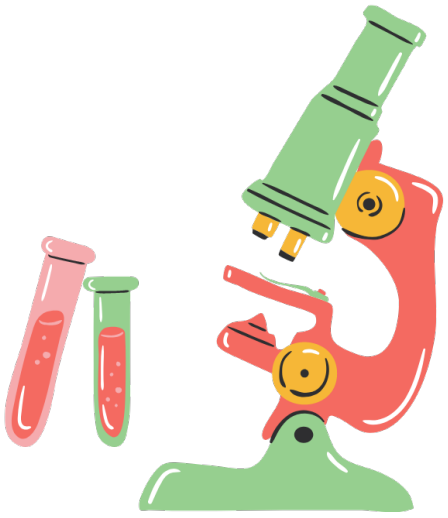
# CELEBRATING SCIENCE: AN ORIENTATION

**Tuesday, August 23, 2022**

## DOCTORAL PROGRAMS IN THE SCIENCES
## BIOCHEMISTRY, BIOLOGY, CHEMISTRY, PHYSICS

THE GRADUATE CENTER
CITY UNIVERSITY OF NEW YORK



# Celebrating Sciences: Orientation
## Biochemistry, Biology, Chemistry & Physics
## August 23, 2019

## AGENDA

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**Posters and Conversation**

CUNY Science Research – Poster Session arranged by Discipline. Open table conversations with researchers and departmental representatives or interested groups.

**Poster Session 1**

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|---|---|---|
| Biochemistry and Biology | 10:00 am - 1:30 pm | **Main Concourse** |

**Poster Session 2**

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| Chemistry and Physics | 2:00 pm - 4:30 pm | **Main Concourse** |

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**Program Meetings with New Students**

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| Biochemistry | 12:15 pm - 1:15 pm | **Science Center** |
| Chemistry | 12:15 pm - 1:15 pm | **Proshasnky Auditorium** |
| Biology | 1:45 pm - 2:45 pm | |
| Physics | 4:30 pm - 5:30 pm | |

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**Please visit https://gcsciences.ws.gc.cuny.edu/ for welcome message from Dean Brumberg, and information about resources available to GC doctoral students.**

# CONTENTS

## POSTERS



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## POSTER SESSION 1 – 10:00 am – 1:30 pm

## BIOCHEMISTRY

*PhD Students

**1. Organo-metallic anti-cancer drug design, synthesis and testing- Contel Lab.** Javier E. López-Hernández*, Nazia Nayeem*, Eric Gavrilov*, Jose P. Cerón-Carrasco, María Contel; Presenter(s): Javier Lopez; Brooklyn College, BICM/BC Chem.

The oxidation of platinum(II) is a synthetic strategy developed since 1990s and currently employed by our laboratory to replace outdated platinum(II)-based anticancer treatments. Platinum(II) as anticancer drugs lack selectivity and develop resistance by cancer cells producing high toxicity and unwanted clinical side effects. This strategy allows for minimization of side effects by decreasing secondary reactions with plasma species, reduction of platinum(IV) by producing cisplatin/oxaliplatin in situ, and the release of bioactive axial ligands into the intratumoral environment. Recently, organic bioactive molecules and metal fragments such as Ru(II) and Gd(III) were reported to coordinate the axial positions of platinum(IV). Last decade our group developed heterometallic anticancer agents containing Au(I) fragments attached to Ti(IV) and Ru(II) with high efficacy in vitro and in vivo towards renal cancer with very low systemic toxicity. We report the synthesis, characterization, stability, DNA interactions and anticancer properties of novel Pt(IV)-Au(I) complexes in vitro against genitourinary cancers.

**2. Synthesis of highly functionalized and structurally complex troponoid-containing drug molecules.** Orugbani, Eli*, Murelli, Ryan; Presenter: Orugbani, Eli; Brooklyn College, BICM/CHEM/BC Chem.

Oxidopyrilium [5+2] cycloaddition reactions are useful in the synthesis of highly functionalized and structurally complex troponoid-containing molecules. By far the most widely studied troponoid is colchicine, which has a methoxytropone-trimethoxytropone (AC ring) that binds to tubulin in its aR configuration, and as a result has been of high interest in the field of oncology. Thus, efficient de novo strategies to generate diverse structures containing the tubulin-binding AC ring could be valuable in drug development pursuits. We have developed a strategy to generate functionalized AC rings focused on a key 3-hydroxy-4-pyrone-derived oxidopyrilium cycloaddition/reductive ring opening sequence. In some cases, molecules have been made that are highly stable to enantiomerization, and can be isolated as a single atropisomers. In these instances, we have been able to able to obtain experimental energy barriers. These studies are complemented by computational modeling of the rotational barriers, and profiling their preferred dihedral angles. Ongoing work is directed at studying the anti-cancer and tubulin-binding properties of these molecules, and optimizing for potency and selectivity.

**3. Understanding DNA replication control in eukaryotes.** Ikui, Amy; Presenter: Ikui, Amy; Brooklyn College, BIOL/BIOl/BICM.

DNA replication must occur exactly once per cell division cycle in order to maintain genome integrity. In eukaryotes, this is accomplished by controls on the 'pre-replicative complex' (Pre-RC), composed of the origin recognition complex (Orc1-6), Cdc6, and the hexameric replicative Mcm helicase (Mcm2-7), bound to origins of DNA replication. A stepwise assembly of the pre- replicative complex is required to initiate DNA replication. In our lab, we use two

different unicellular organisms, S. cerevisiae and Chlamydomonas reinhardtii to understand molecular basis of replication control in eukaryotes.

**4. Multi-level approaches to study and mitigate antibiotic resistance in mycobacteria.** Quadri Lab: Biology of Mycobacterial Pathogens; Presenter: Gabrielle Germain*, Manal Fouad Farhat*, Niklas Janisch*, Keith Levendosky*, Malini Prasad*, Luis Quadri; Brooklyn College, Biology-MCD Subprogram; Biochemistry/BC Biol.

Infections by drug-resistant Mycobacterium tuberculosis and several species of opportunistic mycobacterial pathogens (e.g., *M. abscessus, M. kansasii, M. avium*) are rising globally. Drug resistance threatens control of mycobacterial infections, which already requires costly, long-term (months to years), multidrug courses (often 4 or more drugs). A comprehensive knowledge of the biology of these pathogens is needed to illuminate paths to new therapeutics against mycobacteria. Our long-term goals are to understand the biology of mycobacterial pathogens and illuminate new avenues to antimicrobial drug development. Current projects are studying (i) mechanisms of antimicrobial drug resistance in mycobacteria, (ii) mycobacterial genetic determinants involved in iron uptake, (iii) development of antibiotic with novel modes of action, and (iv) essential mycobacterial genes as new drug target candidates. We utilize techniques in molecular biology, enzymology, mutational analysis, bioinformatics, molecular modeling, omics (RNA-Seq, Tn-Seq), inhibitor / antimicrobial testing / assays, mass spectrometry, and more with great collaborators.

**5. Photo-Biooxidation: Dark Processes and Toxicity Priming.** Alexander Greer Lab; Presenter: Alexander Greer; Brooklyn College, BICM/CHEM/BC Chem.

Dr. Greer's group is involved in photosensitized oxidation reactions to sort out reactive oxygen intermediates to study. A crucial step is to solve sequential light and post-illumination processes, which are often mechanistically inaccessible. Our group utilizes both experimental and theoretical methods to research fundamental aspects in the photosciences, including a focus on controlling and amplifying the production of reactive oxygen intermediates. The research provides methods that facilitate the deconvolution of complex photobiological processes. Broader implications are related to latent effects in the phototherapy of ovarian cancer and toxicity of free radical particulates. Our group consists of Ph.D. biochemistry students Lloyd Lapoot and Oliver Turque and postdoctoral fellow Dr. Goutam Ghosh, and is funded by the NSF. Dr. Greer is also a co-chair of the Committee of Concerned Scientists, an Associate Editor of Photochemistry & Photobiology, and past-president of the American Society for Photobiology (ASP).

**6. Influence of maternal choline supplementation on metabolic outcomes of offspring with prenatal and postnatal alcohol exposures.** Xin Yin Jiang Lab; Presenter: Xin Yin Jiang; Brooklyn College, BICM/BC Health Nutrition.

