectively fragment N-terminal to proline residues. This preferential cleavage can confound automated peptide sequencing algorithms. The proline effect results from an enhanced basicity at the proline amide as well as the rigidity of the proline ring. Differing adjacent residues affect the prevalence of the selective cleavage. This research seeks to determine the influence of adjacent residues on the basicity of proline-containing peptides. By experimentally and computationally evaluating the proton affinity of all thirty-nine proline-containing dipeptides, a better understanding of this preferential fragmentation can be gleaned. Experimental results were determined using the extended kinetic method in an ESI triple quadrupole mass spectrometer. Computational Boltzmann-weighted proton affinities were obtained from multiple low-energy conformers of each dipeptide using geometries at the B3LYP/6-31+G(d) level of theory and single point energies at the B3LYP/6-311++G(d,p) level.

**DAY 1 PRESENTER – 8/5**

**Emily Chapa**

2020 Beckman Scholar  
Biology (Genetics)  
Texas A & M University



**Circadian Clock Control of tRNA Synthetases in *Neurospora crassa***

Half of eukaryotic proteins accumulate with a circadian rhythm. Our lab discovered that the circadian clock in *Neurospora crassa* controls translation initiation by regulating the activity of eIF2 $\alpha$  kinase CPC-3, the homolog of mammalian GCN2, and that CPC-3 activity is controlled by binding of uncharged tRNAs to CPC-3. Based on these data, I hypothesized that clock control of tRNA synthetases is necessary for rhythmic CPC-3 activation and mRNA translation in *N. crassa*. To test this hypothesis, I selected RS's that are predicted to be clock-controlled at the RNA level in fungi and mammals, and I have independently confirmed clock control of *N. crassa* PheRS and GlnRS protein levels. Experiments are currently underway to abolish rhythmic PheRS and GlnRS protein accumulation to determine how loss of rhythmicity of the RS alters rhythmic CPC-3 activity and mRNA translation. These findings will provide insights into the mechanism of circadian clock control of protein production and a rationale to connect clock control of protein synthesis to other vital cellular processes.

**Megan Coolahan**  
2020 Beckman Scholar  
Biology (Marine Biochemistry)  
Haverford College



**Investigating the effects of a bacterial signaling molecule on a master regulator of DNA repair in marine phytoplankton**

Interactions between marine phytoplankton and bacteria drive global biogeochemical cycling. 2-heptyl-4-quinolone (HHQ), a quorum-sensing molecule produced by the marine bacterium *Pseudoalteromonas piscicida*, induces immediate and reversible S-phase arrest in the globally distributed phytoplankton *Emiliana huxleyi*. HHQ causes upregulation of poly(ADP-ribose) polymerase (PARP), a master regulator of the DNA damage repair response, and is known to inhibit human PARP. The goal of this study was to determine whether HHQ inhibits EhPARP by heterologously expressing EhPARP in *Escherichia coli*, purifying EhPARP using affinity chromatography, and testing the activity of EhPARP exposed to HHQ in a biochemical assay. Additionally, the effect of a known PARP inhibitor veliparib on *E. huxleyi* was tested using a phytoplankton growth inhibition assay. While EhPARP was expressed in *E. coli*, the protein could not be fully purified due to persistent proteolysis. However, veliparib exhibited similar effects to HHQ on *E. huxleyi* growth rate and chlorophyll content. These results suggest that bacteria use quorum-sensing compounds to manipulate fundamental cellular processes in phytoplankton and shape microalgal population dynamics on a global scale.

**DAY 1 PRESENTER – 8/5**

**Lauren Davis**

2020 Beckman Scholar  
Biology (Bioengineering)  
Clemson University



**Structural Analysis of Polymeric Surgical Mesh Fibers and Pores in Varied Loading Conditions**

Polymeric surgical mesh implants provide support for damaged or weakened tissues in the abdominal wall and pelvic floor. Literature suggests that mesh structure and mechanical behavior signals the cellular response, but these characteristics are rarely reported in clinical outcome studies. The objective of this work was to specify imaging parameters to distinguish gross mesh structure of polymer fibers and pores after *in vivo* function and during simulated physiological loading. Six mesh types were evaluated including *ex vivo* mesh explants from clinical cases (n=25) and unused mesh controls (n=36). Control samples underwent uniform biaxial tension (0.039 N) and were imaged with optical microscopy. Pristine samples were mounted in a biaxial test system and imaged from 0.1N to 22N at 0.2mm/s. On average, pore sizes of mesh increased 4% to 69% as polymer fibers tightened during loading. Interlacing loops consisted of 3 to 13 overlapping fibers with total heights from 510 to 700  $\mu\text{m}$ . In conclusion, mesh under physiologically relevant load conditions exhibit altered pore structure. Analysis of explants and correlation with patient outcomes is ongoing.

**Nicholas Dulock**  
 2020 Beckman Scholar  
 Chemistry (Physical Chemistry)  
 Boston College



**Enabling Lithium Metal Anode in Nonflammable Phosphate Electrolyte with Electrochemically Induced Chemical Reactions**

Lithium metal anodes reserve high energy density, and thus are very promising for future battery applications. The formation of dendrites and uneven deposition of lithium during cycling, however, leads to low coulombic efficiency, lifetime, and safety. Therefore, it is essential that a stable passivation layer known as the solid-electrolyte interphase (SEI) be achieved. To further address safety issues, doing so in a nonflammable electrolyte is a critical goal. This project therein sought the reversible stripping and plating of lithium within triethyl phosphate (TEP)— a known flame retardant. The TEP solution was observed to produce  $\text{Li}_3\text{PO}_4$  and polyphosphates during its electrochemical reduction and initial decomposition in the presence of oxygen, resulting in a thin, stable SEI layer that greatly improved cycling. More than 300 cycles of stripping and plating were measured at a current density of  $0.5 \text{ mA} \cdot \text{cm}^{-2}$ . Fabrication into  $\text{Li-O}_2$  and  $\text{Li-ion}$  prototype batteries further supported its effectiveness as a scalable electrolyte. Predicted mechanisms for formation are supported by DFT calculations, and supported by successful detection of relevant intermediates and products.

**DAY 1 PRESENTER – 8/5**

**Elliott Einstein**

2020 Beckman Scholar  
Chemistry (Biochemistry)  
University of California, Irvine



**Co-pigmentation in African violets: Two pigments are better than one**

*Streptocarpus* sect. *Saintpaulia* (African violets) are one of the most popular flowering houseplants in the world due to their year-round display of blooms and vivid colors. Our focus is on characterizing the yellow- and ivory-color pigment in these cultivars, which are unusual for African violets because of their lack of chromoplast, an organelle responsible for the production and storage of both carotenoids and xanthophyll pigments normally responsible for visible yellow and orange colors, respectively. We sought to elucidate why these plants exhibit a yellow phenotype despite not having carotenoid or xanthophyll pigments, which led us to attempt to find the biochrome or biochrome conjugates responsible for the yellow coloration in one African violet species and seven cultivars: *S. ionanthus*, 'Ethel's Wild Side', 'AE-Blue System', 'Rebel's Splatter Kake', 'Peach Perfect', 'Emerald Love', and 'Majesty.' Using liquid chromatography-mass spectrometry (LC-MS) in combination with a novel ultra-performance liquid chromatography–quadrupole time-of-flight mass spectrometry (UPLC–Q-TOF-MS/MS) method, we established a characterization protocol to identify the yellow pigment from African violet petals.

