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Epithelial

T cells?

Endothelial cells, fibroblasts?



Celebrating Science across the CUNYverse PhD Programs in Biochemistry, Biology, Chemistry, and Physics

Sign-In (Concourse Level Foyer) 12:30 – 1:00 pm

New Student Welcome (Proshansky Auditorium) 1:00 – 1:30 pm

Welcome	Joshua Brumberg, President
Program Overview	Brian Gibney
	Interim Dean for the Sciences
Some useful information	
Career Planning	Jennifer Furlong, Ph.D.,
	Career Planning
The Teaching and Learning Center	Luke Waltzer, PhD.,
	Director
Research and Sponsored Programs	Huyuni Suratt,
	Executive Director
Responsible Conduct of Research	Brian Gibney, PhD
	Interim Dean for the Sciences
Library	Mason Brown,
	Science Resource Librarian

Program Breakout Meetings

Biochemistry – C203 Biology – C204 Chemistry – C205 Physics – C195

Poster Session and Networking Event

light refreshments provided Posters may be mounted at 1:30 pm. Posters and their corresponding boards are numbered.

2:30 – 5:00 pm

1:30 – 2:30 pm

Words of Wisdom

"It's okay if you fail sometimes as long as you get up every single time and keep trying because that's what's going to make the difference between succeeding and not succeeding," Morán Ramirez said. "If it's not today, it'll be tomorrow. You've got this."



– Denice Morán Ramirez, Biology

"Don't be afraid," she said. "I grew up in Sri Lanka. I didn't know the culture. I didn't know the language. Everything was new to me. I never thought I would pass all the exams and finish the Ph.D. with two kids. If I can do it, I feel that anybody can do it."

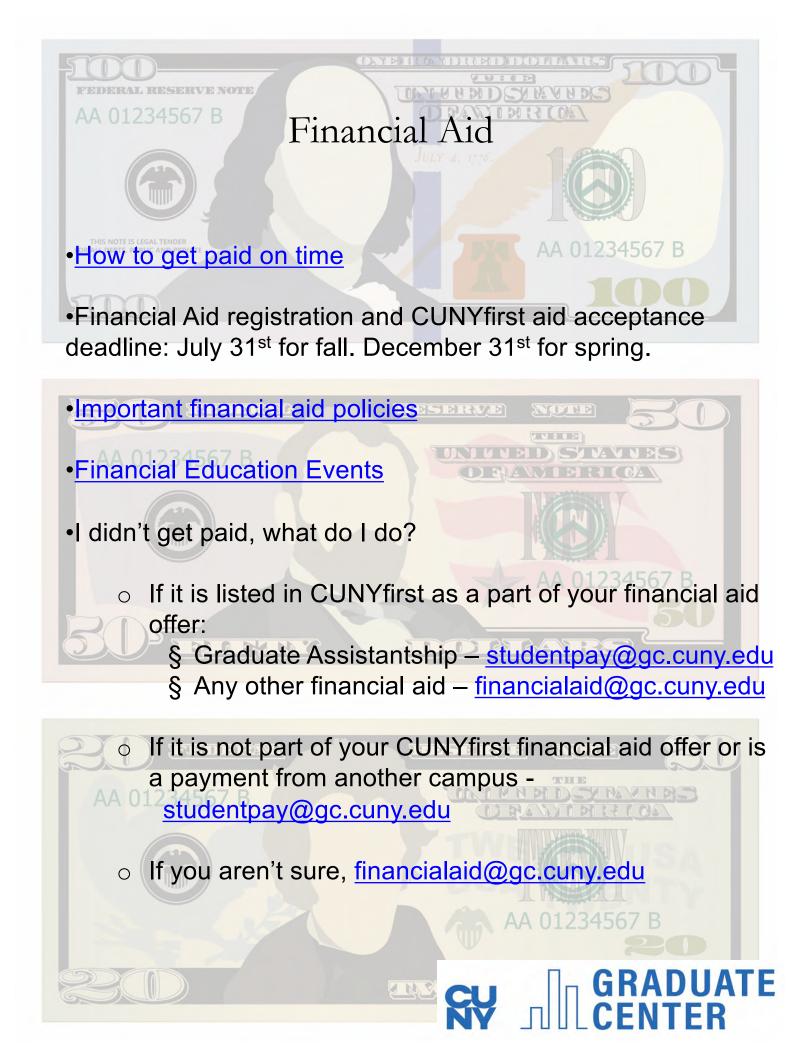
– Nishani Jayakody, PhD, Physics

"Surround yourself with people who are doing or have what you want to achieve in the future," he says. "Stay ambitious and make 1% progress every day, as this will compound over time and help you achieve your goals." — Mike Cornejo, Chemistry

"Graduate school is a marathon, not a sprint," he said, "hence the need to be dedicated and resilient." He added, "Always ask questions and accept new ideas because no wise man has ever attained perfection, and constructive criticism is important for progress."

- Augustine Onyema, Biochemistry









Christopher Blair, Ph.D. *Executive Officer*



Moh Moh Aung *Assistant Program Officer*

SY JACENTER

- MCD Prof. Mark Emerson
- EEB Prof. Mike Hickerson
- PS Prof. Renuka Sankaran
- NS Prof. Leora Yetnikoff





Integrated stress response associated with dark microglia contributes to neurodegeneration.

Pinar Ayata, ASRC Neuroscience Initiative

Microglia, the brain's primary resident immune cells, can assume various phenotypes with diverse functional outcomes on brain homeostasis. In Alzheimer's disease (AD), where microglia are a leading causal cell type, the identity of microglia subsets that drive neurodegeneration we identify microglia remains unresolved. Here, а phenotype characterized by a conserved stress signaling pathway, the integrated stress response (ISR). Using mouse models to activate or inhibit ISR in microglia, we show that ISR underlies the ultrastructurally distinct "dark" microglia subset linked to pathological synapse loss. Inducing microglial ISR in murine AD models exacerbates neurodegenerative pathologies, such as Tau pathology and synaptic terminal loss. Conversely, inhibiting microglial in AD models ameliorates pathologies. ISR these Mechanistically, we present evidence that ISR promotes the secretion of toxic long-chain lipids that impair neuron and oligodendrocyte homeostasis in vitro. Accordingly, inhibition of lipid synthesis in AD models ameliorates synaptic terminal loss. Our results demonstrate that activation of ISR within microglia represents a pathway contributing to neurodegeneration and suggest that this may be sustained, at least in part, by the secretion of long-chain lipids from ISR-activated microglia.

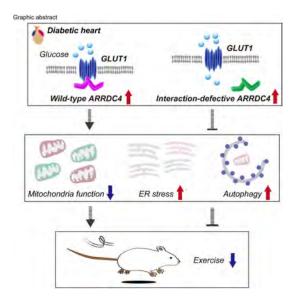


The City College of New York

Hyperglycemia-induced ARRDC4 limits cardiac function and exercise capacity in diabetes

Jun Yoshioka, MD, PhD Department of Molecular, Cellular & Biomedical Sciences CUNY School of Medicine, The City College of New York e-mail: <u>jyoshioka@med.cuny.edu</u>

Despite its clinical importance, the underlying basis of diabetic cardiomyopathy remains unclear. We discovered that arrestin domaincontaining protein 4 (ARRDC4) is a glucose-responsive protein that mediates mitochondrial dysfunction, ER stress, and cardiac dysfunction in diabetes mellitus. ARRDC4 is a member of the ancient family of arrestin-fold proteins with conserved roles in regulating nutrient transporter trafficking as adaptor proteins. Using cellular and animal models, we have found that deletion of Arrdc4 reduces metabolic stress by diabetes and protects the cardiac and skeletal muscle against apoptosis. These results define the outlines of the pathway that strongly links hyperglycemia with diabetic cardiac/skeletal myopathy.



Nakayama et al. *Circ Res* **2024** Jul 1. doi: <u>10.1161/CIRCRESAHA.123.323158</u>

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The City College of New York

Characterization of Indonesian Pteropus alecto Immunoglobulin Genes

Thongthai Thavornwatanayong, Sigit Wiantoro, EmilySegovia, Matthew Kantorski, Kanelly Reyes, Bao Q.Vuong, Susan M. Tsang

There is a need to understand bat immunity to address challenges in public health and conservation. Previous studies of bat immunity have focused primarily on genes related to innate immune response, yet our understanding of bat adaptive immunity, in particular, immunoglobulins (Igs), remains limited. In this study, we reconstructed the evolutionary relationships of the constant region of bat IgM, IgA, and IgG genes and calculated dN/dS ratios to understand selection pressure on each gene. Our phylogenetic reconstruction of each gene yielded topologies that generally agreed with known evolutionary relationships between bat families, with some minor variation in positioning for families that were not well-represented in this study. The dN/dS ratio relative to B. taurus suggested purifying selection for the constant region of all the bat Ig genes. However the significant purifying selection relative to *M. daubentoniid* were only observed in P. a. gouldi, P. a. alecto and P. vampyrus suggesting conservation of IgA among these three flying foxes. Such finding may have implications about the roles of Igs in bat immune response.

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The City College of New York

Reexamination of Nrl regulation with implications for the formation and evolution of photoreceptors

Brandon P. Webley, Miruna Ghinia Tegla, Thabelo Lekoetje, Brendon Patierno, Mark M. Emerson

The Maf family transcription factor NrI is a key regulator of mammalian rod photoreceptor identity. Both gain-of-function and loss-of-function studies have identified NrI as sufficient and necessary for the promotion of rod transcriptional programs and the repression and the identification of gene regulatory networks that set this expression are of critical importance to our understanding of cone and rod photoreceptor formation. Previous studies have used a NrI promoter region to generate a transgenic GFP reporter line (NrIProm::GFP) that has been widely used in studies, often with the purpose to serve as a faithful proxy for endogenous NrI expression and for rod photoreceptor fate. However, the developmental fidelity of the NrI promoter element through examination of the cell types lineage traced by a NrIProm::Cre activity. In addition, Cre protein expression was observed in developing cones, but not adult cones, which supports the conclusion that the propose. The most proteceptors have a history of NrIProm::GFP line to identify S-opsin positive cells as rod photoreceptors was in error and the NrIProm::GFP-positive cells were in fact cones. To address this, we used theriting at postnatal day 0 to unambiguously identify cells generated after birth such as rods, and not cones, which are ports: GFP-positive cells were in fact cones, which are ports. We found almost no S-opsin positive cells do not express S-opsin in the early stages of their formation. Lastly, we used developmental ATAC-See profiling to identify several regions of open conclusion that the previous use of the restriction of NrI expression to rod photoreceptors. The suggest that further elucidation of the mechanisms that regulate NrI expression is necessary to accurately generate a model so photoreceptors. The suggest that the restriction of the mechanisms that regulate NrI promoter is differentially active during to the supports the conclusion that the previous use of the mouse postnatal retina. We hypothesized that the previous use of the mouse p

https://elifesciences.org/articles/54279

Emersonlabccny.com



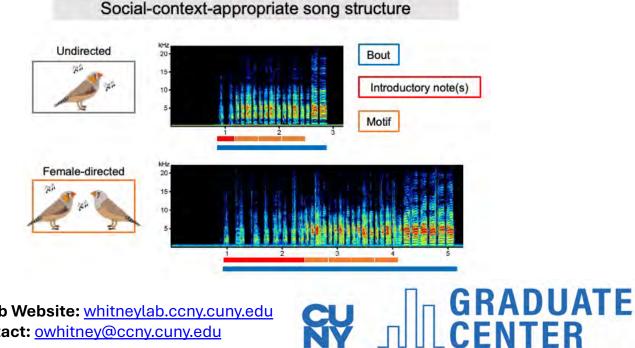
The City College of New York



Oxytocin mediates social-context-appropriate singing

Katherine L. Anderson^{1,2}, Violet Doolittle¹, Aongkita Biswas¹, & Osceola Whitney^{1,2} ¹Biology, CUNY City College of New York; ²Biology PhD Program, CUNY Graduate Center

Modifying behavior is a skill shared between many social animals, including humans and songbirds. In the zebra finch (Taeniopygiaa guttata), adult males modify a learned song depending on the intended audience. Compared to undirected song, femaledirected song (song used for establishing or maintaining pair-bonds) has more introductory notes per bout and more motifs per bout. Brain circuits that control socialcontext-appropriate singing, are assumed to be sensitive to oxytocin. Here, we investigate the consequences of antagonizing the oxytocin receptor on contextappropriate song modifications. We intranasally delivered either an oxytocin receptor antagonist or a saline vehicle control to 8 adult male zebra finches, and then recorded their singing behavior in a female-directed and an undirected context. Compared to the control group, oxytocin receptor antagonism increased the delay to begin singing in an undirected context, but not a female-directed singing context. In both undirected and female-directed singing contexts, males who received the oxytocin receptor antagonist sang fewer introductory notes per bout than those who received saline. Finally, birds who received the oxytocin receptor antagonist sang more motifs per bout in the femaledirected condition than in the undirected condition. Overall, these data indicate that, in adult male zebra finches, the oxytocin receptor may contribute toward the modification of learned vocal behavior.