Objectives: This study investigated how maternal choline supplementation may modify metabolic health of offspring with prenatal and postnatal alcohol exposures (PAE). Methods: C57BL/6J female mice were fed either a Lieber DeCarli liquid diet with 1.4% ethanol between embryonic day (E) 9.5 and E17.5 or a control Lieber DeCarli diet. Choline was supplemented to 4 x concentrations versus control throughout pregnancy. At postnatal week 7, offspring mice were exposed to 1.4% ethanol for females and 3.9% ethanol for males for 4 weeks. Results: Prenatal choline supplementation led to better glucose tolerance in male PAE offspring. Postnatal alcohol exposure led to lower expression of carnitine palmitoyltransferase 1a (Cpt1a), an important

enzyme that mediates fatty acid β-oxidation, but prenatal choline supplementation prevented this alteration. Conclusions: Maternal choline supplementation has a modest effect on normalizing liver metabolic gene expression that is altered by alcohol exposure.

**7. Graduate Research at the Computational Molecular Biophysics Laboratory at Brooklyn College.** Emilio Gallicchio; Presenter: Emilio Gallicchio; Brooklyn College, BICM/ BC Chem.

The Computational Molecular Biophysics Laboratory at Brooklyn College works with industry and experimental and computational modeling collaborators to develop and deploy sophisticated molecular theories, efficient algorithms, and powerful computers to characterize fundamental chemical and biological mechanisms. Recent focus has been on the modeling of protein-ligand binding free energies for applications in structure-based drug discovery. The lab strives to offer advanced research opportunities to give students access to high-quality industrial and academic positions. Visit www.compmolbiophysbc.org for more information.

**8. Causes and outcomes of inheriting uncommon number of chromosomes.** The Schvarzstein lab; Presenter: Mara Schvarzstein; Brooklyn College, Biology (MCD) and Biochemistry.

The Schvarzstein lab research focusses on uncovering the causes and consequences of inheriting abnormal number of chromosomes (aneuploidy) or abnormal number copies of the genome (polyploidy). Aneuploidy is a major driving force for cancer development, are responsible for most miscarriages and a large proportion of sterility in humans and are responsible for congenital birth disorders and genetic syndromes. Whereas cell and tissues polyploidy are a key step in normal development (e.g. platelet production by megakaryocytes), wound healing, and a key step in cancer formation, whole organism polyploidy is a key step in evolution, crop domestication, speciation, and adaptation to stresses. To uncover molecular and cellular mechanism regulating accurate chromosome inheritance in regular and specialized cell divisions, the Schvarzstein lab takes a comprehensive approach that combines omics, live and fixed high- and super resolution imaging with developmental genetics technologies in the transparent nematode C. elegans. In this poster, we will discuss some of the ongoing projects in the lab, as well as our future research goals.

**9. Biochemistry research at CSI: Structural Biology, Biophysics and Nanobiochemistry.** Rupal Gupta, Sharon Loverde, Sebastien Poget, Ming Tang and Shuiqin Zhou; Presenter: Rupal Gupta; CSI, Biochemistry / Chemistry.

Brief outline of biochemistry research in the Gupta, Loverde, Poget, Tang and Zhou labs.

**10. Biochemistry Research at CSI: Neurobiochemistry, Bioorganic Chemistry, Molecular and Developmental Biology.** Alejandra Alonso, Cesar Arenas-Mena, Probal Banerjee, Jimmie Fata, Krishnaswami Raja and Chang-Hui Shen; Presenter: Rupal Gupta; CSI, Biochemistry / Biology and Chemistry.

Brief outline of the biochemistry research in the Alonso, Arenas-Mena, Banerjee, Fata, Raja and Shen labs.

**11. Molecular Dynamics Simulations of the Structural Effects of Oncogenic Mutations in the Nucleosome.** Augustine C. Onyema*, Phu K. Tang*, Prabir Khatua and Sharon M. Loverde; Presenter: Augustine Onyema*; CSI, Biochemistry/Chemistry.

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

dynamics of the NCP together with DNA binding proteins drive cellular processes including replication and transcription. However, these dynamics are biochemically exploited by tumor cells to aid their proliferation in different cancer types including glioblastoma, leukemia, lung carcinoma, and chondroblastoma[1]. Mutations in the core histone proteins (H2B and/or H4) seen in uterine cancer have been shown to destabilize the H2B-H4 protein interface[2]. We performed a 12 μs all atomistic simulation of the H2B E76K mutant of the NCP (1kx5) on Anton 2[3]. We noticed a destabilization of the H4-H2B (α3_H4 and α2_H2B) helix interface characterized by a decrease in interhelical polar contacts. To investigate similar behavior for the histone H4 R92T mutant system, we ran a 100ns all atomistic simulation after a 10ns equilibration. We observed a decrease in interhelical hydrogen bond in the mutant system at the H4-H2B interface compared to the wild type (1kx5). We also observed that the strong interhelical polar contacts favors the formation of π- π interaction between Y83 (H2B) and Y88 (H4). The binding free energy in both systems was similar after 100ns. Also, His75 on histone H4 and Leu97 on histone H2B were major contributors to the free energy. We intend to run longer simulations to understand the stability at the helix interface in the R92T mutant. Observing the structural effects of oncogenic mutations in the histone may shed light on how mutations affect the stability of the histone core proteins.

**12. Structural basis of Protoxin-2 modulation in pain channel Nav1.7.** Joekeem Arizala*, Ryan Schroder*, Abba Leffler, Sebastien Poget; Presenter: Joekeem Arizala; CSI, Biochemistry/Chemistry.

Voltage sensing drives the movements in voltage-gated sodium channels (Nav). This ability to sense membrane voltage is confined to channel regions known as the voltage-sensing domain (VSD). Due to its function, the VSD region became the target of gating modifier toxins (GMTs). Protoxin-2 is a GMT known to inhibit the activation of pain channel Nav1.7 by targeting its VSD from repeat 2. For this reason, Protoxin-2 has gained interest as an analgesic candidate. However, a deeper understanding of the Protoxin-2 binding mechanism is required to utilize its pharmacological potential. It is therefore our goal to map the interaction sites between Protoxin-2 and VSD that may be important in toxin binding and gating function. First, we optimized the recombinant expression and purification of Protoxin-2 and Nav1.7 VSD2. The purified and refolded Nav1.7 VSD2 exhibits a near-native fold as demonstrated by the Protoxin-2 binding during microscale thermophoresis. We then explored other binding sites by making point mutations in the VSD2. Information gathered from toxin binding experiments of VSD2 mutants will be used to create an accurate model of toxin-channel interaction. Finally, we want to unravel the role of the membrane in Protoxin-2 docking using a combination of fluorescence and solution NMR.

**13. Catalytic activity of iron-containing enzymes: Biophysical and Computational Study.** Rupal Gupta and Angelo Bongiorno; Presenter: Rupal Gupta; CSI, Biochemistry and Chemistry/Chemistry.

Transformation of chemical bonds in nature is efficiently performed by enzymes bearing a metal cofactor. Understanding the Chemistry of enzymes is critical for the development of next generation of industrial catalysts capable of performing complex chemical reactions. In this project, we combine biochemical and spectroscopic methodologies along with quantum chemical calculations to gain a deeper insight into the structure and functions of iron enzymes

**14. The Amyloidogenic Propensity of the Helix 1 Region of Serum Amyloid A is Influenced by Key Charged Amino Acids.** Marvin M. Bilog, Ruel Z. B. Desamero and Adam A. Profit; Presenter: Marvin Bilog*; YC, Biochemistry/Chemistry.

**15. Biochemistry Research Opportunities at Queens College.** Uri Samuni; Presenter: Uri Samuni; QC, Biochemistry / Biology and Chemistry and Biochemistry.

Cutting edge research at Queens College covers a wide range of Biochemical research topics. The poster describes the Biochemistry research opportunities at Queens College and provides an overview of the campus, research facilities and research environment. Biochemistry faculty at Queens College are members of the Department of Chemistry and Biochemistry or of the Biology Department. The poster highlights research performed at the laboratories of Biochemistry faculty at Queens College with whom Biochemistry students can mentor. Interested students can contact potential mentors directly or email Prof. Uri Samuni the Queens College campus Biochemistry program representative (uri.samuni@qc.cuny.edu).

**16. Silica based sol-gels/nanogels and their applications.** Uri Samuni; Presenter: Uri Samuni; QC, Biochemistry/Chemistry and Biochemistry.

