

*Science Preparatory Research
Opportunities for
Underrepresented Teens
(SPROUT)*

August 19, 2021



Program

Welcome and Introduction

Michael L. Klein, FRS
Dean, College of Science and Technology
Temple University

Presentations

Theoretical and Computational Nuclear physics

Porous Materials for Capture, Detection, time-consuming
and Destruction of Chemical Warfare Agents

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Predicting deep-sea coral distribution for effective
management

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Closing Remarks

Erik Cordes, Ph.D.
Professor and Vice-Chair
Department of Biology
Temple University

Theoretical and Computational Nuclear Physics

Geonni Gee

Principal Investigator(s): Martha Constantinou, Ph.D.

Abstract: Over the course of eight weeks, I've gotten the opportunity to take a closer look at the visible world we know at a microscopic level. Using numerical simulations on supercomputers and the supporting theory of Quantum Chromodynamics (QCD), we can study the mass of the smallest building blocks of matter, called the hadrons. The theory of Quantum Chromodynamics, or QCD, essentially describes what we know as the Strong Force. It is one of the four fundamental forces in nature and contributes immensely to the visible universe. The Strong Force is responsible for the formation of particles by the name of hadrons. Hadrons are at the core of our visible universe. Examples of the hadrons we have studied this summer include, what we know as, pions and kaons. We focus on calculating the mass (weight) of these particles. The term mass is more appropriate for microscopic elements since the relation of weight and energy are interchangeable based on Einstein's famous formula $E = mc^2$.

The calculations are performed using a discretization formulation of the space (three spatial directions) and time on a hyper-cubic grid (four-dimensions), called lattice QCD. To obtain the masses of these particles requires the calculation of special functions called the two-point correlation functions. These allow the evolution of a particle in time and the measurement of its energy. The results are then analyzed to extract the mean values and the appropriate errors. The analysis is performed using the Mathematica package, and we find that the mass of the pion is 258 ± 1 MeV and the kaon is 0.532 ± 1 MeV. MeV (Mega electron-volts) are the appropriate energy units to describe the mass (weight) of microscopic matter.

Porous Materials for Capture, Detection, and Destruction of Chemical Warfare Agents

Isaiah Weekes

Principal Investigator(s): Eric Borguet, Ph.D. and Venkata Swaroopa Datta, Devulapalli

Abstract: Metal-organic frameworks (MOFs) are 3D porous compounds that act as effective catalysts in degrading chemical warfare agents (CWAs) and their simulants. However, synthesizing MOFs is time consuming and tedious. This study seeks to guide the selection of optimum metals, for synthesizing MOFs, which catalyze the hydrolysis of dimethyl 4-nitrophenyl phosphate (DMNP- a simulant of the CWA Soman).

By investigating the catalytic ability of their corresponding metal precursors, we provide insight into and compare the efficiencies of several MOFs before their synthesis. NbCl_5 , $\text{Ti}(\text{C}_4\text{H}_9\text{O})_4$, ZrCl_4 , HfCl_4 , FeCl_3 , ScCl_3 , ZnCl_2 , and SnCl_2 were tested for DMNP hydrolysis under basic (pH: 10) buffer conditions (4-ethyl morpholine) and their reactivity was observed to be by their Lewis acidity. Based on reported research, we predict that the reactivity of these metal salts would correspond to the catalytic ability of their corresponding MOFs, to which the metals were precursors.

Metals in Medicine: Titanium Anticancer Compounds

Kera McCarthy

Principal Investigator(s): Ann Valentine, Ph.D.

Abstract: With a focus on biologically relevant metals sensitive to hydrolysis, the Valentine Lab's research in bioinorganic chemistry explores the relationships between Biology and difficult metals like iron and titanium. In a proteomic experiment utilizing one such metal, the lab analyzed the effect of titanium citrate on the regulation of yeast proteins.