Whitney Lab Website: whitneylab.ccny.cuny.edu Contact: owhitney@ccny.cuny.edu

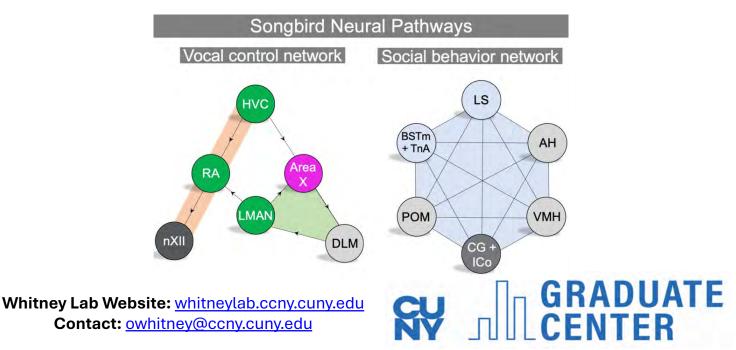
The City College of New York



Visualizing Oxytocin and Vasotocin in the Zebra Finch Brain

Melanie Carcamo¹, Sen Haur Lin¹, Katherine L. Anderson^{1,2}, & **Osceola Whitney^{1,2}** ¹Biology, CUNY City College of New York; ²Biology PhD Program, CUNY Graduate Center

Social behavior derives from the integration of emotional, cognitive, and motivational processes that occur in response to internal and external stimuli. Two neuropeptides, oxytocin and vasotocin, regulate the social behaviors and potentially song production of songbirds. Zebra finch songbirds possess sophisticated neural networks that facilitate vocalmotor control and social behavior. This "social behavior network" is highly connected with the paraventricular nucleus of the hypothalamus (PVN), a major site for synthesizing oxytocin and vasotocin. Avian studies have also highlighted that there are direct and indirect pathways between the social behavioral and the vocal-motor control networks, implicating that social context influences the production of song. Here, we hypothesize that PVN is transporting oxytocin and vasotocin protein to hypothalamic and social behavior network regions in the zebra finch brain. We evaluate this hypothesis by performing fluorescent immunohistochemistry against oxytocin and vasotocin in adult male and female zebra finches. We observed immunoreactive expression of oxytocin and vasotocin synthesis in PVN and projections surrounding VMH. This expression provides correlative evidence of how these neuropeptides function in songbird social behaviors. In pair with anatomical data, oxytocin and vasotocin signaling from PVN may work to convey social context to hypothalamic nodes of the social behavior network, eventually contributing toward regulation of singing based on social context.





Spatiotemporal Characterization of Nucleolin Phosphorylation at Threonine 76 and 84 in Cell Cycle Regulation and DNA Damage Response

Hanjun Jeon^{1,2}, Rukayat Agbona¹ and Anjana Saxena^{1,2}

¹Biology Department, Brooklyn College, Brooklyn, New York, USA, ²City University of New York, Graduate Center, New York, USA.

Abstract

Nucleolin (NCL) is a multifunctional protein that plays pivotal roles in ribosome biogenesis, chromatin structure maintenance, cellular stress responses, and cell cycle regulation. This study aims to investigate the phosphorylation status of NCL at threonine 76 (T76) and threonine 84 (T84) under various stress conditions and during different phases of the cell cycle, focusing on the regulatory mechanisms involved. Previous studies suggested Protein Phosphatase 1 Beta (PP1 β) might regulate these phosphorylation sites. However, our findings indicate that silencing PP1 β does not alter the phosphorylation status of NCL at T76 and T84 in response to UV, hydroxyurea (HU), and etoposide (ETP) treatments, suggesting that other phosphatases may be involved.

Using U2OS cells engineered to express exogenous 3x FLAG-tagged NCL, we treated cells with UV, HU, nocodazole (Noco), camptothecin (CPT), and ETP. Western blotting was employed to analyze the phosphorylation and expression levels of NCL. Our results show that UV treatment leads to a significant decrease in NCL levels and a complete loss of phosphorylation at both T76 and T84. Similarly, ETP and HU treatments result in the loss of detectable phosphorylation at these sites. Conversely, CPT treatment reduces phosphorylation, while Noco treatment strongly induces phosphorylation at T76 and T84, with significant increases in NCL expression.

These findings suggest that the phosphorylation of NCL at T76 and T84 is differentially regulated under various stress conditions and highlight the complexity of NCL regulation. The data imply that PP1 β is not the primary phosphatase for these sites. Future directions include utilizing Phos-tag SDS-PAGE for detailed phosphorylation analysis and exploring the subcellular localization of phosphorylated NCL. Understanding these mechanisms may reveal novel therapeutic targets for modulating NCL function in response to cellular stress and DNA damage.





Exploring a Unique Comparative Model of Immune Deficiency: Adaptive Immunity in the Seahorse

Tony Wilson PhD Program in Biology Department of Biology Aquatic Research and Environmental Assessment Center e-mail: <u>twilson@brooklyn.cuny.edu</u>

The adaptive immune system is a key innovation of the vertebrates, and central to their evolutionary success. While the genes of the Major Histocompatibility Complex (MHC) have long been thought to be essential for adaptive immunity and immune memory, the recent discovery of species lacking key components of the MHC challenges this paradigm. Seahorses and pipefish (family Syngnathidae) are one of the only known examples of this phenomenon, and while *Hippocampus* seahorses maintain a minimal MHC II system, *Syngnathus* pipefish have lost the MHC II/CD4 axis considered essential for immune memory - How are such species able to mount an effective immune response? We are developing molecular tools that will allow us to interrogate this unique evolutionary experiment to identify structural and functional changes associated with the loss of key components of the adaptive immune system, and potential alternative mechanisms of immune protection. These tools will be used to screen immune activation and memory in immune challenge experiments with MHC II+/+ and MHC II-/- animals.

Wilson Lab



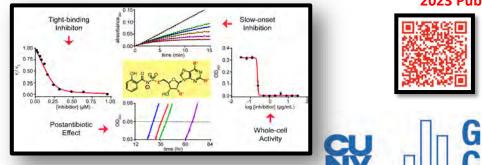


The Quadri Lab Biology of Mycobacterial Pathogens

Luis Quadri PhD Program in Biology PhD Program in Biochemistry Department of Biology e-mail: LQuadri@brooklyn.cuny.edu

The Mycobacterium genus includes obligate pathogens such as Mycobacterium tuberculosis and Mycobacterium leprae, the causative agents of tuberculosis and leprosy, respectively. The genus also includes ubiquitous environmental species recognized as opportunistic human pathogens. Among them, Mycobacterium kansasii, Mycobacterium abscessus, and Mycobacterium avium are the most pathogenic. These pathogens cause tuberculosis-like disease in individuals with pre-existing conditions, such as those who are immunocompromised or have suboptimal lung function due to various medical conditions. Mycobacterial infections are difficult to control and eradicate. Current treatments require long-term (months to years) multidrug (often four or more) regimens with adverse side effects. The rise of drugresistant mycobacterial strains is a global phenomenon of increasing concern. Comprehensive knowledge of the biology of mycobacterial pathogens is needed to illuminate paths to new and more efficacious therapeutics. Our long-term goals are to expand the understanding of mycobacterial pathogens' biology and illuminate new potential avenues for antimicrobial drug development.

Link to Lab Publications, Grants, and More



2023 Publications



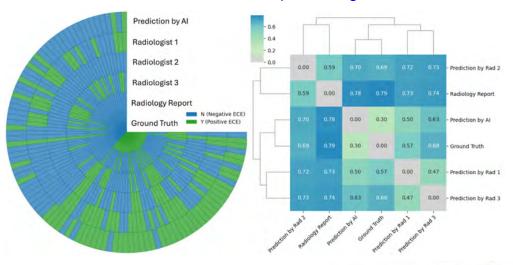
GRADUATE



Deep Learning Enhances Detection of Extracapsular Extension in Prostate Cancer from mpMRI of 1001 Patients

Professor Pegah Khosravi PhD Programs in Biology and Computer Science New York City College of Technology Department of Biological Sciences Email: <u>pkhosravi@citytech.cuny.edu</u>

Extracapsular extension (ECE) is detected in approximately one-third of newly diagnosed prostate cancer (PCa) cases at stage T3a or higher and is associated with increased rates of positive surgical margins and early biochemical recurrence following radical prostatectomy (RP). This study presents the development of AutoRadAI, an end-to-end artificial intelligence (AI) pipeline designed for the identification of ECE in PCa through the analysis of multiparametric MRI (mpMRI) fused with prostate histopathology. The dataset consists of 1001 patients, including 510 pathology confirmed positive ECE cases and 491 negative ECE cases. AutoRadAI integrates comprehensive preprocessing followed by a sequence of two novel deep learning (DL) algorithms within a multi-convolutional neural network (multi-CNN) strategy. In the blind testing phase, AutoRadAI achieved an area under the curve (AUC) of 0.92 for assessing image quality and 0.88 for detecting the presence of ECE in individual patients. Additionally, AutoRadAl is implemented as a userfriendly web application, making it ideally suited for clinical applications. Its datadriven accuracy offers significant promise as a diagnostic and treatment planning tool. Detailed instructions and the full pipeline are available at https://autoradai.anvil.app and on our GitHub page at https://github.com/PKhosravi-CityTech/AutoRadAI. P. Khosravi et al. medRxiv 2024, DOI: https://doi.org/10.1101/2024.05.21.24307691



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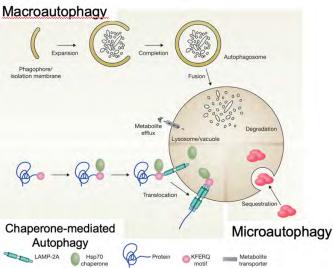




Autophagy in Development and Aging

Prof. Alicia Meléndez

Biology and Biochemistry PhD programs, Graduate Center Biology Department, Queens College, The City University of New York Flushing, NY 11367, Email: <u>Alicia.Melendez@qc.cuny.edu</u> https://aliciamelendezcuny.wordpress.com/



Autophagy is the major cellular pathway for degrading long-lived proteins and cytoplasmic organelles. Autophagy is involved in the progression of cancer, promotes longevity and prevents neurodegenerative diseases. We use a combination of genetic, molecular and cellular biological approaches, in the genetically tractable model organism C. *elegans*, to determine the role of autophagy in development, and aging. We were the first to implicate a direct role for autophagy in longevity and in the remodeling that occurs during dauer formation, a response of *C. elegans* to lack of nutrients early in development (Meléndez et al., Science 2003). Several conserved longevity pathways are known to extend lifespan, and interestingly, they all require autophagy. More recently, we showed that autophagy is required for lipid homeostasis (Lapierre et al., Current Biology 2011), and for stem cell proliferation (Ames et al., Current Biology 2017). Projects in the lab aim to:

- I. Determine the role of autophagy in germ cell stem cell progenitors (Ames et al., 2017 Current Biology), meiosis, and DNA damage repair (Hoffman et al., 2014 PLos One).
- II. Investigate compensatory mechanisms for autophagy. We have found that autophagy *atg-4.1* mutants are more resistant to Tunicamycin/ER stress and will determine the compensatory mechanisms involved.
- III. Microautophagy consists of engulfment of cytoplasmic cargo directly by septation, protrusion or invagination of the lysosome membrane or of endosomal vesicles (eMI). It may involve a specific sequence motif that is highly conserved in the *C. elegans* proteome. We will identify the genes involved in this process employing advanced genetic approaches.
- IV. Al-powered cross-level cross-species omics data integration to elucidate mechanisms of elevated longevity. Novel molecular targets, biomarkers, pharmaceutical agents, and personalized treatments identified by AI will be verified in *C. elegans*, where several pathways have been shown to increase longevity and all so far require autophagy.



Department of Biology 65-30 Kissena Blvd. Natural Sciences Building E102/104 Flushing, NY 11361 Sebastian Alvarado@gc.cunv.edu

What can a water flea teach us about collective behaviour and gene-by-environment interactions?

Alice Lin, David Young, Oleg Kogan, Sebastian Alvarado

Animal behaviour is finely tuned to receive, process, and respond to diverse and dynamic environmental stimuli. Within a species, these behaviours can translate into motor movements and emerge into collective dynamics across tens to hundreds of individuals. The Alvarado Lab, in Collaboration with the Kogan Lab, have adopted *Daphnia magna* as a model system to understand the behavioural and morphological variation as a function of a changing environment. We have engineered and optimized tools using high throughput platforms to track individual daphnids (Trex) and screen morphological variation in fixed animals using flowcell microscopes (PlanktonScope). Our approach will reveal environment-by-gene interactions that can be complemented with molecular screens of the transcriptome/(epi)genome and validation using antisense knockdowns, CRISPR, and pharmacology. Since daphnids are parthenogenetic, we expect that these gene-by-environment changes can be resolved down to epigenetic substrates and tractable towards experimental evolution studies. Our data will inform a broader understanding of the intersectional processes that generate (epi)genetic variation across cells, tissues, and whole organisms.





a 2024 - Weanesdays a 11.10a 3B D-139	
Aug 28 Organizational Meeting	
Sep 4 Sebastian Alvarado, Queens College Department of Biology Behavioral and morphological plasticity in an African cichlid, Astatotilapia burtoni	Savage-Dunn
Sep 11 Anke Kloock, NYU Grossman School of Medicine Rictor regulates the Growth of Germline Stem Cells non-autonomously	Savage-Dunn
Sep 18 Yu-Chieh David Chen, New York University Wiring up the brain during development: Coordination and propagation of cell fate choic assembly	Savage-Dunn ce in neural circuit
Sep 25 Peter Compo, former director DuPont Ventures Recognizing Natural Selection as a Dynamical Law: Key to Understanding Creativity and in Culture	Lahti Evolution
Oct 2 No class	
Oct 9 Robert Kozol, St. John's University Investigating novel behaviors in the blind Mexican cavefish: How evolution shapes neuro and nutrient-poor environment	Alvarado al circuits in a dark
Oct 16 Lei Xie, Hunter College Omics, AI, and systems medicine	Meléndez
Oct 23 Jennifer Salerno, George Mason University	DuBuc
Oct 30 Christopher Rongo, Rutgers University Using <i>C. elegans</i> to understand the role of mitochondria in aging	Savage-Dunn
Nov 6 John Patton, Indiana University Bloomington Replication of the Rotavirus Genome: Secrets Revealed by Reverse Genetics	Dennehy
Nov 13 Rabindra Mandal, Hunter College Exploring Gut Bacteroides in Severe Malaria Anemia: Challenges and Way Forward	Dennehy
Nov 20 Vanessa Ezenwa, Yale University Helminth-microbe coinfection: insights from a natural system	Coleman
Nov 27 <i>No class – Friday schedule</i>	
Dec 4 Herminia Gomez, USDA Federal Employment Opportunities for Bio Majors	Alvarado
Dec 11 Néva Meyer, Clark University Worms do it differently: Dual autonomous and conditional neural specification in anneli	DuBuc d s



Bacterial sibling inhibition, a novel discovery and its potential for antibiotics

Prof. Hai-Ping Cheng, PhD

Biology and Biochemistry PhD Programs, Graduate Center Biology Department, Lehman College, The City University of New York Bronx, New York 10468, Tel: 718-960-7190 (O), <u>haiping.cheng@lehman.cuny.edu</u> <u>https://www.lehman.edu/academics/natural-social-sciences/biology/profile/fac-cheng/</u>

Our world is facing an increased possibility of a worldwide bacterial infection pandemic especially with the deadly combination of the continued rise of antibiotic-resistant bacteria and the lack of novel antibiotics. Our lab accidently discovered that most bacteria have a previously unknown mechanism that allows them to inhibit other unrelated bacteria and even siblings in close range. We have shown that this sibling inhibition mechanism and the sibling inhibitor appear to be shared by many very different bacterial so that a common lab bacterium *Escherichia coli* is able to rely on its secreted sibling inhibitor to inhibit wide range of different bacteria. The sibling inhibitor caused bacterial cells to explode in contact. We are currently focusing on this *Window of Opportunity* to identify the structure of this amazing sibling inhibitor and the bacterial cellular process that is targeted by the sibling inhibitor.