Silica sol-gel derived matrices have advantageous properties including extremely large porosity, chemical inertness, structural stability and transparency in the UV/Vis spectral regions. These advantages lead to utilization of sol-gel matrices in a variety of fields including chromatography, sensing, catalysis and drug delivery. Many of these applications involve entrapment of analytes within the sol-gel's -Si-O-Si-O- amorphous network, such as entrapments of proteins that can serve as biosensors. Indeed, the sol-gel environment is an exceptionally good host for biomolecules, leaving them intact and functional. Recent development in the field is extension of the sol-gel method to fabrication of colloidal particles and nanoparticles (nanogels). This allows to combine the silica sol-gel matrix advantageous properties with those of nanoparticles, namely the large surface area and the particles small size. Hence, nanogels could serve in a variety of applications including to imaging and drug delivery. The Samuni lab is developing fabrication methods for encapsulation of enzymes and biologically active molecules within silica based sol-gel matrices and nanogels and explores their applications.

**17. Title: Organic, Medicinal, & Natural Products Chemistry @ Hunter College.**
**Presenters:** Wayne Harding, Akira Kawamura, David R. Mootoo, Shengping Zheng; Hunter, Biochemistry/ Chemistry

This poster presents recent research activities of four organic groups at Hunter Chemistry Department.

***Also see Poster No. 19 listed under Biology:***
**Autophagy in Development.** Alicia Meléndez; Presenter: Alicia Meléndez; QC, Biology/ Biochemistry.

## POSTER SESSION 1 – 10:00 am – 1:30 pm

## BIOLOGY

*PhD Students

**18. Models and mechanisms of malaria-induced acute kidney injury.** Johanna Bensalel*, Angelica P. Piña*, Kiara Hernandez*, Winifred Prempeh*, Daniela Basave*, Alberto Lazaro, Julio Gallego-Delgado; Presenter: Johanna Bensalel; Lehman, Biology.

In 2020, there were an estimated 627,000 deaths from malaria of which most are in children. It has been reported that 40-60% of severe malaria patients present with MAKI which often results in renal failure and/or long-term complications. There are currently no specific therapies to treat this complication and there are no suitable rodent models that replicate the condition in humans. The removal of one kidney from wild-type mice and subsequent infection with Plasmodium berghei NK65 has resulted in development of kidney injury in mice, evident by elevated levels of urinary and serum acute kidney injury (AKI) biomarkers and increased expression of AKI-associated proteins in renal tissue. Establishment of this in vivo model of MAKI is critical as it can be used to elucidate the molecular pathways implicated in MAKI, delineate the development of the disease, identify biomarkers for early diagnosis and prognosis, and test potential adjunctive therapies.

**19. Autophagy in Development.** Alicia Meléndez; Presenter: Alicia Meléndez; QC, Biology/ Biochemistry. *(crosslisted with Biochemistry)*

Macroautophagy (autophagy) delivers intracellular constituents to the lysosome to promote catabolism. Autophagy is required during development, as it mediates various cellular processes, including survival during starvation, programmed cell death, phagocytosis, secretion, and organelle recycling. Our current understanding of autophagy has been enhanced by developmental biology research during the last quarter of a century, as we have learned about the mechanisms involved and how this degradation process is involved in disease. My lab investigates the role of autophagy in germline development, meiotic fidelity, DNA damage, and aging in C. elegans. We are also starting a new project to investigate the role of microautophagy, where endosomal or lysosomal membranes generate invaginating vesicles that internalize proteins carrying a penta-peptide (KFERQ) motif. We have developed a sensor for microautophagy and plant to dissect the genetic and molecular mechanisms involved in turnover by the KFERQ-motif and determine its physiological relevance.

**20. Pre-replicative complex dynamics in Chlamydomnas reinhardtii.** *Gavin Duckett, Amy Ikui; Presenter: Gavin Duckett; Brooklyn College, Biology.

We have examined the cell cycle-dependent abundance and localization of pre-replicative complex components ORC1, CDC6, and MCM4/6 in the green alga Chlamydomonas reinhardtii, using time lapse microscopy and immunofluorescence. Formation of the pre-replicative complex on DNA, beginning with binding of the origin recognition complex (ORC), establishes origins of replication by loading the helicase MCM2-7 as a double hexamer, to be later activated to create a pair of replication forks. This process, known as origin licensing, is therefore a critical point of control for the cell cycle. We found that CDC6 and MCM4/6 are nuclear bound throughout the Chlamydomonas division cycle except during mitosis when they transiently enter the cytoplasm

due to loss of nuclear membrane integrity. In contrast, ORC1 is present in the nucleus only during mitosis, when it becomes DNA bound, followed shortly by CDC6.

**21. Quadri Lab: Biology of Mycobacterial Pathogens.** Gabrielle Germain*, Manal Fouad Farhat*, Niklas Janisch*, Keith Levendosky*, Malini Prasad*, Luis Quadri; Presenter: Malini Prasad; Brooklyn College, Biology-MCD Suprogram; Biochemistry.

Infections by drug-resistant Mycobacterium tuberculosis and several species of opportunistic mycobacterial pathogens (e.g., M. abscessus, M. kansasii, M. avium) are rising globally. Drug resistance threatens control of mycobacterial infections, which already requires costly, long-term (months to years), multidrug courses (often 4 or more drugs). A comprehensive knowledge of the biology of these pathogens is needed to illuminate paths to new therapeutics against mycobacteria. Our long-term goals are to understand the biology of mycobacterial pathogens and illuminate new avenues to antimicrobial drug development. Current projects are studying (i) mechanisms of antimicrobial drug resistance in mycobacteria, (ii) mycobacterial genetic determinants involved in iron uptake, (iii) development of antibiotic with novel modes of action, and (iv) essential mycobacterial genes as new drug target candidates. We utilize techniques in molecular biology, enzymology, mutational analysis, bioinformatics, molecular modeling, omics (RNA-Seq, Tn-Seq), inhibitor / antimicrobial testing / assays, mass spectrometry, and more with great collaborators.

**22. The DEAH-box family RNA helicase associated with AU-rich element (RHAU) regulates immunoglobulin class switch recombination.** Thongthai Thavornwatanayong*, Simin Zheng†, Sabine Jean Guillaume, Bao Q. Vuong; Presenter: Thongthai Thavornwatanayong; City College of New York, Biology (MCD).

Class switch recombination (CSR) permits B cells to produce alternative immunoglobulin isotypes (IgG, IgE, IgA). AID initiates recombination of the immunoglobulin heavy chain (IgH) locus by deaminating intronic switch (S) regions. Current models posit that AID localizes to S regions by G-quadruplex (G4)-forming RNA or DNA; however, the molecular mechanism that transfers AID from RNA to DNA remains uncharacterized. RNA pull-down assays identified RNA helicase associated with AU-rich element (RHAU) as an S transcript binding protein. Genetic inactivation of Rhau in B cells reduced CSR to IgG1 in vivo and in vitro without affecting CSR to IgG3. Future experiments will examine if RHAU specifically unwinds G4 in Sg1 transcripts and how RHAU could mediate the binding of AID to G4-RNA or S region DNA during CSR.

**23. Tracking Cryptic SARS-CoV-2 Lineages in NYC Wastewater.** Smyth DS, Trujillo M, Gregory DA, Cheung K, Gao A, Graham M, Guan Y, Hoxie I*, Kannoly S, Kubota N, Lyddon TD, Markman M, Rushford C, San K, Sompanya G, Spagnolo F, Suarez R, Daniels M, Johnson MC & Dennehy JJ. ; Presenter: John Dennehy; Queens, Biology: MCD/EEB.

Tracking SARS-CoV-2 genetic diversity is strongly indicated because diversifying selection may lead to the emergence of novel variants resistant to naturally acquired or vaccine-induced immunity. To monitor New York City (NYC) for the presence of novel variants, we deep sequence most of the receptor binding domain coding sequence of the S protein of SARS-CoV-2 isolated from the New York City wastewater. Here we report detecting increasing frequencies of novel cryptic SARS-CoV-2 lineages not recognized in GISAID's EpiCoV database. We offer several hypotheses for the anomalous presence of these lineages, including the possibility that these lineages are derived from unsampled human COVID-19 infections or that they indicate the

presence of a non-human animal reservoir. Evidence suggests that these lineages are derived from long-term persistent infections of immunocompromised patients.