**DAY 2 PRESENTER – 8/6**

**Christine Fasana**

2020 Beckman Scholar  
Chemistry (Materials Science &  
Development)  
Furman University



**Bottom-Up Assembly of Nanomaterials and Thin Films**

Self-assembly capitalizes on the fundamental chemical forces at the nanoscale to drive the formation of elaborate structures from simpler units. The research herein investigated the bottom-up assembly of nanomaterials and thin films. Tetrahedrite nanoparticles synthesized via a modified polyol process were studied to determine the effect of nano-structuring and doping on the material's thermal stability. Tetrahedrite ( $\text{Cu}_{12}\text{Sb}_4\text{S}_{13}$ ) is a thermoelectric material and therefore maintains the ability to convert waste heat into electricity (and vice versa). Therefore, it is of paramount importance to understand how these materials withstand high temperatures. Employing differential scanning calorimetry and thermogravimetric analysis, we successfully demonstrated that nanostructuring reduces thermal stability, while first row transition metal dopants stabilize the material. As the thermoelectric investigation concluded, I focused on a new study that explores the growth mechanisms of surface-anchored metal organic frameworks (surMOFs), which are a class of nano-porous thin films assembled from metal-based nodes and bridging organic ligands. The goal of this study is to control surMOF morphology by altering deposition parameters and characteristics of the underlying self-assembled monolayer.

**DAY 1 PRESENTER – 8/5**

**Benjamin Fefferman**  
2020 Beckman Scholar  
Chemistry (Biochemistry)  
University of Chicago



### **Bioinformatics Analysis of 5-Hydroxymethylcytosine Profiles in Colorectal Cancer**

5-hydroxymethylcytosine (5hmC), a chemical modification in DNA, has recently been recognized as a promising cancer biomarker. Over the past decade, it has been determined that 5hmC residues are associated with active gene expression, and are derived from the more abundant 5-methylcytosine (5mC) via oxidation by Ten-Eleven Translocation (TET) enzymes. 5hmC can either be an oxidative intermediate from active demethylation by TET enzymes, or 5hmC residues may emerge de novo. Changes in 5hmC correlate with gene expression changes in several cancers. In this poster, I present bioinformatics analysis of 5hmC gDNA profiles in NGS data from colorectal cancer patients. I have performed pairwise analysis of colonocytes and stromal cells, as well as of tumor and normal tissue. The data below indicate that 5hmC profiles in gDNA separate tissue type, over disease state, from CRC, while 5hmC profiles in cfDNA may separate disease state, over tissue type, in CRC. Such epigenetic analysis has promising implications toward methods for less invasive “liquid biopsies” of circulating cell-free DNA (cfDNA).

**Johanna Fowler**

2020 Beckman Scholar  
Chemistry (Biophysical Chemistry)  
Haverford College



**The membrane-bound conformational distribution of alpha-synuclein Parkinson's disease-linked mutants can be studied with site-specific infrared spectroscopy.**

Alpha-synuclein ( $\alpha$ S) is a protein expressed in neurons whose  $\beta$ -sheet aggregation is linked to Parkinson's Disease (PD). Six point mutations in  $\alpha$ S have been directly linked to familial cases of PD.  $\alpha$ S is intrinsically disordered, but is known to adopt a mostly helical secondary structure upon binding to lipid membranes. Three putative membrane-bound conformations have been proposed to be in dynamic equilibrium, primarily based on magnetic resonance experiments. The "non-amyloid beta component (NAC) liftoff" conformation is particularly notable because it involves solvent exposure of the protein region central to aggregation. Additional magnetic resonance experiments suggest the PD-linked mutations of  $\alpha$ S could shift the membrane bound conformational distribution towards NAC liftoff. This project investigated how PD-linked mutations of  $\alpha$ S impact the membrane-bound conformational distribution using site-specific infrared (IR) spectroscopy. Cyanylated cysteine probes were incorporated at four sites in N-terminally acetylated  $\alpha$ S (wild type and two PD-linked mutants). Preliminary IR lineshape analysis suggests a continuous, rather than discrete, NAC liftoff which potentially occurs more frequently in the PD-linked mutants compared to wild type.

**DAY 1 PRESENTER – 8/5**

**Jessica Freed**

2020 Beckman Scholar  
Chemistry (Biochemistry)  
Boston College



**A Hybrid Approach to Phage Engineering Towards Targeted Treatment of Bacterial Infections**

Antibiotic resistance is one of the greatest threats to public health today and can largely be attributed to the overuse of broad-spectrum antibiotics. This project seeks to test the feasibility of a novel strategy to develop new narrow-spectrum antibiotics in the form of engineered bacteriophages: viruses which target bacteria. We hypothesize that *mcr-1*, which confers colistin resistance through bacterial lipopolysaccharide modification, also confers bacteriophage T3 resistance. We also hypothesize that attaching a *mcr-1* (+)-cell-targeting motif (MAK30) to T3 will restore T3's ability to target *mcr-1* (+) *E. coli*. Here, we investigate the relationship between *mcr-1* and *E. coli* sensitivity to T3. We also use CRISPR-Cas9 to genetically engineer cysteine residues onto the T3 tail fiber protein tip, which we will use as a site-specific conjugation site for the peptide probe MAK30. These engineered phages will be tested for restored activity against *mcr-1* (+) *E. coli*. Through our hybrid approach of genetic and chemical engineering, we hope to further expand the field of phage therapy.

**DAY 2 PRESENTER – 8/6**

**Sasha Gill-Ljunghammer**  
2020 Beckman Scholar  
Chemistry (Materials Science)  
University of California, Los Angeles



**Novel One-Pot Synthesis of Cobalt Ferrite Nanocrystals for Improved Morphology and Size Distribution**

Metal oxide nanoparticles hold great promise for application in a wide variety of fields due to their exploitable physical properties, which are size dependent. These materials have commonly been synthesized in a solvothermal reaction that proceeds via a burst nucleation event, followed by nanoparticle growth. Under this classical growth scheme, precise size control of synthesized nanoparticles is difficult due to the rapid nature of the nucleation step, thus presenting a problem for the industrial application of the particles. This work demonstrates the improved size and shape uniformity of cobalt ferrite (CFO) nanoparticles produced via a novel esterification synthesis method as compared to the commonly used solvothermal procedure using TEM imaging and ImageJ software. It is shown that the more gradual continuous growth scheme allows for more precise control in the selection of desired particle properties and allows for the formation of smaller particles than possible with the classical method. Furthermore, particles grown via this method follow a less continuous growth scheme at higher temperatures, likely due to an additional nucleation pathway.

**DAY 1 PRESENTER – 8/5**

**Samantha Grecco**

2020 Beckman Scholar  
 Chemistry (Biochemistry)  
 Pennsylvania State University



**Gene-specific pulldown for targeted *in vivo* RNA structure probing**

When *Escherichia coli* experiences environmental stressors it initiates regulatory responses to maintain homeostasis. In response to a specific stress, small non-coding RNAs (sRNAs) change the expression of target mRNAs by altering mRNA stability and translation efficiency. The sRNA RyhB is expressed under iron-limiting conditions and regulates the iron sparing response.<sup>1</sup> The majority of RyhB targets have not been characterized and the role of RNA structure in the sRNA-mRNA interactions is unknown. It is hypothesized that the target mRNA secondary structure influences the ability of RhyB to bind and that the interaction may induce a structural rearrangement to alter gene expression. To analyze the role of RNA structure in RyhB regulation four putative RyhB targets (*cirA*, *fliA*, *sufAB*, *frdA*) were selected. Then gene expression profiling was performed, and a gene-specific pulldown was developed for targeted *in vivo* structure probing. This research will provide a deeper understanding of the regulatory systems in *E. coli*, which could help combat pathogenic infections and antibiotic resistance.