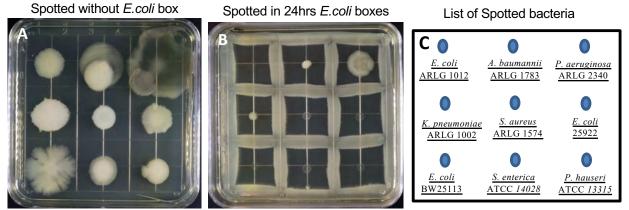


Figure. *E. coli* was streaked onto LB agar and incubated for 1-day. Gram-negative and positive bacteria, including multi-drug resistant clinical isolates, were spotted in the center of the grids or onto fresh LB agar only. Data shows *E. coli* can surprisingly inhibit the growth of other bacteria.

Representative Publication: Ertan Kastrat and Hai-Ping Cheng. 2024. Escherichia coli has an undiscovered ability to inhibit the growth of both Gram-negative and Gram-positive bacteria. Scientific Report 14, 7420. **link** ->









High-throughput cell phenotype screening coupled with ion mobility spectrometry of American *Aconitum*

Yi Zhao^{a,b}, Dennis Y. Liu^c, Trevor N. Clark^c, Roger G. Linington^c, Edward J. Kennelly^{a,b}

^a Department of Biological Sciences, Lehman College, The City University of New York, Bronx, 10468 NY, United States
^b Biology Ph.D. Program, The Graduate Center, The City University of New York, New York, 10016 NY, United States
^c Department of Chemistry, Simon Fraser University, V5A 1S6 British Columbia, Canada.

Aconitum plants have been widely used as traditional medicine in Asian countries for centuries. However, there are few records about how American Aconitum has been used medicinally, despite its phylogenetic closeness to medicinally important Asian species (Luo et al., 2005). This study aims to discover the bioactive compounds in American Aconitum based on a systematic molecular network strategy integrating both mass spectrometric data and a high-throughput phenotype screening assay, cell painting. The chemical profile in different parts of two American Aconitum species was obtained by ion mobility spectrometry technique and compared with non-American Aconitum species. Image analysis and feature extraction were performed on four different concentrations of Aconitum extracts assayed in cell painting, resulting in 2,090 unique morphological features per extract. In conjunction with the TargetMol library of 4,400 compounds with known mechanisms of action, 198 unique hierarchical clusters were established after a feature selection strategy known as Fast Correlation-Based Filtering, which reduced the number of features to 429. An overall activity heuristic called CP score was calculated for each sample. After integrating CP score and spectrometric data, a molecular network containing higher CP scores was constructed and the compounds with high activity were targeted and being identified. The molecular network showed that American Aconitum is more active than non-American species in the cell painting assay.

Keywords: Aconitum, cell painting, mass spectrometry, molecular network, drug discovery

Presenting author. Yi Zhao E-mail address: <u>yzhao6@gradcenter.cuny.edu</u>

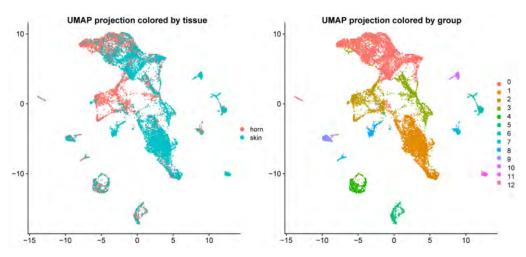


Barich COLLEGE

Building a single nucleus atlas of the fetal horn bud

Zachary T. Calamari

The genetic underpinnings of bovid horn growth are of great interest in agriculture, as horned livestock represent a significant danger to other animals and their handlers. Although polled (genetically hornless) breeds mediate some of the danger posed by horns, the adoption of these breeds is limited to certain industries. Breeding for polled animals also may reduce genetic diversity in livestock and introduce other undesirable traits, thus targeted genetic approaches to prevent horn growth are needed. Nevertheless, there has been limited research on the earliest stages of horn development *in utero*, when horn-forming tissues (the horn bud) differentiate from other cranial tissues. To address this limitation, I am pursuing single nucleus sequencing of fetal horn buds. Working with collaborators at University of Idaho, we collected the left and right horn buds from a 70-day post conception fetal cattle, capturing the time point when early morphological differentiation between horn bud and other cranial soft tissues is distinct. Sequences from these tissues will form the first atlas of cell types and gene expression values for fetal cattle horns.



GRADUATE CENTER

Representative publication: Calamari and Flynn *Commun Biol* 2024 7:509 https://doi.org/10.1038/s42003-024-06134-4

calamarilab.com





Effects of Matrix Rigidity on Glial Morphology and Function

Maria Pereira

The regulation of chronic pain is influenced by the neuroinflammatory response of microglia. Microglia play a crucial role in maintaining brain homeostasis, but when over-activated or uncontrolled, they can contribute to various brain diseases, promoting neuronal cell death in neurodegenerative conditions like Alzheimer's, Parkinson's, Huntington's, and ALS [1]. Similarly, recent advancements indicate that the extracellular matrix undergoes remodeling in neurodegenerative diseases. This remodeling influences the release of pro- and anti-inflammatory cytokines, shaping the fate of immune, glial, and neuronal cells [2]. These comprehensive insights fuel our interest in understanding microglial responses to matrix rigidity and contribute valuable knowledge to the broader field of neurobiology.

Aim:

Investigate how matrix rigidity influences microglial behavior, function, and epigenetic programming In vitro.

Methods:

To investigate the role of substrate biomechanics on BV-2 cell morphology and function in different matrix rigidities of 0.2 kPa, 0.5 kPa, 2.0 kPa, 8.0 kPa, 16.0 kPa, 32.0 kPa, and 64.0 kPa. The cells are cultured in F-12 HAMS, FBS, and STREP media in 6-well plates coated with various extracellular matrix conditions.

- 1. Morphology: Microglial morphology will be analyzed in terms of area, circularity, and process complexity.
- Engulfment: Functional assessments will be performed by placing carboxyl beads into the cultured microglia in 6-well ECM-coated plates. After incubation, the dynamics of glial engagement with the carboxyl beads will be recorded and analyzed.
- 3. Epigenetic Programming: the result of microglia's engagement with the ECM will be studied using DNA methylation patterns, histone modifications, and gene expression analysis.
- 4. Microscopic videos will be recorded to generate predictive computational models for microglial behavior.

Results:

Our preliminary results suggest that substrate biomechanics affects the branching of BV-2 processes as well as cellularity and engulfment(function). These analyses are currently being completed. We are currently working on researching changes in DNA methylation patterns, histone modifications, and gene expression.

Conclusion:

This study aims to understand the role of the extracellular matrix in glial behavior and function. The results can open avenues for biomarker discovery. Such biomarkers could serve as diagnostic tools for early detection and intervention in diseases like Alzheimer's and Parkinson's. In addition, understanding the mechanics of the extracellular matrix is a new therapeutic approach. Instead of targeting microglia, we can explore treatments that alter how the extracellular matrix behaves, to develop potential approaches to treat neurodegenerative diseases.





Investigating the effect of direct current stimulation on axonal regrowth and motor function recovery after spinal cord injury in mice

Dr. Zaghloul Ahmed PT PhD

Investigating the effect of direct current stimulation on axonal regrowth and motor function recovery after spinal cord injury in mice

Background. To date, Axonal regeneration following spinal cord injury (SCI) is not achievable. One promising approach to this problem is using electrical stimulation to activate the pathways that would create a conducive environment for axonal regeneration. Applied electrical stimulation creates a voltage gradient that has both stimulatory and guidance effects on neurite growth. However, there are difficulties in the applications of electrical stimulation.

Methods. Our study uses a novel multipath direct current stimulation system (Mutltipath-DCS). It has 6 surface anode electrodes that are placed on the ventral and dorsal surfaces of the mouse. In addition, a cathodal ionically conductive hydrogel electrode (iCHE) is placed over the injury site. The study included 5 CD-1 mice with SCI. Two of the mice were stimulated with current intensity 1 mA and 4-7 V for 2 hours, 4 times/week for 3 weeks. Neurotracing was done by injecting biotinylated dextran amine below the injury site, and Basso Mouse Scale was used to record locomotor recovery in SCI mice.

<u>Results.</u> The stimulated mice showed significant improvement in their locomotor recovery with forelimb-hindlimb coordination, plantar stepping, parallel paw position and tail up position. In addition, we were able to visualize axons at the injury site in the stimulated group only.

Conclusion. We suggest that the specific distribution of the electrodes of multipath-DCS provides guidance of axonal regrowth from both directions towards the injury site. In addition, the composition of iCHE improves the delivery of the stimulating current to the tissue as it allows us to use high current intensity for prolonged duration of stimulation.





Elucidating the Behavior of Charged Peptides Using The SIRAH-CG Model

Presenting Author: Tania Rajpersaud PI: Sharon M. Loverde

Mixtures of oppositely charged polyelectrolytes can engage in Liquid-liquid Phase Separation (LLPS). It is well known that the properties of this phase separation depend on the molecular composition of the complex polymers. However, the exact relationship between phase behavior and molecular composition remains unknown. Understanding this relationship would lend itself to applications in developing novel drug delivery systems and responsive materials. Here, we compare the phase behavior of six peptide-based polyelectrolyte complexes using both all-atomistic and coarse-grained molecular dynamics. These systems were initially designed by Lorraine Leon laboratory (University of Central Florida) to probe the relationship between hydrophobicity and condensate stability by incorporating either Glycine, Alanine, or Leucine within poly-lysine and poly-glutamic acid strands. In all-atomistic simulations we observe sensible trends between the hydrophobicity of the peptide, chain conformation, and degree of backbone hydrogen bonding, aligning qualitatively with experimental FTIR results. We also observe similar trends in the coarse-grained simulations using the SIRAH-CG force field (developed by Sergio Pantano, Institut Pasteur de Montevideo), but with a significantly larger radius of gyration values, suggesting expanded conformations of the peptide chains. Our results suggest that the SIRAH-CG force field can be used to characterize LLPS for oppositely charged chains, and we suggest an approach to improve the model to better predict the phase separation behavior of these peptide-based polyelectrolyte complexes.

"Molecular Dynamics Simulations of Polylectrolyte Complexes," Tania Rajpersaud, Sara Tabendeh, Lorraine Leon, and Loverde, S. M., *Biomacromolecules*, 2024.

https://sites.google.com/site/loverdelaboratory GRADUATE

Biochemistry



Sebastien Poget, Ph.D. Executive Officer



Denise Charles Assistant Program Officer

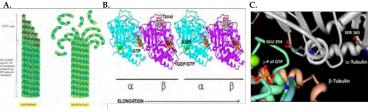




Exploring the α/β -Tubulin Toggle Switch in Human Breast Cancer <u>Susan A. Rotenberg</u> (Queens College), Maria Nagan (Stony Brook-SUNY), Nathalia Holtzman (Queens College)

 α/β -Tubulin heterodimers are building blocks of microtubules or spindle fibers that respectively support the phenotypes of cell movement and cell division, respectively. Protein kinase C (PKC) is a key enzyme in signaling pathways that control these phenotypes in human breast cells. Previous work from the Rotenberg lab demonstrated that PKC phosphorylated a-tubulin at Ser¹⁶⁵ in human breast cells, engendering the assembly of α/β -tubulin subunits into microtubules, and thereby promoting cell movement. Similarly, others demonstrated that b-tubulin undergoes phosphorylation at Ser¹⁷² by cyclindependent kinase-1 (Cdk-1) which consequently promoted proliferation, a process that is dependent on the assembly of α/β -tubulin subunits into spindle fibers in preparation for cell division. The possibility that phosphorylation of one or the other tubulin subunit favors the appearance of a specific phenotype may provide a breakthrough in our understanding of how the cell is instructed to transition between the programs of cell movement and cell proliferation. Phosphorylation of a-tubulin or b-tubulin could determine whether a breast cancer cell metastasizes to a remote site or proliferates into a primary tumor. (NIH R16 GM153696-01)

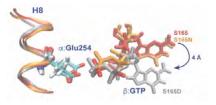
Figure 1: Structural Models of $\alpha/\beta\text{-Tubulin}$



Biochemistry

Key publications from the Rotenberg Lab Maddula *et al.*, *Biochemistry* 61: 1508-1516, 2022 Markovsky *et al.*, *Cell Signaling* 52: 74-82, 2018 De *et al.*, *Cytoskeleton* 71: 257-272, 2014 Abeyweera *et al.*, *J. Biol. Chem.* 284:17648-17656, 2009 Sun and Rotenberg, *Cell Growth & Diff.* 10: 343-352, 1999 Figure 2: The Toggle Switch Model describes the effects of

Figure 3: Molecular dynamics of E-site GTP in mutant α-tubulin (phosphomimetic S165D, negative control S165N). Maddula *et al.*, *Biochemistry* 61: 1508-1516, 2022





QUEENS

Multiscale Modeling and Simulation of Replication/Transcription Complexes of Emerging RNA Viruses

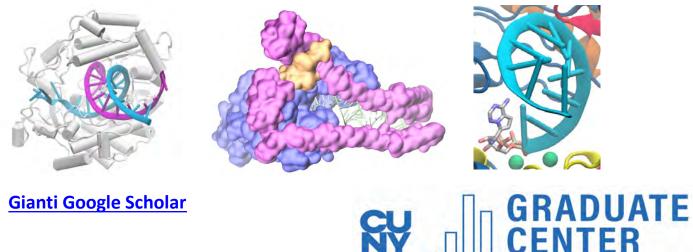
Hannah Gibbs¹, Ben Shabtian², Preston Moore¹, Eleonora Gianti^{2*}

- 1. Department of Chemistry and Biochemistry, Saint Joseph's University
- 2. Department of Chemistry and Biochemistry, CUNY Queens College

Presenting Author and PI: *Eleonora.Gianti@qc.cuny.edu;

The emergence of RNA viruses with pandemic potentials, such as SARS, MERS, SARS-CoV-2, ZIKA virus (ZIKV), etc., has underscored the critical need for advanced computational approaches to understand the complex mechanisms underlying viral replication and transcription. The **Gianti Lab at CUNY Queens College** uses multiscale modeling and simulation to bridge the gaps between molecular-level interactions and cellular-scale phenomena in these processes. Specifically, we integrate approaches across various scales—from first-principles molecular dynamics (MD) simulations within hybrid quantum mechanics/molecular mechanics (QM/MM) implementations for atomistic level interactions, to enhanced sampling techniques for investigating protein conformational changes at longer time scales, and up to coarse-grained (CG) models capturing the behavior of large biomolecular complexes. Furthermore, we work at the crossroads of molecular modeling with data mining, machine learning (ML) and computer-aided drug design (CADD).