**24. Molecular basis of microglial response to insoluble aggregates.** Dvir Avnon-Klein, Shawn Kilpatrick, Pinar Ayata; Presenter: Dvir Avnon-Klein; ASRC, Neuroscience.

In age-associated diseases, cellular proteins misfold and assemble into insoluble aggregates. These aggregated proteins, which acquire new physical and chemical characteristics, are then perceived as non-self by the immune cells and subsequently targeted by defense mechanisms. Microglia are the brain's primary immune cells and first responders to accumulating protein aggregates. To understand how microglia respond to insoluble aggregates, we fabricated spherical microparticles that mimic the size and stiffness of the dense-core amyloid plaques in Alzheimer's Disease. We found that microglia in the proximity of the particles polarized toward and then corralled around them. A subset of cells took up multiple particles and built a cluster of these particles. Our current studies address the molecular basis of this response.

**25. Cellular events that shape microglia identity in Alzheimer's disease.** Thi Ngo, Anna Flury, Leen Aljayousi, Dvir Avnon-Klein, Pinar Ayata; Presenter: Thi Ngo, Anna Flury, Leen Aljayousi; ASRC, Neuroscience.

Genetics implicates microglia—the brain's primary immune cells—as significant determinants of Alzheimer's Disease (AD) risk. In AD, microglia can assume phenotypes with protective or harmful functional outcomes. We found that a subset of microglia, which drives this harmful aberrant synapse loss, displays disrupted metabolic and protein homeostasis (proteostasis). Many diverse genetic and non-genetic risk factors for AD and related dementias also disrupt proteostasis in microglia. Therefore, we hypothesized that the disruption of proteostasis by risk factors induces metabolic-epigenetic reprogramming of microglia and primes the expansion of microglia that drive an aberrant synapse loss. We tested the functional outcome of proteostasis challenge in microglia in vitro and in vivo using a novel chemogenetic mouse model. We found that disruption of proteostasis in microglia results in long-lasting metabolic and epigenetic changes. Our current studies address the functional outcome of these changes.

**26. Aging effects on the density of dopamine-glutamate neurons in the ventral midbrain.** Jacquelyn N. Tomaio*, Sixtine Fleury, Yoon Seok Kim, Lief Ericsson Fenno, Charu Ramakrishnan, Karl Deisseroth, Susana Mingote; Presenter: Jacquelyn N. Tomaio; ASRC, Biology/Neuroscience.

Dopamine (DA) neurons in the ventral midbrain express vesicular glutamate transporter 2 (VGLUT2) and can co-release glutamate (GLU). Fate-mapping experiments in mice have shown 100% of DA neurons co-express VGLUT2 (Poulin et al., 2018; Steinkellner et al., 2018) during early development, which changes to 30% in the ventral tegmental area (VTA) and 10% in the substantia nigra pars compacta (SNc) (Mingote et al., 2019; Steinkellner et al., 2018) in adulthood. However, how aging affects eurotransmitter switching in mice has not been addressed. We used INTRSECT 2.0 viral vectors in transgenic mutant mice to label two subpopulations of DA neurons (DA-only with mCherry, and DA-GLU with yellow fluorescent protein). We quantified neurons in the VTA and SNc in 3-, 12- and 24-months aged mice and showed a significant decrease in SNc DA-GLU neuron density in old (24) aged mice. We also showed a significant reduction of VGLUT2 transcripts in the VTA, with a trending decrease of VGLUT2 transcripts in DA-GLU neurons.

**27. Role of Ventral Midbrain Dopamine Neurons in Familiarity.** Rhonda Kolaric1* , Sixtine Fleury1 ,Jacquelyn Tomaio1* , Andreas Toft Sørensen2 , Ulrik Gether2 , Susana Mingote1; Presenter: Rhonda Kolaric; ASRC, Biology.

It is well established that dopamine (DA) neurons in the ventral midbrain signal novelty by increasing their bursting activity, while decreasing it after repeated inconsequential stimulus presentations 1,2,3,4. Thus, the lack of DA neuron burst activity is a physiological signature that a stimulus has become familiar. We tested the hypothesis that decreasing DA neuron activity while animals explore objects for the first time enhances familiarization and improves subsequent novel object recognition (NOR). NOR is dependent on the amount of pre-exposure to the familiar object, and here we show that only one familiarization session is not sufficient to induce NOR. The lack of exploration on the novel object is thought to reflect a stage of equal attention allocated to the familiar and novel stimulus. To investigate whether decreasing DA neuron activity prompts gain-of-function in NOR, we chemogenetically inhibited DA neurons in the ventral tegmental area (VTA) during the familiarization session of a NOR paradigm that results in poor novelty discrimination.

**28. The Cortical Barrel a Window into Development.** Joshua C. Brumberg; Presenter: Joshua C. Brumberg; Queens, Biology/Psychology/Neuroscience.

The Brumberg Lab utilizes the mouse-whisker-to-cortical barrel to study how sensory experience impacts neural development. Utilization a synthesis of physiogical, behavioral and anatomical techniques how changes in sensory experience (deprivation) impact neuronal structure and function is assayed as well as the impact on non-neuronal components such as glia and the extracellular matrix.

**29. BMP Signaling in Regulation of *C. elegans* Lipid Homeostasis and Immune Response.** Kat Yamamoto* and Cathy Savage-Dunn; Presenter: Kat Yamamoto; Queens College, Biology.

Research on innate immunity has focused on aspects that decrease pathogen load, including physical barriers and the upregulation of antimicrobial peptides (AMPs). Less is known, however, about the role of host metabolism in supporting survival independently of anti-bacterial responses. Bone Morphogenetic Proteins (BMPs) are secreted peptide growth factors in the TGF-β family, well known for their roles in development and differentiation, but emerging as homeostasis modulators. In *C. elegans*, impairment of BMP signaling results in increased infection susceptibility and decreased survival after exposure to bacterial pathogens. The BMP pathway also regulates lipid metabolism in *C. elegans*, where impairment of signaling results in decreased quantities of lipid stores, and fewer, smaller lipid droplets. Altered lipid metabolism is one potential mechanism for immune tolerance, an alternative response that does not depend on reducing pathogen load. Here we begin to explore the relationship between host metabolism and pathogen tolerance.

**30. Preclinical Evaluation of a Potential Ruthenium-Based Chemotherapeutic Agent for the Treatment of Triple Negative Breast Cancer.** Nazia Nayeem, Maria Contel; Presenter: Nazia Nayeem; Brooklyn College, MCD.

Triple negative breast cancer (TNBC) is an aggressive subtype of breast cancer that is defined by the absence of expression of progesterone, estrogen, and human epidermal growth factor 2 receptors. Due to the inability to target a receptor, treatment is mostly limited to

nonspecific chemotherapy. A potential water-soluble ruthenium-based chemotherapeutic agent has been developed, which promisingly showed a 56% tumor shrinkage in a preliminary in vivo study with TNBC MDA-MB-231cell line xenograft. Preclinical evaluation of this complex has revealed significant anti-angiogenic, anti-invasive, and anti-migratory properties, along with subcellular accumulation in the mitochondria with increased ROS generation and an apoptotic mechanism of cell death. Proteomic analysis has implicated the inhibition of PI3K/Akt pathway as a potential target of this drug, and in vivo studies are currently underway to view the potential use of this drug in combination and monotherapies clinically.

**31. Identification of molecular pathways in neurodegeneration and neuroprotection in nematode excitotoxicity.** Zelda Mendelowitz*, Adem Idrizi, Ayesha Chowdhury*, Shirley Chan, and Itzhak Mano; Presenter: Itzhak Mano; CUNY Sch of Med, MCD; CNC / MCBS.

Excitotoxicity is a prevalent form of neurodegeneration seen in stroke and in a rage of progressive neurodegenerative diseases. While we know that excitotoxicity is triggered by excessive accumulation of the neurotransmitter Glutamate (Glu) and hyper-activation of Glu Receptor/Channels (GluRs), our understanding of the process that leads from GluR hyperactivation to necrotic cell death remains highly controversial, and its progression remains untreated in the clinic. Surprisingly, the degenerative process is also partially mitigated by a neuroprotective process that depends on GluR-activated transcriptional programs. The Mano lab focuses on the study of a model of excitotoxicity in the nematode. We use this model to decipher the pathways that lead to necrotic neurodegeneration, and to understand how neurodegeneration is mitigated by transcriptional neuroprotective programs. We hope that identifying molecular mediators of neurodegeneration and neuroprotection in nematode excitotoxicity can be informative in the future development of strategies to mitigate neuronal damage in brain ischemia.