**Elora Greiner**

2020 Beckman Scholar  
Biology (Developmental Biology)  
Smith College



**Glow with the Flow: Visualizing Bioelectric Patterns and their Relationship to Axis Determination in *Danio rerio***

Bioelectrics, or the different membrane potentials that exist across a tissue and whole organism, is emerging to be an important, yet understudied, mechanism that may influence a variety of developmental processes. Although evidence is mounting to support a role for bioelectric signaling during regeneration, much less research has been done to explore its involvement in the formation of an embryo. Our lab has begun an investigation into the roles that bioelectrics may play during early axis determination in the developing zebrafish embryo (*Danio rerio*). Using voltage sensitive dyes and transient expression of genetically encoded voltage indicating constructs, we show here preliminary data suggesting that a gradient of differential membrane potentials does exist from the dorsal to ventral axis of the developing blastula and gastrula. Moreover, to monitor changes in bioelectric patterns over time, we are currently generating stable transgenic lines expressing different genetically encoded voltage indicators, namely Marina, FlicR1, and ArcLight. Lastly, we present our pharmacological and genetic strategies to interrogate whether specific modes of bioelectric signaling are required for axis determination.

**DAY 1 PRESENTER – 8/5**

**Hunter Hansen**

2020 Beckman Scholar  
 Chemistry (Organic Chemistry)  
 Whitman College

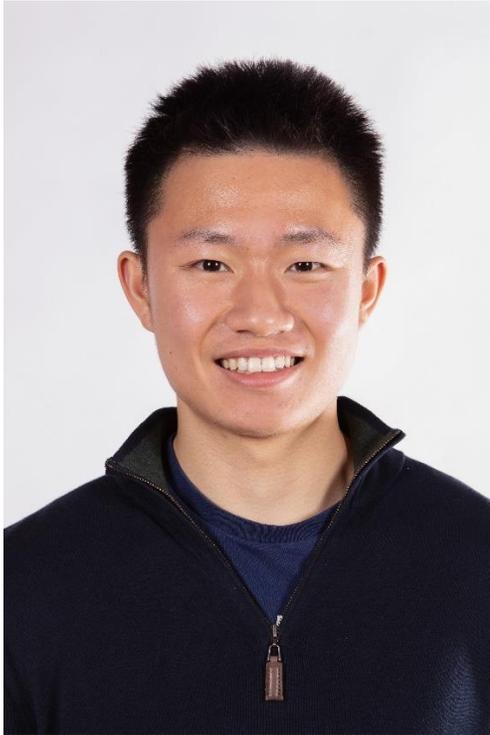


**Synthesis and evaluation of macrocyclic peptide epoxides as potent and selective inhibitors of the 20S proteasome**

The multicatalytic human 20S proteasome is a threonine protease responsible for the breakdown of intercellular proteins. It is a promising chemotherapeutic target for treatment of multiple myeloma due to its role in regulating cellular processes, including the breakdown of tumor suppressors (p543) and activation of growth and proliferation regulators (NF-κB). Multiple myeloma is currently treated with proteasome inhibitors such as the peptide epoxyketone carfilzomib. Although current inhibitors are clinically effective, off-target inhibition from a lack of specificity causes severe and even life-threatening side effects. Other highly selective proteasome inhibitors include synthetically challenging peptide macrocycles, such as TMC-95A, a fungal peptide metabolite. This research aims to enhance the selectivity of epoxyketones by combining the epoxyketone electrophilic trap of carfilzomib with the macrocyclic oxindole moiety of TMC-95A. The most potent analog inhibits the human 20S proteasome in the low micromolar range ( $IC_{50} = 0.17 \mu M$ ) and is selective against other representative proteases. The crystal structure confirmed the presence of additional hydrogen bonding between the oxindole moiety and the proteasome active site residues.

**James He**

2020 Beckman Scholar  
Biology (Molecular & Cell Biology)  
University of Connecticut



**DAY 1 PRESENTER – 8/5**

**Identifying the Cell Composition and Clonal Diversity of Supratentorial Ependymoma Using Single Cell RNA-Sequencing**

Ependymoma is a primary solid tumor of the central nervous system. Supratentorial ependymoma (ST-EPN), a subtype of ependymomas, is driven by an oncogenic ZFTA-RELA fusion in 70% of cases. We introduced this fusion into neural progenitor cells of mice embryos via in utero electroporation of a non-viral binary piggyBac transposon system containing ZFTA-RELA. To define the cellular composition and subclonal diversity of ST-EPN tumors, we used single cell RNA-sequencing to derive a transcriptomic profile of the heterogeneous cell types. Among the 20,000 cells sequenced, two-thirds of the cells did not express the oncogene. These cells represent various types of immune, stromal, and neural cells. Although ZFTA-RELA has been shown to activate NF- $\kappa$ B effector genes, there was not a ubiquitous upregulation of such genes across the cells enriched for ZFTA-RELA expression. Subclustering these tumorigenic cells revealed distinct subpopulations characterized by upregulation of non-NF $\kappa$ B pathways involved in cell proliferation, extracellular environment reorganization, and immune activation. We identified a list of specific markers for these cellular conditions to better characterize the processes underlying ST-EPN aggressiveness and immunological response.

**Grace Heiting**  
2020 Beckman Scholar  
Biology (Animal Physiology)  
Union College



**Effects of Oxygen on Jump Performance and Lactate Production in the American Locust**

Grasshoppers are among the most evolutionarily successful animals in part due to their air-filled tracheal respiratory system and air sacs. A recent study showed that late-stage grasshoppers undergo physiological changes that hinder their oxygen delivery capacity and jump performance compared to early-stage grasshoppers (Kirkton et. al 2012).

We forced early- and late-stage 6th instar grasshoppers to jump in artificial atmospheres (5%, 10%, 21%, 40% oxygen) and predicted that if oxygen delivery is compromised then late-stage jumping performance would correlate with oxygen level. Grasshoppers were individually placed in a chamber and stimulated to jump for five minutes. Jump rate was recorded and then the grasshoppers were frozen in liquid nitrogen to later analyze lactate production and HIF protein expression.

Our initial results show that oxygen levels affect late-stage grasshoppers more than early-stage grasshoppers during repeated jumping. At 5% and 10% oxygen, late-stage grasshoppers jumped significantly less than the early-stage grasshoppers. At 40% oxygen, early-stage grasshoppers jumped significantly less than late-stage grasshoppers. These results suggest that jump performance is impacted by age and oxygen levels.

**Ashley Hirt**

2020 Beckman Scholar  
Biology (Neuroscience)  
University of Virginia



**High-throughput, single-cell methods expand our knowledge of touch and pain cells**

Precisely controlled development of the somatosensory nervous system is essential for detecting pain, itch, temperature, touch, and the body's position in space, with defects in this process causing various sensory disorders. To comprehensively investigate the development of somatosensory cell types, we performed single-cell mass cytometry on mice dorsal root ganglia each day, from embryonic day E11.5 to postnatal day P4. Measuring 41 protein markers from over 3 million cells, we identified over 40 molecularly distinct neuron states and tracked the changes in protein expression for neuronal and glial cell types across development. Overall, our work demonstrates the utility of mass cytometry as a high-throughput platform to rapidly phenotype somatosensory ganglia and other neural tissues.