Herein, we present some of our recent computational efforts to unravel the intricate dynamics of viral RNA synthesis, replication fidelity and interactions of enzymes and cofactors in SARS-CoV2 and closely related emerging viruses. Our insights are crucial for identifying new antiviral drug targets and designing more effective therapeutic strategies against highly pathogenic viruses. Not only our work highlights recent advancements in multiscale modeling and simulation, but also emphasizes their application to RNA virus replication/transcription complexes, ultimately paving the way for addressing the currently open challenges in this rapidly evolving field.

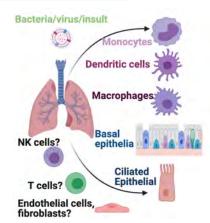




Cell Death Programs as Mediators of Inflammation and Multi-Organ Injury

Pratyusha Mandal, PhD, Dept of Biological Sciences, Lehman College, Biology (MCD) and Biochemistry Doctoral Faculty, the Graduate Center Email: pratyusha.mandal@lehman.cuny.edu

Cell death programs (including but not limited to, apoptosis, necroptosis, pyroptosis, ferroptosis) are genetically regulated pathways that serve as the first line of defense against invading pathogens or cellular abnormalities. Even though the primary function of cell death programs is to eliminate infected or abnormal cells, these pathways also dictate inflammation and tissue injury. Release of immunogenic cellular materials from dying cells contributes to the initial stages of inflammation (also called acute inflammation). As infection/insult is mitigated, acute inflammation is resolved with onset of tissue repair processes. However, if insult/infection continues, acute inflammation is not resolved, the persistent inflammation continues to injure tissues and subsequently leads to fatal organ damage. The key research areas of Mandal laboratory is a) to study how cellular death programs dictate organ injury during bacterial and herpesvirus infections (with a focus on identifying role of cell death in the different lung cells, during acute pneumonia and chronic lung disease e.g. fibrosis); b) to study how cellular death programs can be modulated via chemical or biological modulators for therapeutic purposes. Prajakta Sawant, PhD student Biology (MCD) is currently investigating how cellular death programs are modulated in lung cells during chemotherapy and progression of lung cancer. Mandal laboratory is funded by NIH grant and recruiting new students. Work highlight: in vitro biochemistry, mouse genetics, in vivo infections, co-infection studies to mimic clinical conditions.



https://www.ncbi.nlm.nih.gov/pmc/articles/PMC 4512186/ https://pubmed.ncbi.nlm.nih.gov/30021146/ https://www.ncbi.nlm.nih.gov/pmc/articles/PMC 9986559/

mandallaboratory.com (coming soon)

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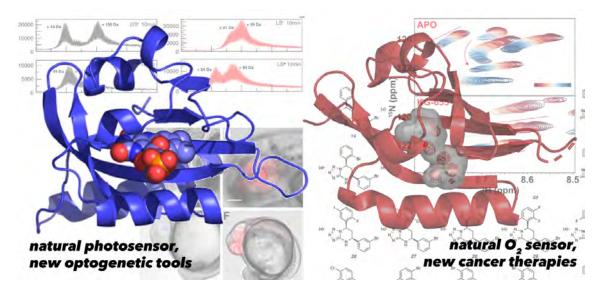




Studies and applications of environmentallyswitched proteins

Kevin H. Gardner, ASRC Structural Biology Initiative

Environmental cues regulate many biological processes, coordinating cellular responses to changing conditions. Such regulation is often initiated by sensory protein domains which use small molecule ligands to convert environmentally-triggered changes into altered protein/protein interactions. Combining biophysics, biochemistry and chemistry, we study the mechanistic controls of such domains to understand fundamentals of biological signaling and how these might be altered in disease or artificially controlled for therapeutic or biotech purposes. Here I will present examples of this principle, showing how our work into light- and oxygen-regulated proteins has led to novel optogenetic tools and a novel anti-cancer therapeutic (Merck's belzutifan HIF-2 inhibitor).



Example publication: Dikiy, Swingle, et al., J. Biol. Chem. 2023 (https://doi.org/10.1016/j.jbc.2023.104934) Group website: https://kglab.org

> SY A GRADUATE CENTER



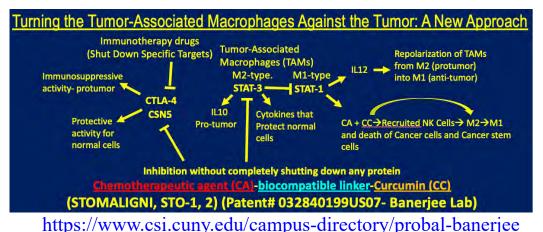
A Novel Gemcitabine Derivative as an Effective Agent Against Pancreatic Cancer

Callistus Onyeagba, Shubhasmita Mohapatra, Adrian Guerrero, Jing Wu, Joel Friedman, and Probal Banerjee

probalbanerjee@yahoo.com

GRADUATE CENTER

Pancreatic ductal adenocarcinoma (PDAC) disproportionately impacts Black Americans who suffer from inferior survival and presentation of a more advanced disease than the white patients. Initiation and progression of PDAC is associated with a major infiltration of far more innate immune cells such as macrophages than adaptive immune cells. Therefore, if activated selectively inside the PDAC tumor, the tumor-associated macrophages (TAMs) may prove to be most effective in PDAC therapy. The Banerjee lab has used a synthetic strategy to reversibly link the PDAC drug Gemcitabine (Gem) to the dietary anticancer agent curcumin (CC). The proprietary prodrug thus invented, STO-2, was greater than two-fold more effective than Gem in killing the mouse pancreatic cancer Pan02 cells in vitro. We and others have established that CC repolarizes the tumor-promoting M2-type TAMs into the tumoricidal M1 state, but inhibits such inflammatory effects in non-cancerous tissue. This project begins by testing the efficacy of STO-2 against pancreatic cancer in a syngeneic mouse model created through heterotopic implantation of the Pan02 cells in C57BL/6 mice. We have observed that topical application of STO-2 dissolved in a proprietary neutral gel caused a major suppression of tumor growth. Further studies are in progress to reveal the mechanism of this therapeutic activity of STO-2 against pancreatic cancer.



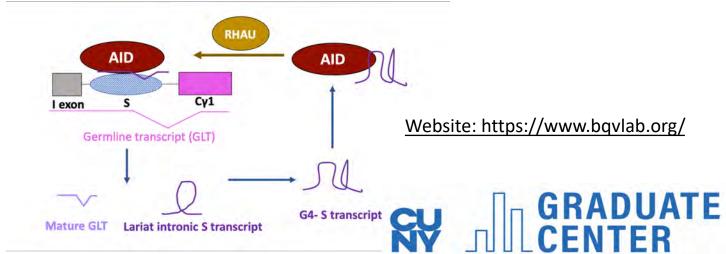
Mohapatra et. al (2023) <u>International Journal of</u> <u>Molecular Science</u>, 24, 5026 Mukherjee et. al. (2018) <u>Journal of Experimental &</u> Clinical Cancer Research, 37, 168. The City College of New York

The DEAH-box helicase RHAU regulates immunoglobulin class switch recombination

Sadman Shawraz, Thongthai Thavornwatanayong, Sabine Jean Guillaume, Kanelly Reyes, Simin Zheng, Bao Q. Vuong

Contact: <u>bvuong@ccny.cuny.edu</u>

During a humoral immune response, B cells produce alternative immunoglobulin isotypes (IgG, IgA, IgE) through class switch recombination (CSR). Initiation of CSR requires AID-mediated deamination of switch (S) regions in the immunoglobulin heavy chain (IgH) locus. G-quadruplex(G4)-forming S region RNAs bind to AID and localize AID to sequence specific S region DNA sequences; however, the molecular mechanism that transfers AID binding from G4-RNA to DNA remains uncharacterized. We hypothesize that helicases disrupt G4-RNA to permit the base-pairing of the S transcript to the complementary DNA sequence in the IgH locus during CSR. An S region RNA pull-down assay identified the RNA Helicase associated with AU-rich element (RHAU), a DEAH-box RNA helicase, as an S transcript binding protein. To examine the role of RHAU in CSR, we genetically deleted a floxed *Rhau* allele (*Rhau^F*) in mouse B cells expressing Cre recombinase under the control of the CD23 promoter (CD23-Cre) to produce a deleted Rhau allele (*Rhau*^{Δ}). *Rhau*^{Δ/Δ} mice produced less serum IgG1, IgG2b, IgG2c, and IgA but comparable IgM and IgG3 as compared to wild-type, CD23-cre⁺, and *Rhau^{F/F}* mice. In vitro stimulated Rhau^{Δ/Δ} B cells show decreased IgG1 and IgA CSR that correlates with reduced γ 1- and a-germline transcription (GLT), respectively, as compared to the control genotypes. Surprisingly, IgG3 CSR and γ 3-GLT increased. These data suggest that RHAU regulates GLT during CSR. Whether the altered GLT changes S transcript levels and thus AID localization and deamination remains to be determined.



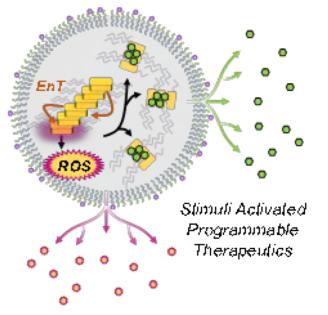


Structured Condensates as Novel Biomaterials

Ankit Jain Assistant Professor PhD Programs in Biochemistry and Chemistry Brooklyn College Cancer Center Department of Chemistry and Biochemistry e-mail: ankit.jain@brookyln.cuny.edu

Biomolecular condensates represent a growing area of research, due to their recognized importance in subcellular organization. While condensates represent an exciting therapeutic target due to their high functional relevance, their foray into novel biomaterials is perhaps equally imperative. An exciting area of development is the application of condensates as a drug delivery platform. One could envisage a next generation of platforms that, instead of being a single phase inside, are made up of multiple stable phases that control the spatial distribution of active components inside, allowing the possibility of reaction systems controlling the therapeutic response. Controlled localized structure in a globally liquid droplet would not only enhances the partition coefficients of prospective drug molecules, but will also be capable of stimuli sensitive, reversible, and multifarious action. Recently, we showed that minimalistic peptides can indeed form localized beta sheet structures inside liquid droplets.¹ In our lab, we intend to explore structured condensates as a viable delivery vehicle with special impetus to stimuli responsive and programmable delivery of anti-cancer drugs.

1. Jain et al. J. Am. Chem. Soc. 2022, 144, 33, 15002–15007



Jain Group Website





Repurposing drugs to treat Alzheimer's disease: exploring their mechanisms of action

Grace Terry (Biochemistry PhD student)

Professor collaborators: L. Xie (Computer), P. Serrano (Psychology), P. Rockwell (Biology) M. Figueiredo-Pereira (Biology)

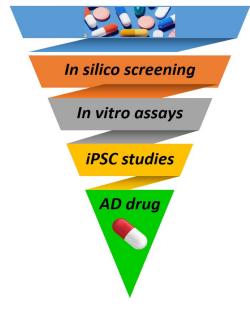
Alzheimer's Disease (AD) is a neurodegenerative disease characterized by amyloid beta plaques, neurofibrillary tau tangles, neuroinflammation, neuronal and synaptic loss, and cognitive decline.

Currently, there are extremely limited treatment options for AD. Bringing a new drug to market is extremely resource intensive in both time and money. Drug repurposing is an efficient route to bring a safe and effective treatment to the clinic.

We use a bioinformatics approach to predict drugs with repurposing potential for AD. We then validate the ability of those drugs to diminish AD pathology, with **induced pluripotent stem cells (iPSCs**). Human iPSCs emerged as a new way to model AD in a fully human based system.

Using iPSCs differentiated into cortical neurons we test drug efficacy and investigate their mechanisms of action. This work will allow us to deeply examine the mechanistic potential of drugs to be repurposed for AD as well as highlight novel therapeutic targets to be further explored.