Proteomics is the study of Proteoms and their functions. It is used to both detect protein expression patterns in response to a specific stimulus at a given time, and to determine what functional protein networks exist at the cell, tissue, and whole organism levels. The fundamental goal of Proteomics is to pinpoint all the proteins in a cell, and to then generate a comprehensive three-dimensional map of the cell indicating each exact protein location.

In this experiment, samples of Baker's Yeast (*Saccharomyces Cerevisiae*, sugar eating fungus) were treated with Titanium Citrate. Using iTRAQ (Isobaric tag for relative and absolute quantitation), the protein score and percent coverage of each protein was measured using 114:115-114:117 ratios, 114 being the control group. iTRAQ is a quantitation technique that allows the simultaneous identification and relative quantification of hundreds of proteins in just one experiment.

Predicting deep-sea coral distribution for effective management

Kylee Mitchell

Principal Investigator(s): Erik Cordes, Ph.D. and Ryan Gasbarro

Abstract: The goal of our research is to find the connection between the abundance of *Lophelia pertusa*, a major reef-building coral in the deep ocean, and species richness of associated fauna. Our research demonstrates the connection between biodiversity and coral cover, along with the importance of protecting them. We annotated imagery from two submersible dives on two coral mounds- a healthy and unhealthy one and calculated the mean percentages of living coral and species richness of invertebrates and fish. There was a clear relationship between invertebrate richness and coral cover, but not between fish richness and coral cover. Richness also varied by site, with more biodiversity associated with the healthier mound. Invertebrates were more likely than fish to be found inside of the coral matrix because of their habitat preferences. Our work shows a clear relationship between biodiversity and coral cover. Predicted losses of healthy coral habitat due to climate change thus threaten seafloor biodiversity.

Finding the evolutionary roots of cancer cell migrations

Maria Awadalla

Principal Investigator(s): Antonia Chroni, Ph.D.

Abstract: Cancer is an evolutionary disease which may spread throughout the body from the primary location as a result of an ongoing progression of cancer cell growth. The spread of cancer cells is known as metastasis. It is the main cause of death in cancer patients. To fundamentally understand the disease's progression investigating the origin and trajectories of cancer cells is key. Here, we infer the clone migration histories of patients with breast cancer and explore the number of clones seeding new metastasis, the presence of reseeding events (clones seeding their tumor of origin), and the source of metastasis. We used computational tools (PathFinder and CloneFinder) and clone migration histories in patients with breast cancer. We concluded that in breast cancer patients presented metastasis in different locations. There were unique patterns in the number of clones seeding new metastasis, presence of reseeding events, and the metastasis pathway/spread. Future investigations should include more patient data with breast cancer and/or other patient types. The development of an effective user-friendly pipeline will be crucial for fully leveraging data and performing comparative analysis. The pipeline along with data analysis provided more insight into cancer cell migrations between tumors in breast cancer patients.

Neurogenomics of incipient speciation in *Drosophila*

Samar Oubbari

Principal Investigator(s): Rob Kulathinal, Ph.D.

Abstract: Identifying genetic connections to the evolution of reproductive isolation and speciation has long been an overarching goal of evolutionary biology. Current studies display that populations of *Drosophila melanogaster* from Zimbabwe yield females who would not mate with *D. melanogaster* males from cosmopolitan populations. These findings demonstrate a possible case of incipient speciation in select African *Drosophila* populations. This study aims to obtain a deeper understanding of the genetic processes that dictate mating behaviors in *Drosophila*.

Phase 1 of the project consists of identifying clusters in *Drosophila* populations through a PCA plot. These clusters could suggest a differentiation of genes between populations that affects mating. The results show expected geographical divides in clusters of flies from the U.S. and France with fly clusters in African populations. In addition, the plots displayed clustering in flies without geographical barriers, indicating a possible case of sympatric speciation in its incipient stages.