**DAY 1 PRESENTER – 8/5**

**Evan Holbrook**

2020 Beckman Scholar  
Biology (Immunology, Virology &  
Infectious Disease)  
University of Colorado, Boulder



***Mycobacterium vaccae*, a soil-derived bacterium, prevents lipopolysaccharide-induced expression of inflammatory genes in human THP-1-derived macrophages**

The Western world is facing a pandemic of inflammatory disease such as inflammatory bowel diseases, asthma, and mental health disorders. It's hypothesized this is due to deficient exposure to beneficial inflammation-regulating microorganisms commonly found in undeveloped environments, but not in developed ones. Previous research has found a soil-derived bacterium called *Mycobacterium vaccae* prevents stress-induced colitis and anxiety in rodents; therefore, it could be a beneficial microbe we've lost touch with since urbanizing. Thus, we investigated whether *M. vaccae* could prevent stress-induced inflammatory disease. Human macrophages were cultured with *M. vaccae in vitro* and inflammatory gene expression was measured after subsequent incubation with lipopolysaccharide (LPS), a chemical stressor meant to trigger an inflammatory stress response. Macrophages incubated with *M. vaccae* were more resilient to an LPS-induced exaggeration of inflammation compared to macrophages that weren't incubated with *M. vaccae*. This finding indicates *M. vaccae* may be a useful therapeutic in the treatment and prevention of conditions arising from stress-induced exaggerations of inflammation such as colitis, asthma, depression, and anxiety.

**Emily Hughes**

2020 Beckman Scholar  
Biology (Microbiology)  
University of Kansas



**Overexpression of RsbW in *Chlamydia* had limited growth defects**

*Chlamydia* is the most commonly reported bacterial sexually transmitted infection in the US, with no vaccine and limited treatment options. This is due to a lack of understanding about its basic biology and pathogenesis, with research being hindered by limited genetic tools. One method to study the role of genes in *Chlamydia* is using an inducible over expression system. *Chlamydia* has a biphasic developmental cycle and is regulated by multiple factors. There are 3 main sigma factors known in *Chlamydia*, but their interaction and regulation hasn't been fully investigated. These sigma factors are targeted by one protein of interest, RsbW, which is a switch-protein kinase. It has been hypothesized that RsbW interacts with the primary sigma factor,  $\sigma^{66}$ . By utilizing RsbW in a Tet system, expression can be induced and changes in transcription of sigma factor regulated genes can be monitored. Upon overexpression, RsbW doesn't show any differences in progeny production, suggesting that  $\sigma^{66}$  is not affected by RsbW. Future studies will look at the remaining sigma factors to determine if they interact with RsbW.

**Isabel Johnson**

2020 Beckman Scholar  
Chemistry (Biochemistry)  
Calvin University



**Structure-Phenotype Relationships in BCS1L-Related Rare Diseases**

Correlating disease genotype with phenotype is a key aspect of understanding rare genetic diseases. Molecular dynamics (MD) simulations support and enhance the interpretation of experimental data allow analysis of the relationships between the movement of individual residues of a protein within a simulated cellular context. Explicit MD simulations were performed on BCS1L in three conformational states to investigate diverse disease phenotypes of BCS1L-related rare. There are unique contacts between different subunits of the heptameric BCS1L protein. The pattern of correlation of other amino acids with residues that cause Björnstad Syndrome, a mild BCS1L-related rare disease, changes after ATP hydrolysis, despite these mutated residues location in a dynamic loop region of the ATPase domain. Residues that cause severe BCS1L Mitopathy when mutated lose correlation in the ATPase domain when ATP is bound. In 3D space these residues are located on the interface between two subunits, suggesting that heptamer assembly is impacted.

**Ramona Johnson**

2020 Beckman Scholar  
Biology (Molecular & Cell Biology)  
Case Western Reserve University



**Dysbiosis During Methadone Use Impacts Gut Barrier Function**

In recent years the United States has been experiencing a serious opioid epidemic, which involves an increased prevalence of opioid addiction and opioid-related deaths. A major side effect of opioid use is gastrointestinal distress, known as opioid-induced bowel dysfunction (OIBD), which includes nausea, vomiting, constipation, and hard stools. This study focused on understanding the influence of methadone maintenance treatment on the composition of the gut microbiota, metabolite profile, and its effect on gut barrier function. An imbalance in key bacterial communities required for production of short chain fatty acids, mucus degradation, and maintenance of barrier integrity was identified. We observed a significant decrease in the abundance of fecal *Akkermansia muciniphila* in participants with chronic methadone use. We also demonstrated that metabolites synthesized by *Akkermansia muciniphila*, but not SCFAs nor outer membrane vesicles, modulate intestinal barrier integrity in vitro by regulating tight junction mRNA and protein expression. Thus, we propose that depletion of *A. muciniphila* in the methadone treated gut leads to a loss of mucin degradation and a compromised mucosal barrier, possibly contributing to OIBD.

**DAY 1 PRESENTER – 8/5**

**Samuel R. Khasnavis**  
 2020 Beckman Scholar  
 Chemistry (Inorganic Chemistry)  
 Pomona College



### Investigating Aprotic Amines in the SuFEx Activation of Sulfamoyl Fluorides

Sulfamides ( $R_2NSO_2NR_2$ ), sulfamates ( $ROSO_2NR_2$ ), and sulfonamides ( $RSO_2NR_2$ ), are sulfur(VI)-nitrogen linkages with established pharmaceutical applications. These linkages were historically produced from sulfur(VI) chloride precursors but, over the past decade, advances in sulfur fluoride exchange chemistry (SuFEx) have increased the viability of sulfur(VI) fluoride precursors, which have increased regioselectivity. The Ball laboratory recently developed a  $Ca(NTf_2)_2$  and DABCO (1,4-diazabicyclo[2.2.2]octane) system that activates previously unreactive sulfamoyl fluorides ( $R_2NSO_2F$ ) to form sulfamides under very mild conditions. However, the mechanism behind activation remains unclear. Herein, we present related mechanistic studies that may provide insight on the role of aprotic amines in S–F cleavage of sulfamoyl fluorides. We further discuss  $^{19}F$  NMR kinetic studies to characterize the rate order of DABCO and Pulse Field Gradient NMR studies to identify the presence of a  $Ca(NTf_2)_2$  mediated sulfamoyl-DABCO activated complex. Understanding the cooperative role of Ca and DABCO will serve as a foundation toward the expanded application of Lewis acid/base pairings and amine activation in SuFEx and synthesis.

**Hope Kirby**  
2020 Beckman Scholar  
Biology (Microbiology)  
Miami University



**DAY 1 PRESENTER – 8/5**

***Acinetobacter baumannii* uses light and temperature as signals for regulation of virulence**

*Acinetobacter baumannii* is a human bacterial pathogen with pronounced mortality rates in immunocompromised patients. With the rise of multidrug-resistant strains, understanding how this bacterium regulates its virulence is imperative for alternative treatments. We previously showed that one such signal to which *A. baumannii* responds is light.

We had determined that the photoreceptor BlsA is primarily responsible for light-mediated regulation at 24°C, regulating multiple virulence factors. We've now broadened BlsA's sphere of influence to include *A. baumannii*'s response to oxidative stress through regulation of catalase and superoxide dismutase activities. Additionally, we've shown that specific amino acid residues of BlsA's C-terminus are critical for this regulation and interaction with protein partners. We've also found that light regulation occurs at the human-host relevant temperature of 37°C, at which BlsA no longer functions as an active photoreceptor. In particular, we have shown upregulation under darkness of the conjugation of a plasmid conferring multidrug-resistance.