FDA approved/Investigational Drugs



Publication links:

https://pubmed.ncbi.nlm.nih.gov/36167438/ https://pubmed.ncbi.nlm.nih.gov/35411386/ https://pubmed.ncbi.nlm.nih.gov/38234827/ https://pubmed.ncbi.nlm.nih.gov/38355687/

Funding: NIH R01AG057555



Chemistry



Yolanda Small, Ph.D. *Executive Officer*



Tricia Plummer Assistant Program Officer









NanoBioNYC Research Traineeship NRT-URoL - Nanoscience Connected to Life

PI: Rein V. Ulijn, co-PIs: Yolanda Small, Stephen O'Brien, Ruth Stark, Sharon Loverde Coordinators: Tasnim Jackson, Alma Perez Perrino

The NanoBioNYC research traineeship program aims to train a new generation of scientists to harness the power of bio-inspired nanoscience to address critical societal challenges. By studying the fundamental principles of life, researchers integrating chemistry, biochemistry, and physics can develop innovative materials and devices with superior performance and sustainability, leading to breakthroughs in electronics, energy, biotechnology, healthcare, and environmental science. The program emphasizes hands-on research, mentorship, and professional development, preparing students for diverse careers in academia, entrepreneurship. By fostering and interdisciplinary industry, collaboration and cultivating a diverse student body, NanoBioNYC seeks to create a positive impact on human and environmental health while addressing workforce needs in a rapidly growing field.





Contact: tjackson1@gc.cuny.edu www.NanoBioNYC.com





The City College of New York

National Institutes of Health Research Training Initiative for Scientific Enhancement (G-RISE) at The City College of New York (CCNY) Ruth E. Stark CUNY Distinguished Professor of Chemistry & Biochemistry City College Department of Chemistry & Biochemistry

<u>Website</u>

34 CCNY faculty members are offering rigorous Ph.D. training and professional development in biochemistry, biophysics, bioorganic (biomedical and chemical) chemistry, engineering, and neuroscience 15-17 trainee cohorts to from groups underrepresented in STEM disciplines. Specific objectives are: (1) to recruit and retain trainees whose biomedical research interests align with the faculty-led teams; (2) to offer rigorous didactic training that combines disciplinary depth with interdisciplinary breadth while building independent research design skills; (3) to provide robust research training that fosters individual skills and creativity, cooperation within a research group, synergy among research groups, and the use of state-of-the-art technology; (4) to build STEM research identity and ethical values, an inclusive and supportive G-RISE cohort, career-ready skill sets and focus; (5) to enhance the numbers and proportions of UR Ph.D.'s who achieve biomedical science and timely graduation in engineering disciplines, while also improving their technical and communication skills, research productivity, and post-Ph.D. workforce placement.



The City College of New York

Biomacromolecular Structure and Assembly: Animal, Vegetable, and Fungal Adventures Ruth E. Stark CUNY Distinguished Professor of Chemistry & Biochemistry City College Department of Chemistry & Biochemistry

The <u>Stark Laboratory</u> uses molecular biophysics and structural biology approaches to study plant protective polymers, lipid metabolism, and potentially pathogenic melanized fungal cells. Nondestructive study of the molecular and mesoscopic architectures underlying the integrity of cuticles in natural and engineered tomatoes and potatoes is undertaken using solid-state nuclear magnetic resonance (NMR), MS, and antimicrobial assays. Ligand recognition and peroxisome proliferator-activated receptor interactions of fatty acid-binding proteins for applications to appetite regulation are under investigation by solution-state NMR and other biophysical techniques. The molecular structure and development of melanin pigments within fungal cells are being probed using (bio)chemical synthesis and solid-state NMR. The members of our research team typically span high school through senior postdoctoral levels.



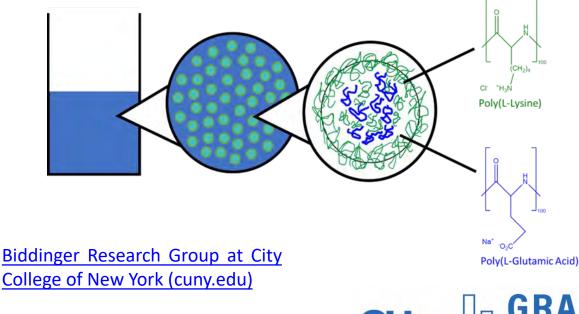
The City College of New York

Characterization of Carbon Dioxide-Reacted Polypeptide Complex Coacervates

Emily N. Charleson¹, Manushi Samarathunga², Elizabeth J. Biddinger^{1,2}, Raymond S. Tu²

(1) Chemistry, CUNY Graduate Center, New York, NY (2) Chemical Engineering, The City College of New York, New York, NY

The reaction of amines with carbon dioxide produces a class of chemicals called carbamates. These chemicals have a variety of applications from agricultural chemicals to pharmaceuticals. As such, we examine the formation of complex coacervates with amine groups for valorization of CO₂ to create these active biomaterials. These complex coacervates are composed of the oppositely charged polyelectrolytes, poly(L-lysine), (Plys), and poly(L-glutamic acid), (PGlu). We create a 'core-and-shell' coacervate droplet using a 2:1 molar ratio of PLys: PGlu, and find that this ratio also results in atypically small coacervates creating larger surface area to volume ratio. Thus allowing for more sites of reaction per coacervate droplet. After coacervation, samples are pH adjusted to convert some of the NH₃⁺ groups of the PLys to NH₂ groups. The desired effect is that the molecule is not fully deprotonated such that the NH₃⁺ groups promote coacervation and the NH₂ groups react with the CO₂. Samples were sparged with CO₂, and the change in their chemistry, size, and charge was explored through Attenuated Total Reflectance Fourier Transform Infrared Spectroscopy (ATR-FTIR), Dynamic Light Scattering (DLS), and Zeta potential.



GRADUATE



Research Opportunities in Chemistry At Lehman College

Benjamin Burton-Pye, Melissa Deri, Thomas Kurtzman, Columba de la Parra, **Yuemei Ye, Chun-I Wang, Donna McGregor**, Pamela Mills, Naphtali O'Connor, Edward Kennelly, Gustavo E. López and **Andrei Jitianu**

Chemistry research at Lehman College is focused on nanomaterials, radiochemistry, drug design, computational chemistry, machine learning, environmental remediation, cancer research, natural products and chemical education. There are many opportunities to collaborate across research groups and students are encouraged to consider a dual-mentor model for their thesis project. Specific areas of research include understanding the metabolism and posttranscriptional regulation of advanced breast cancer, examine phytochemicals with antioxidant activity to prevent cancer and cardiovascular diseases, new computational methods to improve drug design and discovery, integrating machine learning for designing and understanding soft materials, the studies of hybrid sol-gel materials applicable to microelectronics, corrosion protection, and batteries, new hydrogel materials with antimicrobial and wound healing applications, developing green PFAS remediation approaches in drinking water and wastewater treatment and radiochemical applications in energy and biomedical imaging. Graduate students who are interested in teaching and learning in chemical education can also consider conducting an education project as part of the PhD thesis.

Group Website link





Hybrid Anticorrosive Glasses Coatings Obtained by Electrospray Deposition

Andrei Jitianu

Melting gel (MG) materials are hybrid polysilsesquioxanes that possess glass transition temperatures between -18.8 and 27.7°C and consolidation temperatures at ~150°C, above which they irreversibly transform into hybrid-organic inorganic silica based glasses. The main advantage of the MGs is their processing ability. MGs can be processed as a thermoplastic melt into a desired form and then converted into a permanent structure based on this property. In our study, melting gel materials are processed by electrospray deposition in order to investigate the kinetic behavior arising from different experimental conditions and how these affect the final morphologies of MG films. Control of spray composition, substrate temperature, flow rate, and collection distance, translates to tuning of the dynamic evolution of solvent evaporation and MG consolidation. The results reveal that these can be used to controllably tune surface cellular, dense, structure from to to superhydrophobic fractal coatings ACS Applied Materials & Interfaces 11 (3), 3493-3505 ACS Applied Materials & Interfaces 10 (13), 11175-11188

Coatings 13 (3), 599

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Group Website link



Machine Learning-Enhanced Multiscale Simulations for Soft Material Modeling

Chun-I Wang (email: <u>CHUNI.WANG@lehman.cuny.edu</u>) Department of Chemistry, Lehman College

The application of soft materials has transformed a wide range of fields, including flexible electronics, biomaterials, energy storage, and polymer sustainability, driving innovative advancements that are redefining the future of technology. A crucial element in the development of these cutting-edge soft materials is the use of predictive modeling, which adeptly captures the intricate relationships between structure and function across various length and time scales. With the emergence of machine learning (ML), integrating ML with multiscale simulation approaches is opening new avenues for designing and understanding advanced soft materials. Our research group is at the forefront of developing ML-based multiscale simulations to investigate structure-performance relationships in four key application areas:

Facilitate Design of Molecular Biosensors

Addressing the structure-performance relationships of near-infrared fluorescent polymer dots for deep-tissue imaging by using ML-enhanced multiscale simulations

Explore Polyelectrolytes for Li-Ion Battery

Establishing a conformation dataset for polyelectrolytes under diverse solvation and operational conditions, with the goal of optimizing materials for battery design

Control Degradation for Sustainable Polymers

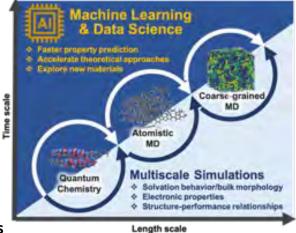
Leveraging ML-based diffusion models of heterogeneous catalytic upcycling to unravel polymer diffusion within and outside catalyst matrices, examine reaction kinetics, and understand chain release processes, all aimed at advancing polymer sustainability

Enhance Charge Transport of Flexible Electronics

Integrating MD simulations, QM approaches, and ML techniques into a unified computing platform to efficiently explore the relationship between charge transport properties and molecular structures, facilitating the design of organic semiconductors

Representative Publication

Chem. Sci., 2024, 15, 8390
 Chem. Mater., 2023, 35, 1470
 J. Chem. Phys., 2020, 153, 214113
 Chem. Sci., 2019, 10, 198



GRADUATE



H₂O₂-catalyzed defluorination of perfluorooctanesulfonate (PFOS) by oxidized vanadium carbide MXene nanosheets and Short-Chain PFAS Removal from Drinking Water with Hydrogel Microbeads

Yuemei Ye (Chemistry department, Lehman College)

Per- and polyfluoroalkyl substances (PFAS) have raising significant concerns due to their acute toxicity, which can lead to tumors, kidney and liver diseases in humans, and immunological effects in aquatic life. The strong C-F bond on PFAS makes these compounds persistent to most degradation methods. Additionally, the adsorption of short-chain PFAS from drinking water remains difficult with current commercial adsorbents due to the reduced hydrophobic interactions.

Our research group is dedicated to developing environmentally friendly, mild, and effective methods for PFAS remediation. We are advancing two primary lines of research: the development of nano-based materials for PFAS degradation, and the creation of functionalized hydrogel beads for the adsorption of short-chain PFAS.

In one of our projects, we have established a green and straightforward method that achieves over 96% defluorination of PFAS using vanadium carbide (V₂C) nanosheets and H_2O_2 at room temperature.

In parallel, we are working on functionalized hydrogels designed to remediate drinking water by leveraging electrostatic interactions between the hydrogel material and short-chain PFAS, such as perfluorobutanoic acid (PFBA). We utilize designed peptides to create microbeads, which offer promising potential for selective PFAS removal. The large surface area provided by the small-sized beads will further enhance the efficiency of short-chain PFAS removal.

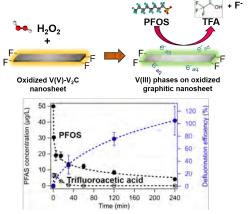


Figure 1. PFAS degradation with nanosheet material.

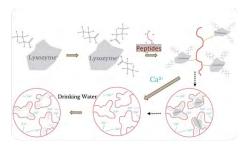


Figure 2. PFAS adsorption with hydrogel microbeads.

GRADUATE

Representative Publication (w/link)

 H_2O_2 -catalyzed defluorination of perfluorooctanesulfonate (PFOS) by oxidized vanadium carbide MXene nanosheets, JMCA, 11 (31), 16803-16814, 2023

Group Website link: <u>https://www.yeenvlab.com/</u>



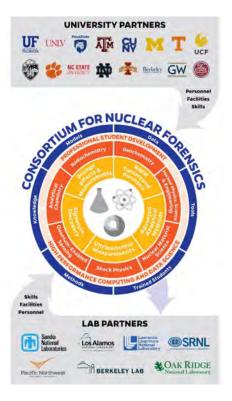
Consortium for Nuclear Forensics

Benjamin P. Burton-Pye^{1,3} and Lynn C. Francesconi^{2,3}

¹Department of Chemistry, Lehman College of CUNY ²Department of Chemistry and Biochemistry, Hunter College of CUNY ³Ph.D. Program in Chemistry, The Graduate Center of CUNY

The overarching theme of the Consortium for Nuclear Forensics (CNF), is the research and development of enabling fundamental science and engineering for the processing, characterization, determination, and quantification of materials for use in nuclear forensics applications. The CNF, consisting of 16 universities and 7 National Laboratories, provides the research, development, and human capital needed to create and develop new scientific discoveries, technologies, and capabilities in support of NNSA's Defense Nuclear Nonproliferation Research and Development (DNN R&D) Office as related to nuclear forensics. The team addresses gaps and challenges within important research fields in nuclear forensics.

CUNY's role is to determine the structural factors that affect our ability to isolate isotopes of interest and to develop the use of luminescence spectroscopy to identify actinide speciation.



Representative publication: https://pubs.acs.org/doi/10.1021/acsomega.4c00393 Consortium website: www.nuclearforensicsconsortium.org





Hunter and Lehman Consortium for inorganic technetium chemistry directed towards Advanced Nuclear Energy Systems and complex legacy waste mixtures from the Manhattan Project

Benjamin P. Burton-Pye, Lynn C. Francesconi Gustavo Lopez, Donna McGregor, Jim Wishart, Anatoly Frenkel

Element 43, technetium, Tc, possesses only radioactive isotopes. The isotope, technetium-99, ⁹⁹Tc, is one of the most prevalent by-products of uranium fission in nuclear energy production and a by-product of plutonium production during the Manhattan Project. For both applications, it is important to separate ⁹⁹Tc from uranium, other fission products, and complex legacy waste mixtures. Understanding the chemical form of ⁹⁹Tc is key to designing effective separation systems. We are funded by the Department of Energy to investigate the fundamental chemistry of ⁹⁹Tc in current nuclear energy systems and in advanced nuclear energy systems, specifically molten salts. We anticipate further funding in September 2024 for examination of ⁹⁹Tc in complex systems such as those found in legacy waste. We are looking for students to carry out both experiments and theoretical calculations at Hunter/Lehman and with partners on-site at Brookhaven National Laboratory, BNL. At BNL, students will perform experiments, including X-ray Absorption Spectroscopy at the synchrotron, and will extend their professional scientific network.