In Phase 2, a pairwise per site F_{ST} analysis will be used to identify the most highly differentiated genes between populations, or “candidate genes.” Additional analysis is required to identify candidate genes and test their impact on *Drosophila* mating behavior. We hypothesize that the most differentiated gene between the populations will be the fruitless genes. Phase 3 entails programming Flytracker and JAABA to interpret and track fly behavior in response to certain candidate genes being knocked down.

Principal Investigators and Student Researcher Biographies

Theoretical and Computational Nuclear Physics

Martha Constantinou, Ph.D. received her bachelor in 2003 and doctoral degree in 2008 from the Department of Physics of the University of Cyprus. In 2012 she was a visiting lecturer at the University of Cyprus and has held Postdoctoral Fellow positions at the University of Cyprus and The Cyprus Institute. As of 2016, Constantinou is an Assistant Professor at Temple in Philadelphia, where she continues her research activities and teaching. She currently teaches Introductory Physics for honors students mostly on a health-professional career path.

Her research is in the areas of Theoretical Nuclear Physics, with a focus on Quantum Chromodynamics (QCD), the theory of strong interaction. The research intersects with Computational Physics, as the calculations are large-scale and are performed in the largest supercomputers worldwide. She is a recipient of the 2019 U.S. DOE Early Career Award. This award is given yearly to about 50 Scientists at the level of an Assistant Professor with an appointment at U.S. Universities across all fields of science. In 2020 she received the Selma Lee Bloch Brown Professorship at Temple University that recognizes early-career female faculty in research and service.

Geonni Gee is a junior at SLA Center City. Some of her interests include reading, sleeping, and skateboarding, which is the newest hobby she's acquired. One thing she dislikes, though, is writing. Not because it isn't fun, but because it is one of her biggest academic insecurities.

Geonni is working with Dr. Constantinou on theoretical & computational nuclear physics. She is optimistic that this research will help her gain the confidence that she needs to accomplish her goal of becoming an engineer! Geonni is very excited about what is in store in the future!

Porous Materials for Capture, Detection, and Destruction of Chemical Warfare Agents

Eric Borguet, Ph.D. is a Professor of Chemistry at Temple University in Philadelphia, PA. He was born in Dublin, Ireland, where he spent his formative years. He attended college in France at the Université de Paris-Sud (XI-Orsay) where he studied chemistry and physics. He traveled to Philadelphia, Pennsylvania in the USA and obtained his Ph.D. in Physical Chemistry at the University of Pennsylvania in 1993, under the mentorship of Professor Hai-Lung Dai where he investigated adsorption and intermolecular interactions on stepped metal surfaces. His post-doctoral training was completed at Columbia University in the group of Professor Kenneth Eisenthal where he carried out nonlinear optical studies of spectroscopy and ultrafast dynamics at liquid interfaces.

Chemical and physical processes at surfaces and interfaces are the principal focus of his ongoing research program at Temple University. His research activities have resulted in over 140 peer-reviewed publications, more than 280 invited talks, and more than 240 contributed presentations.

Eric has mentored 26 graduate students, 18 of whom earned a Ph.D. and went on to post-doctoral fellowships, as well as industrial and academic careers. He has advised over 85 undergraduate researchers, many of whom have continued to graduate studies. His group has welcomed 13 visiting graduate students, as well as 5 sabbatical visiting scholars. He has supervised the training of 17 post-doctoral fellows.

For any additional information please visit:

<https://sites.temple.edu/borguet/eric-borguet/>

Venkata Swaroopa Datta, Devulapalli is the first student to join the Ph.D. program at Temple University under a joint initiative, IISER-TU Dual Doctoral Degree (DMDD), between the Indian Institute of Science Education and Research (IISER) Pune, India and Temple University. As an undergraduate at IISER Pune, he worked on synthesizing complex carbohydrate structures present in glycoprotein 41 (GP 41), employing a novel alkynyl carbonate donor strategy, under the guidance of Dr. S. Hotha. Later, he joined the group of Dr. R. Vaidhyanathan and worked on the synthesis and development of photocatalytic materials, such as boron carbon nitrides (BCN).