Our findings provide a more global insight into how *A. baumannii* uses light as a signal to confer virulence both in and outside of the host.

**Sakin Kirti**

2020 Beckman Scholar  
Biology (Molecular & Cell Biology)  
Case Western Reserve University



**DPP-IV mediates Wnt-induced skin fibrosis**

Fibrosis is defined by the excessive deposition of extracellular matrix (ECM) in addition to the loss of fat in many tissues. Currently, there is no cure for fibrosing diseases. The Atit Lab identified Dipeptidyl Peptidase-4 (DPP-IV) as a new target that may play roles in both aspects of fibrosis. **I hypothesize that DPP-IV promotes fat loss and ECM remodeling in skin fibrosis.** I test the hypothesis by crossing a mouse fibrosis model with genetically *Dpp4*<sup>-/-</sup> mice. Dermal white adipose tissue (DWAT) thickness measurements of control and *Dpp4*<sup>-/-</sup> mice suggest that *Dpp4*<sup>-/-</sup> mice are protected from fibrotic fat loss. To test that DPP-IV promotes ECM remodelling, we used collagen hybridizing peptide (CHP) that marks unassembled collagen to quantify the ECM remodelling process. Compared to controls, we found lower levels of CHP stain in the DWAT layer of *Dpp4*<sup>-/-</sup> mice showing that DPP-IV plays an important role in ECM remodelling in fibrosis. Future studies aim to understand how inhibition of DPP-IV causes fibrotic fat loss, allowing us to devise new treatments for fibrosis using existing DPP-IV inhibitors.

*Project Mentor: Dr. Radhika Atit, Department of Biology, Department of Dermatology, and Department of Genetics*

*Acknowledgements: This work is supported by Beckman Scholars Program (SK), NIAMS- NIH-T32 (AJ), NIAMS-NIH-R01 (RA).*

**Allen Knepper**

2020 Beckman Scholar  
Chemistry (Biochemistry)  
Furman University



**Biofouling Resistant ICP Films for Biologically Triggered Dopant Release**

Intrinsically conducting polymers (ICP) have been electrochemically synthesized to create polycation polymers that require counterions to maintain an overall neutral charge. The counterions are often small anionic molecules that serve as a “dopant” in the polymerization of ICPs. During the treatment of polypyrrole (PPy) films with thiol-terminated poly(ethylene glycol) (PEG), the films undergo surface derivatization that reduces a portion of the film, removing the need for some of the “dopant” counterion, while creating a brush-like hydrolayer. Quartz crystal microbalance (QCM) measurements have demonstrated that the PEG hydrolayer resists the adhesion of fetal bovine serum (FBS) protein solution as compared to unmodified PPy films. When dextran sulfonate is used as a dopant, no change in the QCM resonance frequency is observed. However, when the dopant is dodecylbenzene sulfonic acid (DBSA), exposure of the film to protein causes an increase in the resonance frequency, indicating a loss of mass. XPS measurements demonstrate that the protein triggers the release of the dopant from the composite.

**DAY 1 PRESENTER – 8/5**

**Leah Knor**

2020 Beckman Scholar  
Chemistry (Biochemistry)  
Calvin University



**The Photophysical Properties of Grevillone (6-Hydroxycoumarin) and Methylgrevillone (6-Hydroxy-4-methyl-coumarin)**

Coumarins are bioactive molecules that often serve as defenses in plant and animal systems, and understanding their fundamental behavior is essential for understanding their bioactivity. Many coumarins are fluorescent, weak acids and can therefore be characterized by pKa, quantum yield, and photometric spectral properties. Grevillone (6-Hydroxycoumarin) and methylgrevillone (6-Hydroxy-4-methylcoumarin) are two such acids with very similar structures but notably different properties. Absorbance and emission spectra over a variety of pH values were compared in order to determine the acidity, and fluorescent behavior of these compounds. Though both molecules have the same pKa, methylgrevillone exhibits dramatically red-shifted fluorescence at high pH, as well as a lower quantum yield in water and a higher quantum yield in methanol when compared to grevillone. Furthermore, both compounds can behave as photoacids, meaning they can become more acidic after excitation with light, but methylgrevillone shows a more distinct difference in emission at high and low pH than grevillone.

**Andrew Kubaney**  
2020 Beckman Scholar  
Chemistry (Analytical Chemistry)  
Carnegie Mellon University



### **High-throughput Monitoring of Polymerizations via Ultrasound Imaging**

Atom transfer radical polymerization reactions utilizing ligands of varying activities were monitored in parallel using a commercial ultrasound device. To track the progress of reactions in a high-throughput capacity, custom hardware was fabricated to interface with the ultrasound probe, and software was created to capture images from the ultrasound device in real-time. Additional software was written to aid in processing the image data produced during experiments. Polymerizations that exhibited visible increases in viscosity displayed decreases in ultrasonic signal intensity, while polymerizations that failed to react and had no corresponding change in viscosity displayed little change in ultrasonic signal intensity.

**DAY 1 PRESENTER – 8/5**

**Juliet Lee**

2020 Beckman Scholar  
Chemistry (Inorganic Chemistry)  
Barnard College



**Alkane Monooxygenase's Unique Diiron Center and Reactivity**

Alkane monooxygenase (AlkB) is an integral membrane protein and a class III diiron metalloenzyme that catalyzes the oxidation of aliphatic alkanes to alcohols. In the event of an oil spill, microorganisms that express the *alkB* gene proliferate and metabolize the alkanes in oil, playing an important role in the remediation of the environment and the global carbon cycle. This work provides the first reported characterization of a novel AlkB from a thermophilic organism (AlkB14), a purification protocol and preliminary crystallization of AlkB14, and preliminary EXAFS data supporting an iron-iron distance of 4.1-4.2 Å in the enzyme's active site. AlkB14 oxidizes aliphatic alkanes to their alcohols or aldehydes, with a substrate range of hexane to tridecane, centering around octane. At its highest, AlkB14 converted octane to octanol with a TON of 70.

**DAY 2 PRESENTER – 8/6**

**Justin Lyon**

2020 Beckman Scholar  
Biology (Neuromuscular  
Biomechanics)  
University of Idaho



**Motor Module Comparison Between Strides in Recreational Athletes**

Muscle synergies have been defined as the physiological activation of a group of muscles that contribute to a particular movement. Synergies potentially provide an insight into possible neuromotor control mechanisms used by the nervous system to simplify movement task coordination. As a result, this study seeks to determine if there is a difference in neuromotor control during the acceleration phase of sprinting. Muscle activity levels were collected from twelve recreational athletes and one college sprinter with the use of a forty meter sprinting protocol. The muscle activation signals were normalized using a box step-up task in order to derive baseline muscle activity values. Collected data was analyzed using MATLAB software and associated algorithms to derive the number of muscle synergies for each athlete. Preliminary data showed that that variation between individuals increases with stride number, thus suggesting that the initial strides during the acceleration phase may be more similar across athletes when using a VAF threshold  $>90\%$ . The single collegiate sprinter showed decreased levels of variation with increasing stride number which differed from other participants.