**32. Effective Modulation of Motor Learning with tDCS at 4mA.** Gavin Hsu*, A. Duke Shereen, Lucas C. Parra; Presenter: Gavin Hsu; CCNY, Biomedical Engineering.

Motor learning experiments with transcranial direct current stimulation (tDCS) at up to 2mA have produced mixed results. We hypothesize that tDCS boosts motor learning provided sufficiently high field intensity on the motor cortex. In a single-blinded, between-subject design, N=72 healthy right-handed participants received either anodal or cathodal tDCS at 4mA while they learned to perform a sequence of key presses using their non-dominant hand. A separate sham stimulation group (N=36) established baseline performance. A single HD-tDCS montage with 4 frontal and 4 parietal electrodes for all N=108 subjects was selected from current flow models optimized to target an fMRI-localized hotspot on the motor cortex. We found significant gains in performance with anodal stimulation, which persisted for at least one hour. Sensation ratings were comparable between the active groups and did not exceed moderate levels. The present paradigm shows reliable behavioral effects at 4mA and is well-tolerated.

**33. Causes and outcomes of inheriting uncommon number of chromosomes.** The Schvarzstein lab; Presenter: Mara Schvarzstein; Brooklyn College, Biology (MCD) and Biochemistry.

The Schvarzstein lab research focusses on uncovering the causes and consequences of inheriting abnormal number of chromosomes (aneuploidy) or abnormal number copies of the genome (polyploidy). Aneuploidy is a major driving force for cancer development, are

responsible for most miscarriages and a large proportion of sterility in humans and are responsible for congenital birth disorders and genetic syndromes. Whereas cell and tissues polyploidy are a key step in normal development (e.g. platelet production by megakaryocytes), wound healing, and a key step in cancer formation, whole organism polyploidy is a key step in evolution, crop domestication, speciation, and adaptation to stresses. To uncover molecular and cellular mechanism regulating accurate chromosome inheritance in regular and specialized cell divisions, the Schvarzstein lab takes a comprehensive approach that combines omics, live and fixed high- and super resolution imaging with developmental genetics technologies in the transparent nematode C. elegans. In this poster, we will discuss some of the ongoing projects in the lab, as well as our future research goals.

**34. Chronic Stress Disrupts Safety Learning and Theta-Based Circuit Communication.**
Itamar S. Grunfeld, L Emma Denholtz, Sadiyah Hanif, Itzik Nahmoud, Siddhartha Datta, Sumantra Chattarji, Nesha S. Burghardt, Ekaterina Likhtik.

Chronic stress leads to generalization of fear to non-threatening cues, a key symptom in numerous psychiatric disorders. Here, we test how chronic stress affects safety learning to gain insight into whether this may contribute to stress-induced impairments in discrimination. We used the chronic social defeat stress (CSDS) model to investigate this relationship in 129 Sv/Ev male mice. Following 10 days of CSDS, mice underwent two days of salient safety conditioning, where they were exposed to 5 unsignaled shocks (0.5mA) intermixed with five trials of a safety stimulus. The safety stimulus was a 30s tone that turned on at the same time as a 1s house light (CSsafety) to signal the explicit absence of shock. The next day, animals were tested with 5 presentations of the CSsafety in the same context without shock. We found that non-stressed control mice (n= 15) exhibited defensive freezing to the context, which was reduced during the CSsafety cue. In contrast, stressed mice (n = 15) showed high levels of freezing behavior regardless of the presence of CSsafety, until the last trial, indicating that chronic stress impairs safety learning. To gain insight into the underlying circuits, we used local field potential (LFP) recordings in the prelimbic cortex (PL), basolateral amygdala (BLA) and dorsal hippocampus (HPC) and compared activity in the presence and absence of CSsafety. In the PL of control mice, the theta (4-8Hz):delta (0.1-3.9Hz) ratio was lower when CSsafety was on. In stressed mice, this process is disrupted, as evidence by the lack of change in the theta:delta ratio and increase in theta and delta power during the CSsafety signal, indicating increased drive onto the PL. In the BLA, controls also had a lower theta:delta ratio during the CSsafety cue, whereas the ratio in stressed mice did not change. Furthermore, stressed mice showed significantly lower overall PL-BLA theta coherence than control mice, indicating that chronic stress decreased synchronous theta-based communication in this circuit. Notably, by the end of the retrieval session (trial 5), when stressed animals first suppress defensive freezing to the CSsafety cue, they showed significantly lower PL theta:delta ratio and BLA theta power when the CSsafety signal was on, consistent with a delay in circuit dynamics underlying retrieval of a safety cue. In a separate cohort, we evaluated spine density in the PL after CSDS, and found that CSDS decreased the number and density of PL spines. Currently, we are investigating the contributions of HPC theta-oscillations to CSsafety processing in this circuit.

**POSTER SESSION 2 - 2:00 pm – 4:30 pm**

## CHEMISTRY

*PhD Students

**1. Photo-Biooxidation: Synthesis, Mechanism, and Toxicity Priming.** Alexander Greer; Presenter: Alexander Greer; Brooklyn, Chemistry.

Dr. Greer's group is involved in photosensitized oxidation reactions to sort out reactive oxygen intermediates to study. A crucial step is to solve sequential light and post-illumination processes, which are often mechanistically inaccessible. Our group utilizes both experimental and theoretical methods to research fundamental aspects in the photosciences, including a focus on controlling and amplifying the production of reactive oxygen intermediates. The research provides synthetic and mechanistic studies that facilitate the deconvolution of complex photochemical processes. Broader implications are related to latent effects in the phototherapy of ovarian cancer and toxicity of free radical particulates. Our group consists of Ph.D. students Lloyd Lapoot and Oliver Turque and postdoctoral fellow Dr. Goutam Ghosh, and is funded by the NSF. Dr. Greer is also a co-chair of the Committee of Concerned Scientists, an Associate Editor of Photochemistry & Photobiology, and past-president of the American Society for Photobiology (ASP).

**2. National Institutes of Health Research Training Initiative for Scientific Enhancement (G-RISE)@CCNY**. Ruth Stark; Presenter: Ruth E. Stark; City College.

30 CCNY faculty members are offering rigorous Ph.D. training and professional development in biochemistry, biophysics, bioorganic chemistry, (biomedical and chemical) engineering, and neuroscience to 15-18 trainee cohorts 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 timely graduation in biomedical science and engineering disciplines, while also improving their technical and communication skills, research productivity, and post-Ph.D. workforce placement.

**3. Biomacromolecular Structure and Assembly: Animal, Vegetable, and Fungal Adventures.** Ruth E. Stark; Presenter: Ruth E. Stark; City College, Chemistry/Biochemistry

The Stark Laboratory seeks atomic-level structural and mechanistic understanding of the protection conferred by plant polymer composites, lipid-mediated metabolic signaling by fatty acid-binding proteins (FABPs), and melanin pigment virulence factors in fungal cells. Nondestructive study of the molecular and mesoscopic architectures underlying the barrier function of cuticles (skins) in both native and engineered tomatoes and potatoes is being undertaken using solid-state NMR, atomic force microscopy, and metabolomic profiling. Ligand recognition and macromolecular interactions of FABPs that are implicated in pain and

inflammation are under investigation using protein engineering, fluorescence, and solution NMR. Molecular structure and development of melanin pigments within fungal cells are probed using (bio)chemical synthesis and two-dimensional solid-state NMR. The members of our research team typically span high school through senior postdoctoral levels.

**4. Structural studies of the interaction of gating-modifier tarantula toxins with voltagegated sodium channels.** Krishnakoli Adhikary; Presenter: Krishnakoli Adhikary; CSI, Chemistry.