Datta joined the Borguet group in Fall 2017. He started his research by studying the interactions of 3-D porous materials-metal organic frameworks (MOFs) and covalent organic frameworks (COFs) with simple chemicals such as acetone and earned his Masters's degree from IISER Pune in 2018.

Currently, he studies the interactions of MOF and COFs with toxic industrial chemicals such as NH₃. The stabilities of MOFs, COFs, are analyzed under controlled temperature and pressure conditions (100 K – 1300 K; 10-10 Torr – ambient pressures) which provide insights into processes and factors that determine the complex chemistry of these materials.

Datta also leads the catalysis subgroup where the focus is on developing design rules and synthetic strategies of metal oxyhydroxides for the degradation of toxic organophosphates.

You can find additional info at:

<https://sites.temple.edu/borguet/datta-devulapalli/>

Isaiah Weekes Isaiah Weekes from Masterman High School is an aspiring engineer, economist, bassist, and researcher. He's interested in the problem solving, data interpretation, and executive skills provided by research and the detailed steps involved. This summer for SPROUT, Isaiah will be working with Dr. Borguet in his lab, 'Porous Materials for Capture, Detection, and Destruction of Chemical Warfare Agents.

Metals in Medicine: Titanium Anticancer Compounds

Ann Valentine, Ph.D. is a Professor and Chair of the Department of Chemistry. She is originally a native of Pittsburgh, PA. Her BS (from the University of Virginia) and Ph.D. (from MIT) are both in chemistry, and she's been at Temple for 10 years. Her research is about bioinorganic chemistry - how nature gets certain metals like iron or titanium from the environment, and what it does with those metals when it gets them. She was the Temple University Honors Professor of the Year in 2015 and 2021 and won the Lindback Award for Distinguished Teaching in 2021. She lives in the Philly suburbs with her husband and three kids (ages 13, 10, and 7).

Kera McCarthy Kera McCarthy is a High School Junior at J.R. Masterman Laboratory and Demonstration school. She is passionate about medicine, language, baking, and how she can bring joy to others through

them. After high school, Kera hopes to pursue a career in medicine and is currently interested in Cardiothoracic Surgery. She is a logophile, bubble tea enthusiast, and advocate for diversifying school curriculums. In her spare time, Kera loves reading, playing instruments, spending time by the water, and watching Grey's Anatomy on repeat.

Kera is working in Dr. Valentine's lab, Metals in Medicine: Titanium Anticancer Compounds. She is looking forward to the experiences SPROUT brings to this summer!

Predicting deep-sea coral distribution for effective management

Erik Cordes, Ph.D. received his M.S. from Moss Landing Marine Labs, his Ph.D. from Penn State University, and was a post-doctoral fellow at Harvard University. He has worked on the ecology of the deep sea for over 25 years, spending over a year at sea on 32 research cruises (14 as Chief Scientist) and making 46 dives in the manned submersibles Alvin and Johnson Sea-Link. His work is centered around the ability of organisms to shape their environment and increase habitat heterogeneity but has increasingly become focused on the ability of humans to impact these processes in the deep sea.

Ryan Gasbarro is a marine ecologist with wide-ranging interests in understanding how animal communities are structured within and across dynamic ecosystems, and using data to make predictions that can aid in protecting biodiversity from threats such as climate change. These broad interests have led him to work in systems including the intertidal, fjord basins, hydrothermal vents, submarine canyons, cold hydrocarbon seeps, and cold-water coral reefs. He has been to sea on multiple research cruises, exploring the seafloor with both manned and unmanned submersibles. Ryan

is currently a Ph.D. Candidate and Presidential Fellow in Temple University's Department of Biology with supervisor Dr. Erik Cordes. He earned his M.Sc. in Earth & Ocean Sciences at the University of Victoria, in British Columbia, Canada, and his Bachelor's with Honors at Arizona State University.