**DAY 1 PRESENTER – 8/5**

**Anjali McNeil**

2020 Beckman Scholar  
Biology (Microbiology)  
Pennsylvania State University



**Symbiotic *V. fischeri* strains engage in combat with different Type VI Secretion Systems**

Animals harbor bacterial symbionts that promote host health and development. Symbiont populations often contain multiple bacterial strains, but how strain diversity is established and maintained remains poorly understood. Different strains can fill the same site within the host, providing opportunities for intraspecific competition. The type VI secretion system (T6SS) is one mechanism that facilitates intercellular competition. The T6SS is a contact-dependent system capable of killing neighboring cells through toxin-delivery. The study aimed to investigate interactions between different strains possessing T6SSs, termed T6SS-positive. The squid-vibrio symbiosis served as a model of strain-level symbiont diversity. The Hawaiian bobtail squid forms a multi-strain symbiosis with bioluminescent populations of *Vibrio fischeri*. Previously, we demonstrated that some *V. fischeri* strains eliminate use T6SS to T6SS-negative strains within the host. Here, we characterized a novel T6SS-positive strain and demonstrated that it inhibits another T6SS-positive strain. Using comparisons between T6SS-encoding genes, we identified genes encoding a putative toxin that varies between strains, suggesting a potential factor dictating strain incompatibility. These results increase understanding of strain-level competitive interactions and toxins facilitating T6SS-mediated killing.

**Anna McTigue**

2020 Beckman Scholar  
Biology (Neuroscience)  
University of Colorado, Boulder



**Pair bonding leads to enhanced neural synchrony with a partner which is not disrupted by blockade of oxytocin receptors**

Recording neural activity from multiple animals provides a holistic of social interaction. When animals interact, their neural activity becomes correlated. Prairie voles, which form monogamous pair bonds with a partner, show stronger interbrain correlation with their partner than they do with a novel animal. We hypothesized that oxytocin, a neuromodulator required for pair bonding, may be mechanistically involved in synchrony in the prefrontal cortex. Using fiber photometry and GCaMP, a molecular sensor for calcium and proxy for neural activity, we found that although bonded animals exhibited higher interbrain correlation with their partner than a novel animal, and that this correlation was stronger when animals were together than when they were separated, acute i.p. injection of an oxytocin antagonist had no significant effect on interbrain correlation. To further investigate the relationship between oxytocin and interbrain synchronization, we plan to analyze interbrain correlation between animals during specific behaviors. We also plan to knockout the oxytocin receptor in the prefrontal cortex to examine effects of chronic loss of oxytocin.

**DAY 1 PRESENTER – 8/5**

**Colin Miller**

2020 Beckman Scholar  
 Chemistry (Physical Chemistry)  
 Colgate University



**Heterogeneous oxidative kinetics of ozone-iodide interactions**

Ozone-iodide chemistry is an important part of atmospheric chemistry because it provides a sink for atmospheric ozone and creates halogenated neutral species in marine aerosol. IOO<sup>-</sup> is a potential intermediate that plays a role in the surface environment of aerosol particles but it has not been observed at the particles' surface. Photoelectric charging enables the monitoring of the surface concentration of iodide in atmospherically relevant conditions. Measuring the diminishing photoelectric activity of a sample as a function of different variables (ozone partial pressure and interaction time) serves as a proxy for the changing surface composition of the aerosol particles. The difference of detectability between iodide and the IOO<sup>-</sup> intermediate demonstrates that the decreasing signal serves as the indirect observation of the IOO<sup>-</sup> intermediate forming a substantial fraction of aerosol particle surface coverage at modest ozone pressure. Using pure potassium iodide and low ozone pressures, a steady-state concentration of surface iodide is achieved, only overcome by a significantly greater ozone partial pressure. Preliminary kinetic modeling yielded a rate constant for IOO<sup>-</sup> formation of  $5 \times 10^{-13} \text{ cm}^{-2} \text{ s}^{-1}$ .

**Anneke Moeller**

2020 Beckman Scholar  
Chemistry (Inorganic Chemistry)  
San Francisco State University



**Experimental investigation of  $\text{Ni}_x\text{Fe}_{1-x}\text{OOH}$  and  $\text{Co}_x\text{Fe}_{1-x}\text{OOH}$  in electrocatalytic oxidation of seawater and Python-based simulation of cyclic voltammograms**

Electrocatalytic water splitting is a promising approach to generate clean energy – hydrogen gas ( $\text{H}_2$ ). Of the two half reactions in water electrolysis, oxygen evolution reaction (OER) limits the overall efficiency. Nickel (Ni), cobalt (Co) and iron (Fe) based electrocatalysts can effectively catalyze the OER process in alkaline electrolytes. However as a scarce resource, the use of pure water in large scale electrolysis may be limited. With sea water making up the majority of the water sources on our planet, it could be an alternative for electrocatalytic water splitting. Sea water differs from purified water sources owing to the presence of sodium chloride (NaCl). The four-electron OER process, compared to the two-electron chloride oxidation, has high overpotential, making OER kinetically unfavorable. This project aims to investigate the effects of electro-oxidation of  $\text{Cl}^-$  on the electrocatalytic activities of the OER electrocatalysts,  $\text{Ni}_x\text{Fe}_{1-x}\text{OOH}$  and  $\text{Co}_x\text{Fe}_{1-x}\text{OOH}$ . The ratios of different metal cations and the concentrations of  $\text{Cl}^-$  will be varied. Additional computational work will be conducted to simulate the cyclic voltammograms of redox couples to further elucidate the electron transfer process.

**DAY 1 PRESENTER – 8/5**

**Hieu Nguyen**

2020 Beckman Scholar

Biology (Biochemistry)

University of California, Los Angeles



**Identifying Novel Drugs to Revert DNA-Damage Induced Senescence**

Cellular senescence is an indefinite cell cycle arrest that not only occurs as a result of differentiation or aging, but also can be induced through improper cell division. Cells that are induced into a senescent state may exhibit delayed phenotypes that encourage tumorigenic behavior. Since the extended presence of both oncogene activation and chemotherapeutic regimens may activate cell senescence, reverting cells from senescence can prevent cancer relapse, thus increasing the efficacy of common cancer therapies. To further investigate the relationship between senescence and cancer, our project plans to conduct a chemical screen to identify novel drugs within the FDA panel that will direct senescent cells to a proliferative, apoptotic, or quiescent state. We have formed a stable HeLa cell line which recognizes quiescence through nuclear fluorescence of a mVenus-p27k marker, and identifies senescence through increased nuclear size and lack of mVenus-p27k fluorescence.

**Nicholas Pancheri**  
2020 Beckman Scholar  
Biology (Bioengineering)  
University of Idaho



**Investigating collagen structure and enzymatic crosslinkers as regulators of tendon formation**

Tendons transfer forces between muscle and bone and are highly susceptible to injury or disease. Current tendon tissue engineering treatments are challenged by a limited understanding of the mechanisms governing normal tendon development. This study assessed 1) the underlying collagen structure of Achilles tendons (ATs) and tail tendons (TT) in relation to tendon mechanical properties during development and 2) used TGF- $\beta$ 2 induced tenogenic mesenchymal stem cells (MSCs) as an *in vitro* model to investigate collagen crosslinking as a potential regulator of tendon development. Results identified that changes in collagen structure correlate to changes in some mechanical properties, but not all of them, and in a loading environment-dependent manner (e.g., AT vs TT). Furthermore, lysyl oxidase (LOX), an enzymatic collagen crosslinker, activity increased with TGF- $\beta$ 2 treatment and was sensitive to low levels of mechanical loading (2.5 mPa) but not higher levels (25 mPa). Together, results may suggest future tendon tissue engineering treatments should focus both upon preserving the native collagen structure and facilitating physiologically relevant collagen crosslinking.