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Hunter College Radiochemistry: an interdisciplinary program and area of national need

Anton Oliynyk, Lynn Francesconi, Brian Zeglis

Radiochemistry is interdisciplinary, intersects with multiple disciplines, and is an area of national need. Scientists with radiochemistry experiences are sought after for positions in medical institutions, national laboratories, industry and academia. Zeglis' research is groundbreaking in medical imaging and in radioimmunotherapy of cancer. He has appointments at Memorial Sloan Kettering Cancer Center and Weill Cornell. Francesconi investigates technetium-99 chemistry, that is a high yield by-product of nuclear energy production and found in complex speciation in legacy waste from plutonium production of the Manhattan Project. Olivnyk applies radiochemistry to the study of solid-state reactions. He formation studies the and properties of alloys/intermetallics used as nuclear reactor materials, which need to withstand thermal, mechanical, and radiation stresses. From the fundamental science perspective, he studies metallic Th, U, Np, Pu solid reaction pathways. To guide experimental work, Professor Oliynyk employs computational and machine-learning approaches to predict and explain the formation of solids.







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BRAUNSCHWEIG GROUP RESEARCH @ CUNY ASRC CONTACT: ABRAUNSCHWEIG@GC.CUNY.EDU

Research in the group is focused on exploring the intersection of organic chemistry, biology, biochemistry, and material science. With a multidisciplinary approach that spans mechanochemistry, photolithography, synthetic chemistry and biochemistry, each project is linked by our emphasis on addressing the complex challenges in the energy, health, and environmental sectors.

Molecular Printing and Photolithography

Our main goal is to develop an efficient printing technique capable of fabricating and patterning functional nanometer-scale structures. Using photopolymerizations, these structures can be precisely controlled in 3D space and time to create arbitrary patterns. The resulting polymer brush surfaces are particularly promising for developing stimuli-responsive materials, metamaterials, biosensors, and molecular assemblies for charge transport.

Mechanochemistry

Mechanical force is an invaluable tool in driving reactions, and it has the potential to significantly reduce the usage of solvent and energy in organic synthesis. Our group aims to better understand the kinetics and energetics of these reactions, and develop new chemical reactions driven by mechanochemical activation.

Synthetic Carbohydrate Receptors

The pressing need for broad spectrum antivirals cannot be overstated. We develop small molecules that bind cell-surface carbohydrates through noncovalent and supramolecular interactions. These molecules are bind used for disease detection, drug delivery, and therapeutics in live animals, and eventually, in the clinic.

Comparative Mucomics

Mucus is one of nature's most abundant and functionally diverse biomaterials, playing key roles in adhesion, lubrication, and barrier protection across all animals. Despite its ubiquity, many aspects of its hierarchical structures, material properties, and underlying genetics remain poorly understood. To address these gaps, our group employs a novel comparative approach inspired by modern omics-style analysis to investigate the chemical structures and physical properties of mucus, shedding light on its complex and vital functions.

Biomimetic Glycopolymers

Glycoproteins are used throughout nature to meet numerous material needs. Despite their potential for filling many roles in biochemistry, the lack of synthetic alternatives has hindered the realization of many promising biotechnologies. Our lab seeks to replicate and improve upon these natural biomaterials by combining carbohydrate and polymer chemistry to create synthetic mucins.

https://www.braunschweiggroup.org



Computational Physical Organic Chemistry at Hunter College

Mateusz Marianski^{1,2}

1. Department of Chemistry, Hunter College, The City University of New York, 695 Park Avenue, New York, NY 10065, USA, mmarians@hunter.cuny.edu https://marianski-lab.github.io/

2. PhD Program in Chemistry and Biochemistry, The Graduate Center, The City University of New York, 365 Fifth Avenue, New York, NY 10016, USA

Abstract

Carbohydrates, one of the three important classes of biopolymers, are involved in a range of biological processes: they serve as structural polymer, energy storage, and recognition modules in the immune system and cell-cell communication. Their multiple functions in living organism are facilitated by properties of the monomeric building block; whereas other biopolymers assembles in a linear fashion, several distinct possibilities for glycosidic bond formation bolster the accessible structural space of carbohydrates over those available for nucleotides and peptides.

In the lab, we focus on theoretical understanding of in-depth relation between the carbohydrate sequence and its molecular properties. Our set of tools, selection of which depends on a particular problem we want to tackle, ranges from simple force-field based molecular modeling, through densityfunctional theory, to high-level quantum chemistry methods. The topics of interests include design of synthetic carbohydrate receptors and their antiviral properties, the gas-phase structure formation and dynamics of small oligosaccharides, theoretical understanding of the glycosylation reaction mechanism, and design of new carbohydrate-based biomaterials.

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Assessing Potential Drug-Drug Interactions Involving Δ -9-Tetrahydrocannabinol and Cannabidiol in Healthy Adults Using Physiologically Based Pharmacokinetic Models

Lixuan Qian¹, Tao Zhang², Jean Dinh³, Mary F. Paine⁴, Zhu Zhou¹

¹Department of Chemistry, York College, City University of New York

²Department of Pharmaceutical Sciences, Binghamton University, The State University of New York

³SimCYP Ltd/Certara

⁴Department of Pharmaceutical Sciences, Washington State University

Background. Δ -9-Tetrahydrocannabinol (THC) and cannabidiol (CBD) are the most extensively studied cannabinoids in cannabis. THC is eliminated mainly by cytochrome P450 (CYP) 2C9-mediated metabolism, with a minor role by CYP3A, whereas CBD is eliminated mainly by CYP2C19- and CYP3A-mediated metabolism. As cannabis use for myriad conditions continues to grow, understanding potential pharmacokinetic interactions between THC or CBD and other drugs remains an urgent public health need. The objective of this work was to develop and verify physiologically based pharmacokinetic (PBPK) models of THC and CBD to assess these potential adverse interactions.

Methods. PBPK models for intravenous (IV) THC (1.25-5 mg) and CBD (20 mg) were developed using the Simcyp[™] PBPK Simulator (v22). Physicochemical and pharmacokinetic input parameters were either collected from the literature or optimized. Models for the oromucosal spray route were next developed for a range of cannabinoid doses (THC: 5.4-21.6 mg; CBD 5-20 mg). All PBPK models were optimized and verified using data obtained from published clinical studies involving healthy adults who were administered THC or CBD alone or with known CYP3A and CYP2C precipitant drugs.

Results. PBPK model-predicted plasma AUC and C_{max} of THC and CBD at all cannabinoid doses were within 0.51- to 1.68-fold of the observed values obtained from 12 clinical studies (Fig. 1). The models also well-captured THC and CBD AUC and C_{max} in the presence of three precipitant drugs, specifically rifampicin (CYP3A/CYP2C inducer), ketoconazole (CYP3A inhibitor), and omeprazole (CYP2C19 inhibitor); predicted AUC and C_{max} for THC and CBD were within 0.65- to 2.24-fold of observed values. Predicted AUC ratios (AUC of THC or CBD in the presence to absence of precipitant) were within 0.68- to 1.54-fold of observed ratios.

Conclusions. PBPK models for both IV and oromucosal spray administration of THC and CBD were developed and verified. The models will be further refined by optimizing the absorption model for additional extravascular administration routes. The verified models could be used to help address critical public health needs, including predicting changes in THC or CBD systemic exposure in combination with other enzyme inhibitors/inducers to assess potential safety concerns.

Funding. This work was supported by the ASCPT Darrell Abernethy Early Stage Investigator Award, NIH/NIGMS (R16 GM146679), and NIH/NCCIH (U54 AT008909).





Chemistry at the College of Staten Island II: From computational chemistry to engineered polymers

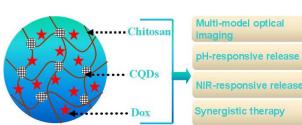
Angelo Bongiorno, Sharon Loverde, Alan Lyons, Chwen-Yang Shew and Shuiqin Zhou

- **Bongiorno** group focuses on atomistic studies of materials using first-principles computational methods.
- Loverde group utilizes molecular dynamics simulations to investigate properties of soft and biological materials, as well as the stability of protein nucleic-acid complexes.
- Lyons group fabricates multi-functional superhydrophobic surfaces for medical and solar applications by controlling the chemistry and morphology of materials.
- **Shew** group develops model, theory and simulation to elucidate the structure of polymeric materials and biological cells.
- **Zhou** laboratory aims to develop responsive polymer-based hybrid nanogels and nanoparticles for catalytic, sensing, imaging, and drug delivery applications.

"Conformational dynamics of the nucleosomal histone H2B tails revealed by molecular dynamics simulations," R. Patel, A. Onyema, P. Tang, and **S. M. Loverde**, J. Chem. Inf. Model. 2024, 64, 4709

https://sites.google.com/site/loverdelaboratory/

"Biocompatible Chitosan–Carbon Dot Hybrid Nanogels for NIR-Imaging-Guided Synergistic Photothermal– Chemo Therapy", H. Wang, S. Mukherjee, J. Yi, P. Banerjee, Q. Chen, **S. Zhou**, *ACS Appl. Mater. Interf.* 2017, 9, 18639



https://www.csi.cuny.edu/campus-directory/shuigin-zhou

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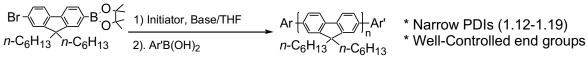
PCA Directions



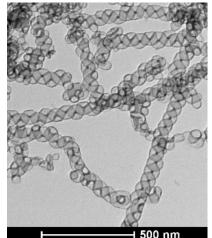
Chemistry at the College of Staten Island I: From polymer synthesis to the development of functionalized nanomaterials

Qiao-Sheng Hu, Shi Jin, Michal Kruk, Ralf Peetz and Krishnaswami Raja

- **Hu group** develops new catalysts and new reactions for organic synthesis and polymer/materials synthesis.
- Jin group focuses on hierarchical structure control of organic semiconducting materials for electronic and optoelectronic applications.
- Kruk group works on design of ordered nanoporous materials and hollow nanoparticles.
- **Peetz laboratory** uses controlled synthesis and macromolecular engineering in development of functional materials.
- **Raja group** works on the development of bioactive polymers, protein based drugs, bioconjugates and green drug development.



- Dong, J.; Guo, H.; Hu, Q.-S. ACS Macro Lett.
 2017, 6, 1301
 Zhang, H.-H.; Peng, W.; Dong, J.; Hu, Q-.S. ACS Macro Lett. 2016, 5, 656
- Beaton, L.; Zhang, S.; Kruk, M. ACS Nano 2021, 15, 1016



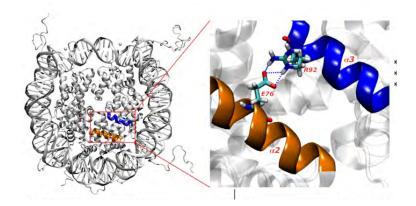
SY JACENTER



Molecular Dynamics Simulations of the Structural Effects of Oncogenic Mutations in the Nucleosome

Presenting Author: Augustine Onyema PI: Sharon M. Loverde

The information available to the cell to initiate, control, or stall metabolic processes is housed in the genome, whose monomeric unit is the nucleosome core particle (NCP). The nucleosome core particle (NCP), in conjunction with DNA-binding proteins like chromatin remodelers and transcription factors, forms the fundamental cellular apparatus essential for transcription, DNA repair, and DNA replication. However, oncogenic mutations within the histone core can disrupt processes, including histone exchange and nucleosome sliding in different cancer types. Mutations in the core histone proteins have been shown to destabilize the H2B-H4 protein interface, impacting histone octamer stability. Here, we ran 36 μs all-atomistic simulations of the wild type (WT) and single point oncogenic mutated systems of the NCP on Anton 2. We show structural and dynamic destabilization of the H2B-H4 interface in the histone core in the mutant systems. We use methods in unsupervised machine learning, such as principal component analysis, to characterize the intermediate states upon destabilization. We are currently working with the Poget laboratory (CUNY College of Staten Island) to characterize the effect of these same mutations on the thermal stability of the NCP and the Yael David (MSKCC) laboratory to characterize the effect of these mutations on in vitro transcription.



https://sites.google.com/site/loverdelaboratory

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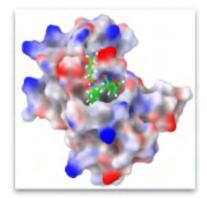


Structure-Based Drug Discovery by Alchemical Free Energy Simulations

Prof. Emilio Gallicchio

PhD Programs in Chemistry and Biochemistry Computational Molecular Biophysics Laboratory Department of Chemistry and Biochemistry <u>egallicchio@gc.cuny.edu</u> <u>https://www.compmolbiophysbc.org/</u>

Lab Publications AToM-OpenMM software



Molecular simulations, novel free energy theories, and an explosion of computer power are increasingly used to help discover new drugs. Our laboratory develops atomistic "alchemical" free energy simulation methods that predict the binding strength between an inhibitor and its target protein receptors. This information is crucial in the early phase of drug discovery to select the most promising compounds to synthesize in the search for drugs against cancer, viral and bacterial infections, drug addiction, and many other diseases and human health issues. Current research in the lab focuses on simulation methods to probe drug selectivity to reduce side effects or increase resilience against cancer and viral mutations. Many biotechnology and B2B technology drug discovery firms, including Genentech, Ensem, SandboxAQ, Psivant, Atommap, Acellera, Ensem, and others, use our methods and software to help discover new drugs. The drug discovery industry competes for the relatively few experts in the field. Graduates from our lab are offered internship and find employment at top biotech companies.