Voltage-gated ion channels are membrane protein complexes which allow the selective flow of their respective ions down an electrochemical gradient in a voltage-depen dent manner. Structurally, they consist of a central ion conduction pore domain that is surrounded by four voltage sensing domains (VSDs). Gating-modifier toxins (GMTs) are peptide toxins found in different animal venoms that bind to these VSDs and change their gating properties. Our laboratory has determined that the GMT GsAF2 from tarantula binds to the VSD of the bacterial sodium channel NaChBac (called BHVSD). GsAF2 and its mutants have been/are being synthesized recombinantly and their functionality has been tested through Automated Patch Clamp electrophysiology.GsAF2 is also known to interact with several other voltage- gated ion channels including Nav1.7. Docking studies have been being performed with the homology model of GsAF2 and the Cryo-EM structure of NaChBac to identify residues of the toxin and channel that could be involved in the interaction and generating suitable mutants for functionality testing. Nuclear Magnetic Resonance experiments will help determining the structure of the toxin and its residues involved in channel binding.

**5. Peptide Acetylation for Improved Stability and Delivery of Au-based Anticancer Agents.** Yaron Marciano; Presenter: Yaron Marciano; Brooklyn College, Chemistry.

Peptide-based supramolecular assemblies have been extensively studied for use as therapeutics (tumor targeting peptides, cell penetrating peptides). They are particularly attractive due to their tunability and biocompatibility. The stability of these assemblies in physiological conditions has always been a concern due to various proteases present in physiological media (human plasma, serum) that can cleave the amide bonds in the peptide backbone. Various modifications have been applied in order to stabilize and decrease proteolysis kinetics, such as cyclization1,2 and incorporation of unnatural amino acids.3 Cyclization changes the peptide structure, and incorporating D-amino acids prevents proteolysis entirely, which may cause toxicity in vivo. Here, we describe a simple modification to decrease proteolysis kinetics, while not preventing it altogether. Capping the peptide by acetylating the N-terminus of peptides while in the solid phase using acetic anhydride, we can greatly improve the stability of peptides and peptide-based therapeutics. The increased stability of these peptide materials makes them viable options as delivery vehicles, specifically for hydrophobic drugs that can sit inside the hydrophobic pocket of the assemblies. We report here on the encapsulation of a Au(I)-NHC complex4 in acetylated supramolecular peptide assemblies. Peptide stability, characterization, encapsulation, and cytotoxicity will be discussed.

**6. Synthesis and Studies of Methylated Colchicine AC Ring Analogs.** Eli Orugbani; Presenter: Eli Orugbani; Brooklyn College, Chemistry.

Oxidopyrilium [5+2] cycloaddition reactions are useful in the synthesis of highly functionalized and structurally complex troponoid-containing molecules. By far the most widely studied troponoid is colchicine, which has a methoxytropone-trimethoxytropone (AC ring) that

binds to tubulin in its aR configuration, and as a result has been of high interest in the field of oncology. Thus, efficient de novo strategies to generate diverse structures containing the tubulin-binding AC ring could be valuable in drug development pursuits. We have developed a strategy to generate functionalized AC rings focused on a key 3-hydroxy-4-pyrone-derived oxidopyrilium cycloaddition/reductive ring opening sequence. In some cases, molecules have been made that are highly stable to enantiomerization, and can be isolated as a single atropisomers. In these instances, we have been able to able to obtain experimental energy barriers. These studies are complemented by computational modeling of the rotational barriers, and profiling their preferred dihedral angles. Ongoing work is directed at studying the anti-cancer and tubulin-binding properties of these molecules, and optimizing for potency and selectivity.

**7. Chemistry at the College of Staten Island I: From polymer synthesis tothe development of functionalized nanomaterials.** Professors Qiao-Sheng Hu, Shi Jin, Michal Kruk, Ralf Peetz, and Krishnaswami Raja; CSI, Chemistry.

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.

**8. Chemistry at the College of Staten Island II: From computational chemistry to engineered polymers.** Professors Angelo Bongiorno, Sharon Loverde, Alan Lyons, Chwen-Yang Shew, and ShuiqinZhou; CSI, Chemistry.

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 laboratory fabricates superhydrophobic and thermally conductive surfaces 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 polymer-based nanomaterials and biomaterials.

**9. Laboratory of Medicinal Chemistry, Computer-aided Drug Design, and Chemical Biology.** Shuai Ma, Ryan Seerattan, Zakir Hossain, Eugene Chung, Diana Rodriguez, Deana Davidova, Hana Chen, Aveta Singh, Valeria Orduna, Jun Yong Choi; Presenter: Shuai Ma; Queens College, Chemistry.

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.

**10. Nanoelectrochemistry:fromfundamental studies to energy and biomedical applications.** Gaukhar Askarova,* Tianyu Bo,* Rui Jia,Xiang Wang, andMichael V. Mirkin; Presenter: *Tianyu Bo,* Rui Jia; Queens College, Chemistry.

Many important chemical and biological systems—form electrocatalysts to living cells—contain nanometer-sized structures and active sites. Nanoelectrochemistry provides powerful tools for high-resolution studies of such systems. Nanometer-sized electrodes can be used to obtain molecular level information about structures and chemical processes and to investigate microscopic systems that cannot be addressed by larger probes. The applications range from molecular electronics to energy conversion and storage to analytical chemistry inside living cells. The focus of this presentation is on the use of nanoelectrodes and scanning electrochemical microscopy (SECM) for high-resolution imaging and quantitative experiments on the nanoscale. The advantages of nanoelectrochemical approaches and remaining challenges are illustrated by two different applications – mapping surface reactivity of individual catalytic nanostrctures and measurements of reactive oxygen and nitrogen species (ROS/RNS) inside breast cancer cells and in subcellular compartments.

**11. Mediating charge carrier transfer from metal halide perovskite nanocrystals through surface engineering.** Chen Wang; Presenter: Jingheng Yuan ; Queens College, Chemistry.

Extracting photo-generated excitons and charge carriers from semiconductor nanocrystals is the fundamental pathway for utilizing light energy stored in their excitonic states. Utilizing the rich surface chemistry properties of nanocrystals, researchers have designed effective strategies for mediating charge carrier migration and energy transfer across the nanocrystal interfaces. Our group develops systematic engineering approaches for handling the overly dynamic surface of metal halide perovskite nanocrystals (PNCs) that are difficult to functionalize using conventional methods. The bound affiliates of various candidate ligands on the PNC surface are evaluated using computational and experimental methods. We identify structures that can stably graft functional groups onto the PNC surface to develop surface modification strategies that can establish strong electronic coupling between PNCs and functional structures. Various molecule-based acceptors, including triplet energy acceptors, such as naphthalene, electron acceptors, such as quinoline, and hole acceptors, such as oligothiophene, are anchored to the PNC surface. Using steady-state and time-resolved optical spectroscopy, we demonstrate that the stable anchoring of these acceptors prominently enhances the efficiency of energy and charge carrier transfer compared to systems with weakly associated acceptors that shuffle on and off the PNC surface. The dynamics of carrier and energy transfer can be flexibly controlled by adjusting the number of bound acceptors. The electron transfer and charge recombination processes from PNCs are also manipulated to mediate photocatalytic cycloaddition reactions of enone.

**12. Comparison of Proton Transfer Paths to the QA and QB Sites of the Rb. sphaeroides Photosynthetic Reaction Centers.** Rongmei Wei; Presenter: Rongmei Wei; City College, Chemistry.

The photosynthetic bacterial reaction centers from purple non-sulfur bacteria use light energy to drive the transfer of electrons from cytochrome c to ubiquinone. Ubiquinone bound in the QA site cycles between quinone, QA, and anionic semiquinone, QA•- , being reduced once and never binding protons. In the QB site, ubiquinone is reduced twice by QA•- , binds two protons and is released into the membrane as the quinol, QH2. The network of hydrogen bonds formed in a molecular dynamics trajectory was drawn to investigate proton transfer pathways from the cytoplasm to each quinone binding site. QA is isolated with no path for protons to enter from the surface. In contrast, there is a complex and tangled network requiring residues and waters that can bring protons to QB. There are three entries from clusters of surface residues centered around HisH126, GluH224, and HisH68. The network is in good agreement with earlier studies, Mutation of key nodes in the network, such as SerL223, were previously shown to slow proton delivery. Mutational studies had also shown that double mutations of residues such as Asp M17 and AspL210 along multiple paths in the network presented here slow the reaction, while single mutations do not. Likewise, mutation of both HisH126 and HisH128, which are at the entry to two paths reduce the rate of proton uptake.