**DAY 1 PRESENTER – 8/5**

**Venkata Patchigolla**

2020 Beckman Scholar  
Biology (Molecular & Cell Biology)  
University of Connecticut



**Enrichment of Non-B-DNA of the *Drosophila melanogaster* Centromeres**

The centromere is a region of the chromosome that provides the foundation for kinetochore assembly, a protein complex essential to proper chromosomal segregation during cell division. The centromeres of most eukaryotes are thought to be epigenetically defined by the presence of a histone H3 variant, centromeric protein A (CENP-A or CID in *Drosophila melanogaster*). CENP-A chromatin is able to recruit the kinetochore machinery and maintain itself faithfully through cell division. The role of centromere associated DNA sequences in specifying centromere formation is largely unknown. Centromeric sequences vary largely from species to species and other than the budding yeast centromeric DNA, no other centromeric sequences are known to sufficiently specify the centromere site. One model proposes that the centromeric identity maybe specified through recognition of an enrichment of non-B-DNA, such as melted, Z, or cruciform DNA. Consistent with this idea, human, mouse, Old World Monkeys and yeast centromeres are enriched for non-B-DNA. Using the *D. melanogaster* centromeres have only recently been sequenced, we find that non-B-DNA is enriched at the centromeres using in silico methods.

**Logan Porrazzo**

2020 Beckman Scholar

Biology (Ecology and Evolutionary  
Biology)

University of Arizona



**DAY 1 PRESENTER – 8/5**

**Assessing the reliability of a method used to identify de novo genes**

De novo genes are functional stretches of DNA that arise from previously noncoding or “junk” DNA. The frequency of de novo gene births in nature is disputed, due to multiple issues that cause overreporting of false positives. These false positives could be deleterious open reading frames (ORFs) that were incorrectly deemed functional or genes that were not born truly de novo. One method for examining gene functionality is the pN/pS ratio test, one that compares interspecies polymorphisms to identify types of selection occurring. When pN/pS is below one, it is sometimes used as evidence that purifying selection is happening so the ORF in question is functional. We hypothesized that under random mutation and chance, a deleterious ORF can have a pN/pS value of less than one and oppose this belief. Due to inefficient simulation runtimes, we were unable to produce timely results that could support or refute our original hypothesis.

**Adriana Gutierrez Ramirez**

2020 Beckman Scholar  
Chemistry (Analytical Chemistry)  
Santa Clara University



**Label-Free Sorting of Activated T-cells**

We have developed a label-free and passive method for the early isolation of activated T-cells and the first technique that enables the isolation prior to the display of cellular surface markers. The isolation of these cells in minutes rather than hours can have broad usage as a biotechnology tool and for the study and selection of T-cells for immunology and immunotherapy.

**Isabel Romov**

2020 Beckman Scholar  
Chemistry  
James Madison University



**Protecting mutations in human desmoplakin with small molecules**

Desmoplakin (DSP) is an integral component of the desmosome, a subcellular structure that links the intermediate filament networks of adjacent myocytes. In cardiomyocytes, the desmosome maintains both cell-to-cell adhesion and promotes electrical synchronization. Four DSP mutations; R451G, S299R, S507F, and S442F, are strongly correlated with arrhythmogenic cardiomyopathy (ACM) in humans. Analysis of these mutations revealed the exposure of a previously-occluded calpain cleavage site, thus making DSP hypersensitive to calpain degradation. Moreover a secondary mutation, L518Y, occludes this exposed cleavage site and partially rescues calpain-dependent DSP mutant degradation. Here we expand these findings and show that small molecules can also act as ‘molecular band-aids’ to prevent mutant DSP degradation. We use both fluorescence polarization assays and computational screenings to monitor the effects of small molecules on DSP stability. This work shows that DSP has a potential ‘druggable’ pocket, and small molecule binding can occlude the DSP calpain cleavage site.

**DAY 1 PRESENTER – 8/5**

**Eric Salisbury**

2020 Beckman Scholar  
Chemistry (Organometallic Chemistry)  
Hope College



**Carbon-Carbon Bond Activation: Rhodium-Catalyzed Decarbonylation of Pyridyl Ketones**

Activation of carbon-carbon bonds using transition metal catalysis could open new synthetic pathways for molecular synthesis. Rhodium has been shown to catalyze decarbonylation of 2-pyridyl substituted aryl ketones. Conditions have been developed to extend this reactivity across a variety of functional groups and substitution patterns in an efficient manner. The methodology also proceeds efficiently in ketones containing heteroaromatic substitutions, which has not been previously observed.

**Michelle Schroeder**

2020 Beckman Scholar

Biology (Immunology)

Georgia Institute of Technology



**VLP-Conjugate Vaccines Produce Diagnostic Monoclonal Antibodies Against Fentanyl Derivatives**

Fentanyl is an opioid responsible for 60,000-80,000 overdose deaths each year. The current lack of fast acting field diagnostics for many fentanyl derivatives hinders the speed at which reversal medication can be administered, therefore limiting positive outcomes.

Monoclonal antibodies (mAbs) have shown tremendous promise in field diagnostic applications due to their specificity, relatively low cost, and portability. Here, mAbs that recognize eight fentanyl derivatives were developed using virus like particle (VLP) conjugate vaccines paired with hybridoma technology. We synthesized PP7 VLPs covalently modified to display one of the chosen derivatives. Mouse serum was monitored for fentanyl specific IgG response over time and those with the highest titer were selected for spleen harvest and hybridoma development. Using this strategy, we found 14 unique binding classes of mAb, 6 of which together can be used to positively distinguish between the 7 of the 8 derivatives tested. These mAbs will be used to improve field diagnostics for fentanyl overdose victims, thereby increasing the speed of treatment and positively impacting survival rates.

**DAY 1 PRESENTER – 8/5**

**Kevin J. Schult**

2020 Beckman Scholar  
Chemistry (Computational  
Biochemistry)  
Tufts University



**Developing a Cyclic-Peptide Inhibitor for Overactive Inflammation**

Tumor necrosis factor alpha (TNF $\alpha$ ) is a signaling cytokine secreted in response to stress, injury, and infection, acting as a significant mediator of the inflammatory response. Overproduction of TNF $\alpha$  is implicated in inflammatory damage in disease states such as arthritis, meningitis, and cancer. TNF $\alpha$  is secreted via the cleavage of a membrane protein by TNF $\alpha$  converting enzyme (TACE). An inhibitor for TACE would be a potential drug to help regulate dangerous inflammation, but problems with specificity or bioavailability have prevented any inhibitors from being successful drug candidates. Based on the interaction between TACE and known inhibitor TIMP-3, and using BE-META simulations and coil library data, we were able to design a potential cyclic-peptide inhibitor for TACE, cyclo-(EASESLadd). Further development of this candidate will be made to ensure that its binding affinity for TACE is comparable to or better than the binding of the TACE/TIMP-3 complex.

**Sonia Sehgal**

2020 Beckman Scholar  
Biology (Biochemistry)  
University of Utah



**Exploring the Role of Biological Probes on MUTYH**

In this project, pharmaceutical drugs were screened to determine if they interacted with a DNA repair enzyme known as MUTYH. MUTYH prevents mutations and is thereby linked to preventing cancer growth. The ability of FDA-approved drugs to dock with the MUTYH enzyme was tested with a virtual screen. The findings suggest that these drugs are able to interact with MUTYH virtually. However, a biochemical assay is needed to further study how the drugs are affecting the enzyme's activity. Studying the molecular interactions of the screened drugs may reveal new treatments for common diseases like cancer. Moreover, understanding the effect of these interactions on other pathways will prevent unintended consequences, such as increased mutation rate that may lead to inflammation.