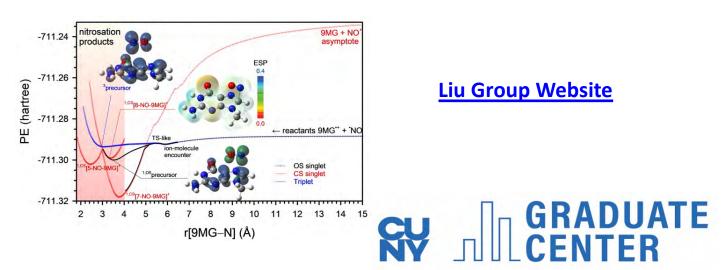


QUEENS

Spin-Orbit Charge Transfer & Nitrosation of Guanine Radical Cations by •NO — Mechanisms, Kinetics, and Dynamics Revealed by Mass Spectrometry

Professor Jianbo Liu (<u>Jianbo.liu@qc.cuny.edu</u>) Department of Chemistry and Biochemistry Quens College and the Ph.D. Programs in Chemistry

As a precursor to reactive nitrogen species formed in biological systems, nitric oxide (•NO) participates in numerous processes, including enhancing DNA radiosensitivity in ionizing radiation-based radiotherapy. Forming guanine radical cations ($G^{\bullet+}$) is another common DNA lesion resulting from ionization and oxidation damage. As such, the interaction of •NO with G•+ may contribute to the radiosensitization of •NO, for which an intriguing aspect is the participation of multiple spin configurations including open-shell singlet ${}^{1,OS}[G^{\bullet+}(\uparrow)\cdots(\downarrow)^{\bullet}NO]$, closed-shell singlet ${}^{1,CS}[G(\uparrow\downarrow)\cdots NO^+]$, and triplet ${}^{3}[G^{\bullet+}(\uparrow)\cdots(\uparrow)^{\bullet}NO]$. We measured kinetic-energy dependent product ions and cross sections for the reaction of • NO with 9-methylguanine radical cations (9MG•+, a guanosine-mimicking model compound) by using electrospray ionization guided-ion beam tandem mass spectrometry. Reaction mechanisms, kinetics, and dynamics were comprehended by interpreting experimental results using spin-projected DFT, coupled cluster theory, and multiconfiguration complete active space second-order perturbation theory, followed by RRKM kinetics modeling. The work has revealed: 1) closed-shell singlet ^{1,CS}[7-NO-9MG]⁺ as the major, exothermic product, and triplet ³[8-NO-9MG]⁺ as the minor, endothermic product; and 2) charge transfer requires surface crossing from the triplet to the closed-shell singlet, during which an electron is transferred from a $\pi^*(NO)$ to a perpendicular $\pi^*(9MG)$, introducing a change in orbital angular momentum — *spin*orbit charge transfer. The charge transfer threshold was measured to exceed 0 K thermochemistry, revealing vibrational excitation in product ions NO⁺. These findings demonstrate synergistic oxidative nucleobase damage in the presence of ionization and nitrosation. https://doi.org/10.1063/5.0160921

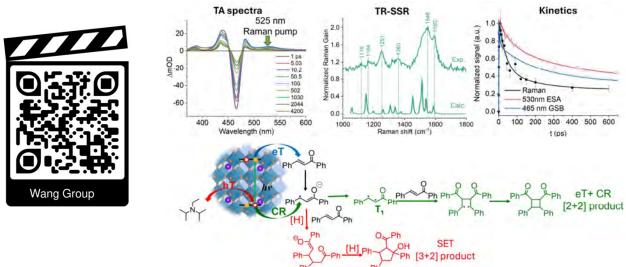




Photocatalysis Mediated by Surface Chemistry of Perovskite Nanocrystals: an Exploration Guided by Time-Resolved Spectroscopy

Aaron Maniloski, Jingheng Yuan, Junwei Pan, Chen Wang*

Photocatalysis provides novel approaches to manipulating chemical bonds for constructing molecular structures that are difficult to attain using conventional synthetic methods. The Wang group exploits the excellent optical properties and rich surface chemistry of metal halide perovskite nanocrystals (PNCs) to develop new photocatalysts for synthetic reactions. We first systematically investigated the surface/ligand interactions and identified two ligand structures, i.e., the aromatic zwitterion (AZLs) and the bidentate chelating ligands, which can stabilize the dynamic PNC surface. Based on the understanding of ligand chemistry, we devised surface engineering strategies to quantitatively functionalize the surface of PNCs, which not only successfully enhanced the stability of the PNC but also facilitated Dexter charge carrier and energy transfer from the PNC. We successfully applied the surface-modified PNCs to catalyze photocycloaddition reactions of enones. Transient absorption (TA) investigation reveals that these reactions undergo a photoredox mechanism. The PNC sensitizes [2+2] cycloaddition resulting in a cyclobutyl motif by generating the triplet excited state of enones through photoinduced electron transfer followed by a charge recombination process. The kinetic information collected by TA predicted the possibility of preserving the anion radicals of enones by introducing appropriate sacrificial electron donors to compete with charge recombination from the PNC. Unlike the triplet excited state, the anionic radicals served as the intermediates for [3+2] cycloaddition and led to cyclopentyl products. The time-resolved spectroscopy data provided the clue to utilize the sensitive solvent effect of charge transfer kinetics to select different reaction pathways. Our work demonstrated that metal halide PNCs are versatile photocatalysts after resolving the stability issue, and mechanistic investigation using time-resolved spectroscopy can guide the design of photocatalytic processes to realize the selection of reaction pathways.



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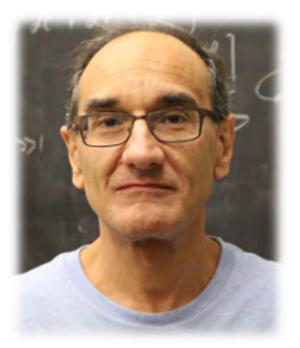
Medicinal Chemistry, Computer-aided Drug Design, and Chemical Biology in the Choi Laboratory at Queens College

Shuai Ma, Diya Sharma, Grace Park, Jenna Lee, Aveta Singh, Jun Yong Choi

The overall objective of my research is to discover specific, target-directed therapeutics for human diseases. This goal will be accomplished by applying a multidisciplinary approach that includes organic synthesis, medicinal chemistry, molecular and structural biology, and computational chemistry and biology. In particular, synthesis of rationally designed inhibitors generated by using computer-aided design techniques is applied to the discovery of novel therapeutic candidate. My research projects include (1) Structure-guided discovery of allosteric inhibitors of kinases; (2) Structure-guided development of specific inhibitors of matrix metalloproteinases; and (3) Development of specific inhibitors of kinases by applying cheminformatics and structural bioinformatics; (4) Development of RPA1 inhibitors for the treatment of trypanosome parasitic diseases; (5) Development of in vivo chemical probes for melanoma and prostate cancers. The discovery and techniques established in the Choi lab advance the chemical and biological science in medical research and drug discovery and facilitate understanding in human diseases for the development of therapeutics.







Alexios Polychronakos, Ph.D. Executive Officer



Daniel Moy Assistant Program Officer

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ITS @ The Graduate Center Initiative for the Theoretical Sciences

Please see https://itsatcuny.org/ for up-to-date information, or inquire at itsatcuny@gmail.com

- Weekly (approximately) seminars on Friday 11am-noon in rm. 5209 (+lunch) mostly condensed matter and many-body physics and field theory, computational and statistical physics; occasionally, experimental talks; organizers: Ganeshan/Oganesyan
- 2) Weekly neuroscience colloquiums on Friday, 3-4pm (room TBD); Organizers: Serrano/Yetnikoff/Amarasingham
- 3) 1~2 day symposia
- 4)

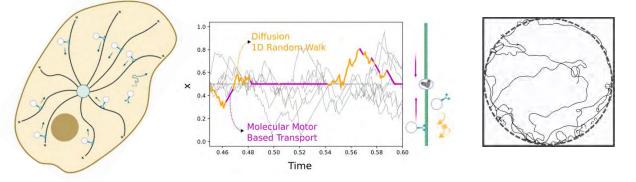
20 SEP 2024, FRI	🔴 All day	Biophysics symposium(D. Schwab)
27 SEP 2024, FRI	🔴 All day	QChem symposium (S.Jang)
25 OCT 2024, FRI	 All day 	Biophysics symposium (D.Schwab)
	All day	Qchem symposium (S.Jang)
31 OCT 2024, THU	 All day 	Quantum algorithms: theory and application, symposium (M. Hillery) (Day 1/2)
1 NOV 2024, FRI	😑 All day	Quantum algorithms: theory and application, symposium (M. Hillery) (Day 2/2)
22 NOV 2024, FRI	😑 All day	Biophysics symposium (D.Schwab)
5 DEC 2024, THU	😑 All day	Precision many body physics TBC (symposium, Kuklov) (Day 1/3)
6 DEC 2024, FRI	 All day 	Precision many body physics TBC (symposium, Kuklov) (Day 2/3)
	All day	Qchem symposium (S.Jang)
7 DEC 2024, SAT	 All day 	Precision many body physics TBC (symposium, Kuklov) (Day 3/3)
13 DEC 2024, FRI	 All day 	tbc "Geometry and Phenomenology of String Compactification" (symposium, Rosenhaus, Franco, Kabat)



Theory of intracellular transport and collective biological dynamics

Professor Oleg Kogan

We are working on problems concerning intracellular transport inside cells – a process that relies on the interplay of diffusion in the cytoplasm and motion of molecular motors on cytoskeleton. We calculate quantities such as residence time of cargo in the vicinity of certain locations in a cell – a quantity relevant for understanding functionality of immune cells, such as cytotoxic T lymphocytes, for example. The work involves collaborations with experimental groups, analytical calculations, and numerical work. We also study collective biological behavior – such as motion of plankton in petri dishes, and theoretical model of swarming called swarmalators.



Representative Publication: Biophysical Reports **4**(3), 100171 (2024). <u>https://www.sciencedirect.com/science/article/pii/S2667074724000302</u>

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Group Website link:

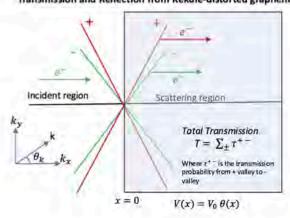
https://physics.qc.cuny.edu/people/faculty/okogan

HUNTER

Dynamical Polarization, Plasmon and Energy Loss of Kekule-Distorted Graphene Under Circularly Polarized Irradiation

Sita Kandel^{1,2} and Godfrey Gumbs^{1,2,3} ¹Department of Physics, Hunter College ²The Graduate School and University Center, CUNY ³Donostia International Physics Center (DIPC), P de Manuel Lardizabal 4, 20018 San Sebastian, Basque Country, Spain

The high frequency electromagnetic irradiation within the off-resonance regime significantly changes the electronic transport and optical properties of Dirac systems. Here, we have studied the effect of circularly polarized irradiation on the energy band, dynamical polarization and the plasmon excitations of Kek-Y phases of graphene. It is found that the large gap is induced between two bands and between two concentric Dirac cones which considerably modifies the polarization function and consequently the plasmon dispersion. The plasmon damping rate and the rate of loss of energy of a charge particle moving parallel to the 2D sheet is calculated numerically. To further explore the electronic transport properties of Kek-Y graphene, the analytical solution for the transmission and reflection coefficients from a potential step are also derived. It is observed that both the reflection and transmission of electrons conserve the energy, and therefore have the finite probability for the particle to transfer not only from one band to another but also from one valley to another. Both intravalley and intervalley transmission contribute to the total transmission in the absence of irradiation. Perfect transmission is observed at normal incidence as it is in non-distorted graphene.



Transmission and Reflection from Kekule-distorted graphene

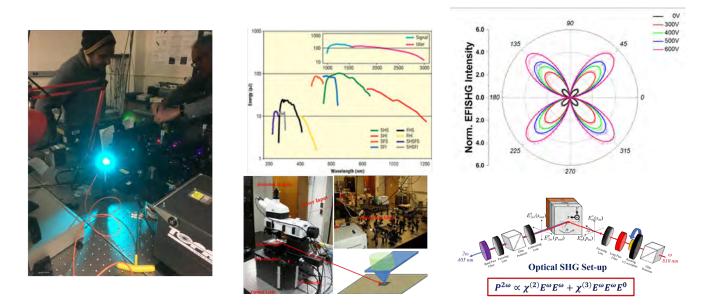


HUNTER

Ultrafast Sciences and Materials Fabrication Group at Hunter College

Professor Yuhang Ren

We are working on the physics of novel dielectric and ferroelectric materials and devices, semiconductor quantum structures, solar cells, energy storage materials, optical response of quantum solids, nano-fabrication and characterization, and coherent ultrafast optical spectroscopy.



Recent Publications: Adv. Electron. Mater. **9**, 2300497 (2023); **8**, 2200465 (2022); Energy Storage Materials **48**, 306-313 (2022). Nano Energy **72**, 104665 (2020); Scripta Materialia **178**, 489-492 (2020); Nature Communications, **8**, 1999 (2017).

Group Website link:

https://www.hunter.cuny.edu/physics/faculty/ren/ultrafast-optics-group

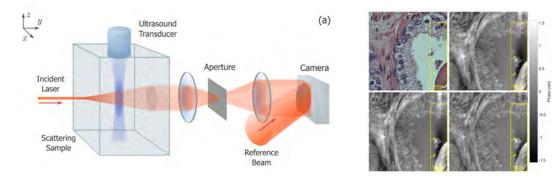


HUNTER

Biomedical Photonics Research at Hunter

Julinda Mujo, Mariia Aleksandrovych, Angel Perez-Martinez, Zichun Xu, Zhuo Yin, Zhesi Wen, and Min Xu

The Biomedical Photonics Laboratory (BPL) at Hunter College develops next-generation spectroscopy and microscopy for imaging structure and dynamics of biosystems and studies the physics of live matter using analytical, numerical, deep learning, and experimental approaches.