**13. Nanoscience in the Braunschweig Group.** ASRC, Chemistry.

Research in the Braunschweig group explores the interface of organic chemistry with biology and materials science to find new solutions to energy, health, and environmental challenges. Supramolecular interactions, nanomaterials, and molecular printing are employed to create functional hierarchical structures from relatively simple starting materials. Emphasis is placed on rational design of target molecules and a fundamental understanding of their assembly and function. Efforts are also made to develop new approaches to increase the efficiency and expand applications of existing technologies. Currently, the laboratory has several ongoing projects. 1) Designing self-assembling supramolecular materials for photophysical applications including energy harvesting and catalysis. 2) Using synthetic carbohydrate receptors with tailorable specificity as antivirals. 3) Employing molecular printing technologies to pattern bioactive and stimuli-responsive features on surfaces. 4) Replicating the structures, and in turn the properties, of animal mucus in synthetic glycopolymers mimicking native polypeptides. 5) Understanding and using mechanical force in the context of chemical processes to expand its applications to rival conventional synthetic methods. Our researchers utilize state-of-the-art synthesis and analytical instrumentation, including electron microscopy. atomic force microscopy, cleanroom nanofabrication, Raman spectroscopy, liquid chromatography, nuclear magnetic resonance, and mass spectrometry. In doing so, we seek to accomplish our mission of meeting society's most pressing material needs in a sustainable and scalable manner. Adventurous students interested in highly interdisciplinary, innovative research are especially encouraged to join the team

**14. Catalytic activity of iron-containing enzymes: Biophysical and Computational Study.** Rupal Gupta and Angelo Bongiorno; CSI, Chemistry.

Transformation of chemical bonds in nature is efficiently performed by enzymes bearing a metal cofactor. Understanding the Chemistry of enzymes is critical for the development of next generation of industrial catalysts capable of performing complex chemical reactions. In this project, we combine biochemical and spectroscopic methodologies along with quantum chemical calculations to gain a deeper insight into the structure and functions of iron enzymes. This research is supported by the National Science Foundation.

**15. Title: Organic, Medicinal, & Natural Products Chemistry @ Hunter College.**
**Presenters:** Wayne Harding, Akira Kawamura, David R. Mootoo, Shengping Zheng; Hunter, Chemistry/ Biochemistry.

This poster presents recent research activities of four organic groups at Hunter Chemistry Department.

**POSTER SESSION 2 - 2:00 pm – 4:30 pm**

## PHYSICS

*PhD Students

**16. Queens College Department of Physics I.** Professors Euclides Almeida, Keaton Bell, Timothy Benseman, Lev Deych; Presenter: TBD; Queens, Physics.

In this poster we present research by Professors Almeida, Bell, Benseman, and Deych . Dr. Almeida's research concentrates on extreme light-matter interactions at the nanoscale, with the goal of creating revolutionary ultrafast, lightweight photonic meta devices with applications in thermal imaging, beam control and nonlinear devices. Dr. Bell's research is focused on discovering planets orbiting white dwarf stars and probing interior structures with stellar pulsations. Dr. Benseman's research is focused on developing compact solid-state terahertz lasers to generate frequencies between 0.3 THz and 2.0 THz, using crystals of high-temperature superconductors. Dr. Deych's research is in theoretical study of optical and optomechanical properties of levitating droplet optical resonators and the photonic molecules based on them.

**17. Queens College Department of Physics II.** Dist. Prof. Azriel Genack, Prof. Mohammad-Ali Miri, Prof. Igor Kuskovsky, Prof. So Takei; Presenter: TBD; Queens, Physics.

In this poster, we present research by Professors Genack, Miri, Kuskovsky and Takei. Dr. Genack studies the propagation of waves in complex structures. Dr. Miri's research spans a broad range of topics in theoretical optics and photonics including nonlinear optics, non-hermitian systems, and inverse problems in optics; his most recent activities are centered around optical computing and analog information processing with light. Dr. Kuskovsky's research is in fundamental properties and applications of so-called type-II semiconductor heterostructures; the current project is focused on investigation of intermediate band solar cells for third generation photovoltaics. Dr. Takei's group theoretically investigates the consequences of strong quantum fluctuations and entanglement in magnetic systems and their potential impact to technology.

**18. The Mu2E Experiment at Fermilab: A High Sensitivity Search for Physics Beyond the Standard Model of Elementary Particle Physics: Charged Lepton Flavor Violation.** Prof. James Popp; Presenter: Prof. James Popp; York, Earth and Physical Sciences.

Mu2e is a world-class experiment! The Muon-to-Electron Conversion Experiment at Fermilab, is a search for a rare and as-yet unseen decay of a muon bound in an atomic Coulomb state directly into an electron and nothing else. Mu2e employs a completely novel charged particle beamline to produce the highest intensity low-energy muon beam to trap muons in orbits about Al nuclei and monitor the endpoint of the decay electron energy spectrum for the unambiguous sign of an excess of 105 MeV electrons in a zero-background experiment. The particle tracker is a one-of-a-kind, leading edge thin-materials technology gaseous detector that lies in a uniform 1T magnetic field, and contained in a large high-vacuum chamber. The Mu2e

Experiment has about two more years of construction remaining: graduate students have the opportunity to get in on the ground floor of this important US Dept of Energy project.

**19. Anisotropic Optical Conductivities of Model Topological Nodal-line Semimetals.** Sita Kandel*, Dist. Prof. Godfrey Gumbs, Prof. Oleg L. Berman; Presenter: Sital Kandel; Hunter, Physics & Astronomy. With the use of simple model we investigated the optical conductivity of nodal line semimetal (NLSM) whose crossing of the conduction and the valance bands near the Γ point in the ( K_x , K_y) plane of the first Brillouin zone can be adjusted by a parameter α. When α=0, these bands touch each other along a continuous close loop but the opening of a band gap corresponding to finite values of α and the varying of the carrier concentration can be adjusted by placing the NLSM in a suitably configured field effect device. This provides a tunable semiconductor gap around Γ and the valance and conduction bands can meet a pair of points within the Brillouin zone. The optical conductivity of such a NLSM is calculated using the Kubo formula with emphasis on the spectral weight redistribution, deduced from appropriate Green's functions, brought about by changes in gap and chemical potential due to modifying α. We derived closed-form analytic expression for the longitudinal and transverse components of the optical conductivity for these model system of NLSM and compare results for chosen α and chemical potential.

**20. Biomedical Photonics: Physics, Computing & Biomedicine.** Prof. Min Xu; Presenter: Prof. Min Xu; Hunter, Physics & Astronomy.

Biomedical photonics is an interdisciplinary field of physics, computing, and biomedicine. This poster will provide a survey of the current work at the Biomedical Photonics Laboratory (BPL) @ Hunter College, including remote spectroscopy, quantitative microscopy, and various computing strategies to address needs in biomedicine. We will also showcase how needs drive innovations.

**21. Linear Optical Implementations of Quantum Communication Protocols.** Pranjal Agarwal*, Saad Bezoui, Prof. Janos A. Bergou; Presenter: Pranjal Agarwal; Hunter, Physics & Astronomy.

We present a straightforward physical implementation of the Bennett two-state and the Barnett three-state protocols in terms of single-photon multiport interferometry using linear optics only. Some general conclusions will be drawn about the general feasibility of quantum networks using linear optical implementations.

**22. Research at the ASRC Photonics Initiative.** Dist Prof. Andrea Alu, Prof. Matthew Sfeir, Prof. Gabriele Grosso; Presenter: Dr. Diana Strickland; Graduate Center, Physics.

An overview of research by the Photonics initiative at the Graduate Center's Advanced Science Research Center.

**23. Interdisciplinary Research at the ASRC.** Dist. Prof. Andrea Alù, Prof. Matthew Sfeir, Prof. Gabriele Grosso, Dr. Viktoriia Rutckaia, Prof. Younes Ra'di, Dr. Diana Strickland; Presenter: Dr. Diana Strickland; Graduate Center, Physics.

An overview of interdisciplinary research by the Photonics initiative at the Graduate Center's Advanced Science Research Center.

**24. Raman scattering multipole moment of OAM light interaction in organic liquids.** Sandra Mamani*, Dist. Prof. Robert R. Alfano; Presenter: Sandra Mamani (CCNY Electrical Engr doctoral student); CCNY, Physics.