**DAY 1 PRESENTER – 8/5**

**Nikita Sivakumar**  
2020 Beckman Scholar  
Biology (Bioengineering)  
University of Virginia



### **Agent-Based Modeling of Multicell Spheroid Patterning Using Synthetic Gene Circuits**

Dynamically activated differential adhesion between cell subpopulations drives multicellular tissue patterning in development and disease. Previous studies have explored this process in heterogeneous spheroids by using synthetically engineered systems, in which initially non-adherent cells engage in bi-directional signaling to activate differential cadherin expression. While synthetic systems provide an excellent in vitro model to observe pattern formation, computational techniques can be leveraged to systematically explore the key parameters that drive the emergence of different patterns. We developed and validated two- and three-dimensional computational agent-based models (ABMs) of cell patterning in spheroids and demonstrated how varying the initial cell seeding ratio, signaling sensitivity, and homotypic adhesion strengths between cells lead to unique spheroid patterns. We developed novel model exploration techniques that use machine learning to identify how combinations of cell-to-cell signaling parameters in this system drive the formation of specific multicell patterns. We also deployed the model in reverse as a tool to design new synthetic cell signaling circuits based on a desired final multicell pattern.

**Saman Tabatabaee**  
2020 Beckman Scholar  
Biology (Developmental Biology)  
University of Chicago



### **Investigating the Role of Phase Separation in the Function of ETS Transcription Factor Yan**

How transcription factor complexes assemble at the correct genomic locations to regulate gene expression dynamics remains poorly understood. While sequence-specific DNA binding plays a central role, protein-protein interactions between transcription factors and cofactors are also essential to assembling functional regulatory complexes. *Drosophila Melanogaster's* Yan, a transcriptional repressor downstream of RTK signaling, provides a good model system to study how protein-protein interactions influence DNA binding and downstream gene expression. Yan contains a SAM domain which is necessary for homotypic polymerization, and two long stretches of low complexity domains whose contributions to function have not been studied. My aim for this project is to explore the mechanisms of Yan aggregation and its functional consequences. My results show that Yan accumulates in nuclear puncta with characteristics typical of phase separating condensates, including fast turnover, fusion of hubs, and sensitivity to cellular environment. By understanding the dynamics of Yan aggregation and the contribution of its different domains my work will produce new insight into how phase separation is used in spatiotemporal transcriptional regulation in vivo.

**DAY 1 PRESENTER – 8/5**

**Hayden Tharpe**  
2020 Beckman Scholar  
Biology (Chemical Engineering)  
Clemson University



### **Engineering a Highly Sensitive and Modular Reaction Cascade Biosensor**

Engineering biosensors for the detection of chemical and biological warfare agents has become increasingly critical, as has the detection of infectious diseases in light of recent global health events. While proteins have been engineered to bind to specific analytes, the larger challenge remains the production of quantifiable output signals. The focus was to engineer three separate single-chain variable fragment (scFv) protein pairs, one pair that can detect small amounts of Protective Antigen (PA), a cell-binding protein of Anthrax, one to detect trinitrotoluene (TNT), and another for SARS-CoV-2, commonly known as COVID-19. These scFv pairs will be expressed fused to split enzymes that can fuel a chain reaction, thus amplifying small sample signals. These biosensors can be used to quickly identify minute amounts of both Anthrax and COVID-19 through a cascading reaction system in the future. This advancement can further the ability to identify chemical and biological weapons of mass destruction as well as infectious diseases in a timely manner to lessen the threat of their impact on daily lives and routines.

**Rory Weeks**

2020 Beckman Scholar  
Chemistry (Materials Science &  
Development)  
University of Utah



**The Effects of Sodium on the Thermal Stability of TiS<sub>2</sub> Nanowires**

Understanding the thermal stability of nanowires is of key importance for the performance and longevity of nanowire-containing devices, particularly where resistive heating may occur. With growing interest in sodium-ion batteries (NIBs) as a more economical and lower environmental impact alternative to lithium-ion batteries (LIBs), and layered transition-metal dichalcogenides (TMDs) as energy storage materials, it is important to determine both the advantages and limitations of replacing lithium-ion conductors with their sodium analogs. Here, an *in situ* heating study to investigate the thermal stability of sodium-intercalated titanium (IV) sulfide (TiS<sub>2</sub>) nanowires, performed in a transmission electron microscope (TEM), is reported. Both sodiated (Na<sub>x</sub>TiS<sub>2</sub>) and non-sodiated nanowires were studied using a specialized heating holder, heating between room temperature and 700 °C. Chemical, morphological, and crystalline changes were observed with increased temperature solely in the sodiated-TiS<sub>2</sub> samples, demonstrating that sodiation profoundly affects the thermal stability of TiS<sub>2</sub> nanowires.

**DAY 1 PRESENTER – 8/5**

**Anneka Williams**

2020 Beckman Scholar  
Biology (Plant, Ecology &  
Environmental Sciences)  
Bowdoin College



**Conifer forest photosynthetic seasonality: exploring the effect of winter severity and the efficacy of different remote sensing methodologies**

Altered seasonal fluctuations of atmospheric carbon dioxide (CO<sub>2</sub>) at high northern latitudes since the 1960's suggest greater photosynthetic activity there as a result of anthropogenic climate change; however, the role of conifer evergreen needleleaf forests (ENF). Here we draw on remotely sensed measurements of photosynthetic phenology of ENF at opposite ends of the latitudinal gradient of NEON sites: Alaska and Florida, which have drastically different winter severities. Phenocam measurements of the green chromatic coordinate (Gcc) varied seasonally at both the FL and AK ENF sites such that values were lower in the winter and peaked during the growing season. Tower-based measurements of solar-induced fluorescence emission (SIF) from the Alaska site showed a marked decline during the winter months from peak values in summer. These remotely sensed measures may serve as an effective means of discerning photosynthetic phenology in ENF. Phenological trends determined from these remote measurements will be compared against leaf-level pigment composition and net ecosystem carbon exchange.

**Julia Vidlak**

2020 Beckman Scholar  
 Chemistry (Inorganic Chemistry)  
 University of Richmond



**Combined Synthetic and Computational Study of Bis(phosphino)pyrrole Ligands and their Transition Metal Complexes for Catalysis**

Bidentate phosphine ligands are ubiquitous with transition metal catalyzed cross-coupling reactions. These small organic molecules bind to metal centers and promote the formation of a variety of new bonds including C–O, C–C, and C–N bonds, in addition to many other transformations that are essential to synthetic chemistry. While phosphine ligands are integral to transition metal catalysis, understanding how the individual steric and electronic properties of these ligands promote or hinder catalytic performance for earth abundant metals requires further investigation. In our work, we address this problem through the development of a library of bidentate bis(phosphino)pyrrole ligands and their nickel complexes for utilization in structure activity relationship (SAR) studies. To accompany our synthetic work, we have utilized Density Functional Theory (DFT) to quantitatively compare the relative electronic and steric properties of each ligand in our ligand library. Finally, we have successfully synthesized a tridentate phosphino(pyrrole) pincer ligand to further elucidate the properties of pyrrole phosphine ligands.

**DAY 1 PRESENTER – 8/5**