Representative Publication:

Opt. Lett. 49, 2349 (2024); *Biomed. Opt. Express*, 14:5833 (2023, Editor's Pick); *Appl. Phys. Lett.*, 119:173702 (2021) Group Website link:

www.hunter.cuny.edu/physics/faculty/xu/home



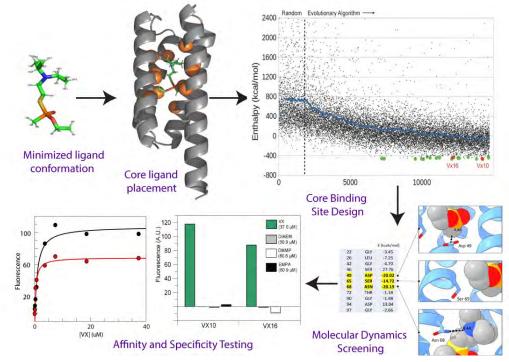
The City College of New York

Biodesign using Machine Learning

Giovanni Crump [‡], Dharshika Malwane [↑], Paul Molinaro [↑], Marlene McKinney [↑], Jim McCann [↑], Ronald L. Koder [↑] \downarrow

[↑]Department of Physics, The City College of New York, New York, NY 10031
 [‡]Department of Biochemistry, The City College of New York, New York, NY 10031
 [↓]Graduate Programs of Physics, Biology, Chemistry and Biochemistry, The Graduate Center of CUNY, New York, NY 10016

The Koder Lab uses computational protein design and machine learning to create novel proteins that offer new functions or physical properties and then integrates them with natural proteins, other designed proteins, or non-protein materials to create solutions for problems in medicine, defense, 'green' industrial catalysis, and green energy production.



Selected References (PDFs available at KoderLab.org or email rkoder@ccny.cuny.edu)

1) Quantum defect sensitization via phase-changing supercharged antibody fragments. (2024) *J. Amer. Chem. Soc.* 146(18):12454–12462

2) Elastin Recoil is Driven by the Hydrophobic Effect (2024) *Proc. Nat. Acad. Sci. USA*. 121(11):e2304009121

3) Design of a Minimal di-Nickel Hydrogenase Peptide (2023) Science Advances 9, eabq199

4) An expandable, modular de novo protein platform for precision redox engineering (2023) *Proc. Nat.* Acad. Sci. USA. 120 (31) e2306046120

5) Liquid to Solid Transition of Elastin Condensates (2022) *Proc. Nat. Acad. Sci. USA* 119 (37) e2202240119

6) Design of a Phase-Changing VX-sensing protein. Science Advances (2022) 8, eabh3421

7) Thermalization of fluorescent protein exciton-polaritons at room temperature Advanced Materials (2022) 34:2109107

8) Designing Heterotropically-Activated Allosteric Conformational Switches Using Supercharging *Proc..Nat. Acad. Sci. USA* (2020) 117(10):5291-5297

The City College of New York

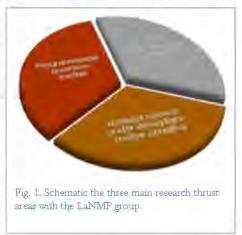
Laboratory for Nano and Micro Photonics: controlling light-matter interaction at the nanoscale

PI: Vinod Menon, Dept. of Physics, The City College of New York

Abstract:

Research in the <u>Laboratory for Nano and Micro Photonics</u> (LaNMP) can be broadly defined as controlling light matter interaction at the nanoscale. The central question we ask is whether hybrid quasiparticles of light and matter, polaritons and their condensates - quantum fluids of light can be

used for computation and materials engineering. Specifically, we are interested in exploring emergent material properties that arise when matter is subjected to artificially engineered electromagnetic environments. The goal is to develop a largely unexplored strategy for quantum materials engineering based on coherently combining material excitations with light. This goal is driven by the quest to understand the ultimate limits of controlling optical transitions, carrier transport, energy harvesting, nonlinear optical response, and quantum effects. We anticipate these fundamental questions to lead to applications in diverse areas such as quantum and classical simulation, photovoltaics, ultrafast light emitters, and catalysis. This theme of "*light engineered matter*" within the group is implemented through three main thrust areas (Fig. 1):



<u>Thrust 1</u>: Programmable quantum matter based on half-light-half-matter quasiparticles [Moore, Keck, DOD, NSF]

Thrust 2: Material Science under strong light-matter coupling [DOE, NSF, DOD]

<u>Thrust 3</u>: Artificial optical media for engineering dielectric properties, light emitters and engineering forbidden optical transitions in nanomaterials [DOD, NSF, Industry].

Some of the key results from the group include demonstration of Bose-Einstein like condensates and their lattices in solid state (*Nano Lett.* 2024), optically dressed magneto-excitons in a van der Waals magnet (*Nature* 2023), the realization of spin correlated exciton-polaritons in an antiferromagnetic insulator (*Nature Nanotech.* 2022), demonstration of highly nonlinear dipolar exciton-polaritons for quantum nonlinearity (*Nature Comm.* 2022), the demonstration of strain engineering (*Science Advances* 2021), use of Rydberg exciton polaritons to enhance nonlinear response in solid state systems (*Nature Comm.* 2021), controlling photo-isomerization in molecules via strong coupling (*Science Advances*, 2021), a polariton LED (*Nature Nanotech.* 2019), and deterministic activation of single photon emitters in 2D materials (*Optica* 2018).

Alumni placement:

Industry: Intel, Quantinuum, Facebook – Meta, Altos Labs, Quantum Circuits *Academia*: Fudan University, Tech Univ. of Munich, Wuhan University, Tata Inst, for Fundamental Research, Indian Inst. Of Technology, CUNY. *National Labs*: Naval Research Lab, Brookhaven National Lab, Air Force Research Labs

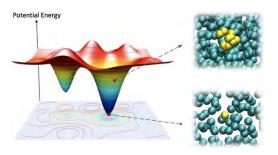
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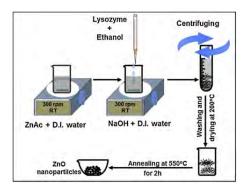
Physics Research at Brooklyn College

Nicolas Giovambattista ngiovambattista@brooklyn.cuny.edu Mim Nakarmi mlnakarmi@brooklyn.cuny.edu Karl Sandeman karlsandeman@brooklyn.cuny.edu Sophia Suarez snsuarez@brooklyn.cuny.edu Ray Tung rtung@brooklyn.cuny.edu

We give an overview of the research facilities and activities of Brooklyn College Physics Department, split over 5 posters. Our faculty's research interests span soft and hard condensed matter, including materials modelling (equilibrium and out-ofequilibrium) The department hosts high school, undergraduate and graduate student researchers, and runs major, minor and MA programs in physics. If you would like to visit the campus at any time, please get in touch with Department Chair Karl Sandeman or Graduate Deputy Nicolas Giovambattista.

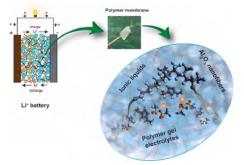


The Harmonic and Gaussian Approximations in the Potential Energy Landscape Formalism for Quantum Liquids Y Zhou, GE Lopez, N Giovambattista Journal of Chemical Theory and Computation, 2024



Optical transitions in lysozyme mediated zinc oxide nanoparticles probed by deep UV photoluminescence N Maharjan, DD Mulmi, ML Nakarmi Optik, 2020

GRADUATE



Structure and dynamics of ILs-based gel polymer electrolytes and its enhanced conductive properties with the incorporation of Al2O3 nanofibers MN Garaga, S Bhattacharyya, D Paterno, S Suarez, S Greenbaum Electrochimica Acta, 2023

Brooklyn College Physics Department Webpage



Absence of Glass Polymorphism in Nanoconfined Water

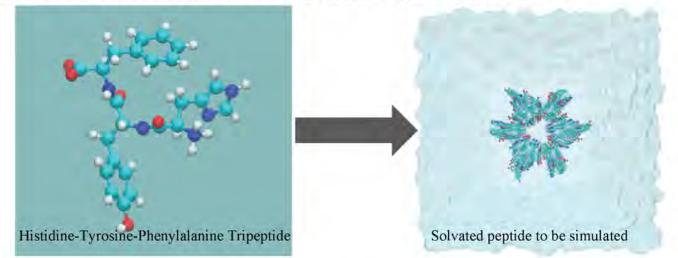
Poster # 56

Bibi A Khan^{1,2}, Gustavo E. Lopez^{2,3}, and Nicolas Giovambattista ^{1,3,4}

Brook

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In general, pure substances exists in one liquid state and, if crystallization is avoided, a single glass state is formed upon fast cooling. The properties of the glass that forms depend on both the cooling and compression/decompression rates. Experiments suggest that water is surprisingly different, having two different liquid states, low density liquid (LDL) and high-density liquid (HDL), and two different glassy states, low density amorphous (LDA) and high density amorphous (HDA); HDA is 20–25% denser than LDA₁. These finding carry significant implications for their potential application in cryogenic technology. For instance, experimental techniques like cryo-electron microscopy require biological samples to be prepared at cryogenic temperatures (T ≈ 100 K), inducing the transformation of water into an amorphous ice state. Nonetheless, the specific properties of the resulting amorphous ice within or at the interphase of the biological sample remains unknown because of the nanoconfinement environment. In the present work we study the properties of water confined in a biomolecular crystal former of HYF tripeptides using the GROMACS software₂.



Specifically, the properties of water in equilibrium (liquid and supercooled states, 240 K < T < 350 K) and in the glassy state (80 K) were computed using classical molecular dynamics. The thermodynamic paths followed to generate the glassy state include: (i) quenching at 1K/ns from 240 K to 0 K, (ii) high pressure cooling at P = 200 MPa and 400 MPa, and (iii) compression/decompression cycles at T = 80 K. The properties of water within the interior, at the interphase, and in the bulk region was obtained by computing the number of molecules in each region, radial distribution functions, density profiles, and the variation in density as a function of pressure or temperature during cooling and compression/decompression simulations.





Physics Research at Lehman College

Eugene Chudnovsky, Dmitry Garanin, Christopher Gerry, Daniel Kabat, Dimitra Karabali

We give an overview of physics research at Lehman College, covering condensed matter, quantum optics and high energy theory.







Astrophysics Research at Lehman College

Luis Anchordoqui, Matthew O'Dowd, Georgios Vernardos

We give an overview of research in cosmology, astrophysics and astronomy at Lehman College.

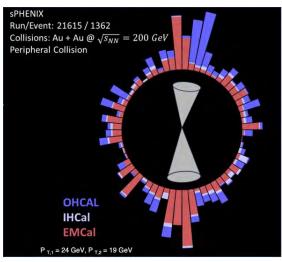


Barich

Probing the hottest matter in the universe with sPHENIX

Stefan Bathe, Skadi Grossberndt, Nikhil Kumar

The sPHENIX Experiment at Brookhaven Lab's Relativistic Heavy Ion Collider (RHIC) will establish the properties of the Quark-Gluon Plasma—an emergent phenomenon of QCD—with precision hard probes (jets, heavy quarks, quarkonia). The experiment was commissioned last year



and is currently taking data in p+p collisions at 200 GeV per nucleon pair. The Baruch experimental nuclear physics group carries a leading role in the experiment. We will present the status and prospects of sPHENIX.

The image shows jet pair in Au+Au collisions.

https://inspirehep.net/literature/2805145 https://www.sphenix.bnl.gov

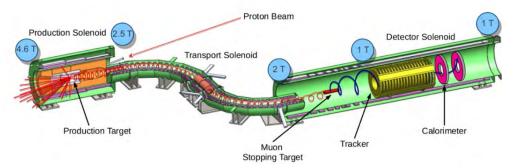




Searching for New Physics with the Muon-to-Electron Conversion Experiment (Mu2e) at Fermilab

Professors James Popp and Andrew Edmonds PhD Program in Physics York College jpopp@York.cuny.edu and aedmonds@York.cuny.edu

The Mu2e Experiment will use the most intense muon beam ever made (10¹¹ muons/sec) to search for neutrinoless muon-to-electron conversion – an unambiguous sign of new physics. The experiment is being built and installed at Fermi National Accelerator Laboratory (Batavia, IL) and will collect data from 2026. This experiment will attain an increase in sensitivity to this rare and as yet unseen decay by a factor of 10,000. Such a leap in sensitivity is accomplished by creating an entirely novel beamline that employs three very large specialized superconducting solenoid magnets; see the central apparatus below.



The results of this experiment will change our understanding of elementary particle physics at energies up to 1000 times greater than those probed at the Large Hadron Collider at the CERN Laboratory in Europe. In other words, the experimental high energy physics team at York is doing science at the leading edge of physics exploration by probing Nature for phenomena at length and time scales at least 1000 times smaller than ever before.

References:

1. Mu2e Run I Sensitivity Projections for the Neutrinoless $\mu \rightarrow e^-$ Conversion Search in Aluminum: <u>https://inspirehep.net/files/1c0c27db504e45b2ff62b5157b64ab26</u> 2. Mu2e Experiment Website: <u>https://mu2e.fnal.gov</u>

> SY J GRADUATE CENTER



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Upcoming Professional Learning Programming



Connect & Collab: Fall Mixer

Wednesday, September 18 | 5:00 - 7:00 PM ET | In-person Free for Science Alliance Members

Join us for an exciting evening of networking and activities at The Academy's fall networking event, brought to you in partnership with <u>Nucleate</u>. Whether you are seeking collaborations, job opportunities, or simply looking to expand your network, this event is the perfect platform to further your career aspirations and cultivate connections with peers.



Course - Mental Health First Aid Certification

Tuesday, November 12 | 12:00 - 5:00 PM ET | In-person Discounted for Science Alliance Members

Similar to First Aid and CPR training, Mental Health First Aid (MHFA) is a key set of skills that allow STEM students, educators, and professionals to assist their students, peers, and colleagues who may be experiencing an acute mental health issue. Join The Academy for a full-day in-person interactive training customized for people in the STEM field. Each participant will receive an online certificate valid for three years upon course completion.



Learn More

Course - Transition to Research Independence: Funding and Grantsmanship Wednesday, December 4 | 6:00 - 7:30 PM ET | Hybrid Free for Science Alliance Members

Learn strategies for concise and persuasive writing that are vital in academia and essential for any career path. This course will be offered both online and in-person at The Academy and taught by Dr. Jaime S. Rubin, Vice Chair for Investigator Development at Columbia University Irving Medical Center, an expert in this field with decades of experience.

For inquiries, contact Zamara Choudhary (zchoudhary@nyas.org).

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