Kylee Mitchell is a rising senior at SLA Beeber. She is working with Dr. Cordes on predicting deep-sea coral distribution for effective management. She will be working on gathering information and synthesizing it to understand the oceanography, geology, biology, and ecology of the regions the lab studies. In the future, Kylee sees herself becoming a math teacher, and hopes to attend Temple University.

Finding the evolutionary roots of cancer cell migrations

Antonia Chroni, Ph.D. is an evolutionary biologist with expertise in molecular evolution, phylogenetics, bioinformatics, molecular ecology, and biogeography of populations, species, and tumors. She is currently investigating cancer metastasis in the context of tumor evolution and heterogeneity. More specifically, Dr. Chroni is using genomics to infer the origin and trajectory of cancer cells between tumors within a cancer patient. She introduced a new field called tumor biogeography and co-developed a computational tool for inferring movements of cancer cells between tumors.

Maria Awadalla is a Coptic Egyptian-American that is entering her senior year at GAMP high school. She is interested in going into a pre-med track out of high school. She is very passionate about healthcare and making sure everyone can receive it. She is interested in research because it is a fun and interesting way to find answers to the many questions she has and gain

knowledge and experience. Some of Maria's hobbies include singing, playing clarinet, and running cross country.

Neurogenomics of incipient speciation in Drosophila

Rob Kulathinal, Ph.D. is an Associate Professor in the Department of Biology and Director of the Ph.D. in Bioinformatics graduate program at Temple University. Dr. Kulathinal is also a founding member of the Center of Computational Genetics & Genomics (CCGG) and the Institute of Genomics & Evolutionary Medicine (iGEM). His lab's primary research interests focus on how rapid evolutionary processes generate remarkable molecular and organismal patterns of diversity across populations and species. Dr. Kulathinal's work on speciation incorporates a broad spectrum of approaches including population, comparative, and functional genomics as well as *Drosophila* behavioral genetics. His lab focuses on the genetics of dynamic reproductive systems, particularly gene networks involved in sexually dimorphic patterns of expression including male fertility. His lab's recent work on sexually dimorphic behaviors is beginning to provide an exciting new neurogenomics framework to study sexual isolation. Dr. Kulathinal further studies the broad implications of this rapid evolutionary framework on a variety of biological phenomena from the effects of anthropogenic distress on deep-sea habitats (e.g., forthcoming Acid Horizon movie) to the rapid proliferation of cancer due to ancestry (e.g., news release). Dr. Kulathinal and colleagues from Management and Information Sciences are also developing an "evolutionary sciences of the artificial" based on their common interest in detecting evolutionary signals from all types of "big" digital data--whether biological, technological, or social (e.g., news release). Dr. Kulathinal teaches "Honors Introduction to Biology", "Evolutionary Genetics & Genomics", and is developing a University-wide course called D.A.T.A. (Data Acquisition, Transformation, and Analysis) that teaches big

data to students from science to business to the arts. Dr. Kulathinal also teaches "Introduction to Graduate Research" to all incoming doctoral students in Biology each fall, and co-teaches an interdisciplinary Studio course on the Bio-Social with Dr. Allison Hayes-Conroy as part of a funded NSF Research Training (NRT) grant.

Samar Oubarri is a rising senior at Central High School, is working with Dr. Kulathinal on the neurogenetics of incipient speciation in *Drosophila*. In her free time, she loves to draw and watch old TV shows! Her research interests include anything in medicine. Medicine is interesting to her as it is such a dynamic field, and in the future, she would like to become a neurosurgeon.

Special Thanks

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Committee**

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Temple University's Science Preparatory Research Opportunities for Underrepresented Teens

Mission Statement

To provide students with low socioeconomic status (SES) early exposure to graduate-level research education, improve the research enterprise through increased diversity, and prepare and recruit passionate students to Temple University's College of Science and Technology.

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