Spontaneous Raman spectra using Orbital angular momentum (OAM) and Spin angular momentum (SAM) from organic liquids with circularly polarized Laguerre-Gaussian (L= 1 and 2) were experimentally observed. For example, methanol shows changes for circularly polarized OAM Raman ranging from 4.5% to 66.8% for different vibrational modes. The relevant enhancement and decrease in Raman intensity from the studied liquids are attributed to the matching up of the multipoles from the vibrational orbital structure from electron clouds symmetry with the multipoles of the OAM light. In summary, we show that the use of OAM and SAM offers a new approach for larger changes of the Raman effect in contrast to with other methods.

**25. Novel Quantum Materials and Nanostructures.** Prof. Lia Krusin-Elbaum
Dr. Xiaxin Ding, Afrin Nahar Tamanna*, Ayesha Lakra*, Entela Buzi*; Presenter: Dr. Xiaxin Ding ; CCNY, Physics.

In our Quantum Materials group (KrusinLab) at the Center for Discovery and Innovation at the CCNY we design new quantum materials and nano-hetero-structures, and study their behaviors at ultralow temperatures (mK range) and high magnetic fields. Our research explores materials designs that could enable harvesting quantum modes for energy sustainability in nanoelectronics, spintronics and in game-changing quantum computing. We focus on topological materials (TIs) □ a new class of quantum solids with robust spin-helical gapless surface states formed by topological effects. These states can host chiral superconductivity and quantized Hall effects that support dissipation-free transport of charge. We have discovered many new exotic topological phenomena and developed new techniques for tuning quantum transport. Among them is an unusual Quantized Anomalous Hall Effect in intrinsic magnetic TIs and invention of a novel electronic tuning of TIs through hydrogenation. Our most recent discovery is hydrogen-tuned magnetic textures and orders in a class of topological magnets important for nanospintronics. Currently, we are developing new TI nano-architectures for exploring proximal magnetism and superconductivity in hybrid devices. We are a partner in the CCNY-Columbia NSF-MRSEC and the NSF-CREST at the CCNY. To learn more about our research, you are welcome to visit our websites http://krusinlab.ccny.cuny.edu; https://HCQM.ccny.cuny.edu.

**26. Laboratory for Nano and Micro Photonics.** Dr. Biswajit Datta, Mandeep Khatoniar*, Rezlind Bushati*, Prathmesh Deshmukh*, Dr. Sitakants Satapthy, Dr. Ravindra Kumar Yadav, Dr. Florian Dirnberger, Prof. Vinod Menon; Presenter: Dr. Biswajit Datta; CCNY, Physics.

Research in the Laboratory for Nano and Micro Photonics (LaNMP) can be best summarized as exploration of light-matter interaction at the nanoscale. We are interested in exploring emergent material properties (classical and quantum) that arise when matter is subjected to artificially engineered electromagnetic environments. The goal is to develop a largely unexplored strategy for realizing programmable matter based on coherently combining material excitations with light – realizing half-light half-matter quasiparticles. We hope to answer fundamental questions related to ultimate limits of controlling light-matter interaction and apply these concepts in applications such as quantum simulators, polariton circuits, energy harvesting, ultrafast light emitters, and catalysis.

**27. From Symmetric Building Blocks to Neural Synchronization in the Connectome.** Dist. Prof. Hernan Makse, Prof. Manuel Zimmer, Pedro Augusto, Dr. Kerem Uzel, Dr. Matteo Serafino, Bryant Avila*; Presenter: Dr. Kuang Liu ; CCNY, Physics.

We develop a theoretical analysis toolbox that identifies various forms of symmetries in the neuronal network of the *C. elegans* worm. Our central hypothesis is that symmetries of the network are important for synchronizing neuronal population activity. In our approach, symmetry features uncovered in our previous study called permutation symmetries form the automorphism group of the graph; a collection of neurons that when swapped preserve the connectivity matrix of the network. Additionally the connectivity matrix of the connectome is used to partition neurons into groups with "balanced coloring" where connections from one group into a neuron of another group depends only on the pair of groups chosen. Graph theory indicates that these quantities predict the cluster synchronization of dynamics among groups of neurons observed experimentally. We verify cluster synchronization in the connectome by ODE simulations of interacting neurons and compare these to experimentally recorded population activity in the motor system.

**28. II-VI Semiconductor nanostructures for photonic applications.** Ahamed Jubair*, Dr. Vladimir Kartazaev, Candice Forrester*, Prof. Maria C. Tamargo, Prof. Swapan K. Gayen ; Presenter: Ahamed Jubair; CCNY, Physics, IDEALS.

Semiconductor nanostructures (such as, II-VI semiconductor heterostructures (SHS), III-V SHS, coupled II-VI and II-V semiconductor structures) are engineered materials with unprecedented structural, electronic and photonic properties. The molecular beam epitaxy (MBE) laboratory at CCNY is a pioneer in synthesis of these novel structures and study of their structural and spectroscopic properties as well as potential device applications. The presentation will provide illustrative examples of some heterostructures, and their potential applications in developing photonic devices such as semiconductor disk lasers (SDLs) and intermediate band solar cells (IBSCs). These research efforts are parts of much wider research activities on nanostructured materials organized as the NSF CREST Center for Interface Design and Engineered Assembly of Low-dimensional Systems (IDEALS II) at CCNY. An overview of IDEALS II research activities and opportunities will be presented.

**29. Faculty and Research Activities At Brooklyn College I.** Faculty of Physics Department ; Presenter: Prof. Nicolas Giovambattista; Brooklyn College, Physics.

Overview of the research activities and facilities available at the Physics Department of Brooklyn College, poster I. Our faculty research interests include condensed matter (eg, semiconductors and photonic materials), liquids, glasses, materials modelling, quantal density functional theory, environmental science, and physics education. The department hosts high school, undergraduate and graduate student researchers, and runs major, minor and MA programs in physics.

**30. Faculty and Research Activities At Brooklyn College II.** Faculty of Physics Department ; Presenter: Prof. Sophia Suarez; Brooklyn College, Physics.

Overview of the research activities and facilities available at the Physics Department of Brooklyn College, poster II. Our faculty research interests include condensed matter (eg, semiconductors and photonic materials), liquids, glasses, materials modelling, quantal density functional theory, environmental science, and physics education. The department hosts high

school, undergraduate and graduate student researchers, and runs major, minor and MA programs in physics.

**31. Overview of Research in the Department of Physics and Astronomy at Lehman College - I.** Presenter: Prof. Dan Kabat; Lehman, Physics & Astronomy.

We give an overview of research in the Department of Physics and Astronomy at Lehman College. Areas of strength include condensed matter theory, high energy theory, quantum optics, astronomy, astro-particle physics and particle phenomenology.

**32. Overview of Research in the Department of Physics and Astronomy at Lehman College - II.** Presenter: Prof. Dan Kabat; Lehman, Physics & Astronomy.

We give an overview of research in the Department of Physics and Astronomy at Lehman College. Areas of strength include condensed matter theory, high energy theory, quantum optics, astronomy, astro-particle physics and particle phenomenology.

**33. TBA**; Staten Island, Physics.

**34. TBA**; Staten Island, Physics.

**35. TBA**; City Tech, Physics.

**36. TBA**; City Tech, Physics.

**Poster Session 1, Biochemistry and Biology**

| Faculty Member | | Poster Number |
|---|---|---|
| Ayata | Pinar | 24, 25 |
| Brumberg | Joshua C. | 28 |
| Contel | Maria | 1, 30 |
| Dennehy | John | 23 |
| Desamero | Ruel | 14 |
| Gallego-Delgado | Julio | 18 |
| Gallicchio | Emilio | 7 |
| Greer | Alexander | 5 |
| Gupta | Rupal | 9, 10, 13 |
| Harding | Way | 17 |
| Ikui | Amy | 3, 20 |
| Jiang | Xin Yin | 6 |
| Kawamura | Akira | 17 |
| Loverde | Sharon | 11 |
| Mano | Itzhak | 31 |
| Meléndez | Alicia | 19 |
| Mingote | Susana | 26, 27 |
| Mootoo | David R. | 17 |
| Murelli | Ryan | 2 |
| Parra | Lucas C. | 32 |
| Poget | Sebastien | 12 |
| Quadri | Luis | 4, 21 |
| Samuni | Uri | 15, 16 |
| Savage-Dunn | Cathy | 29 |
| Schvarzstein | Mara | 8, 33 |
| Vuong | Bao Q. | 22 |
| Zheng | Shengping | 17 |

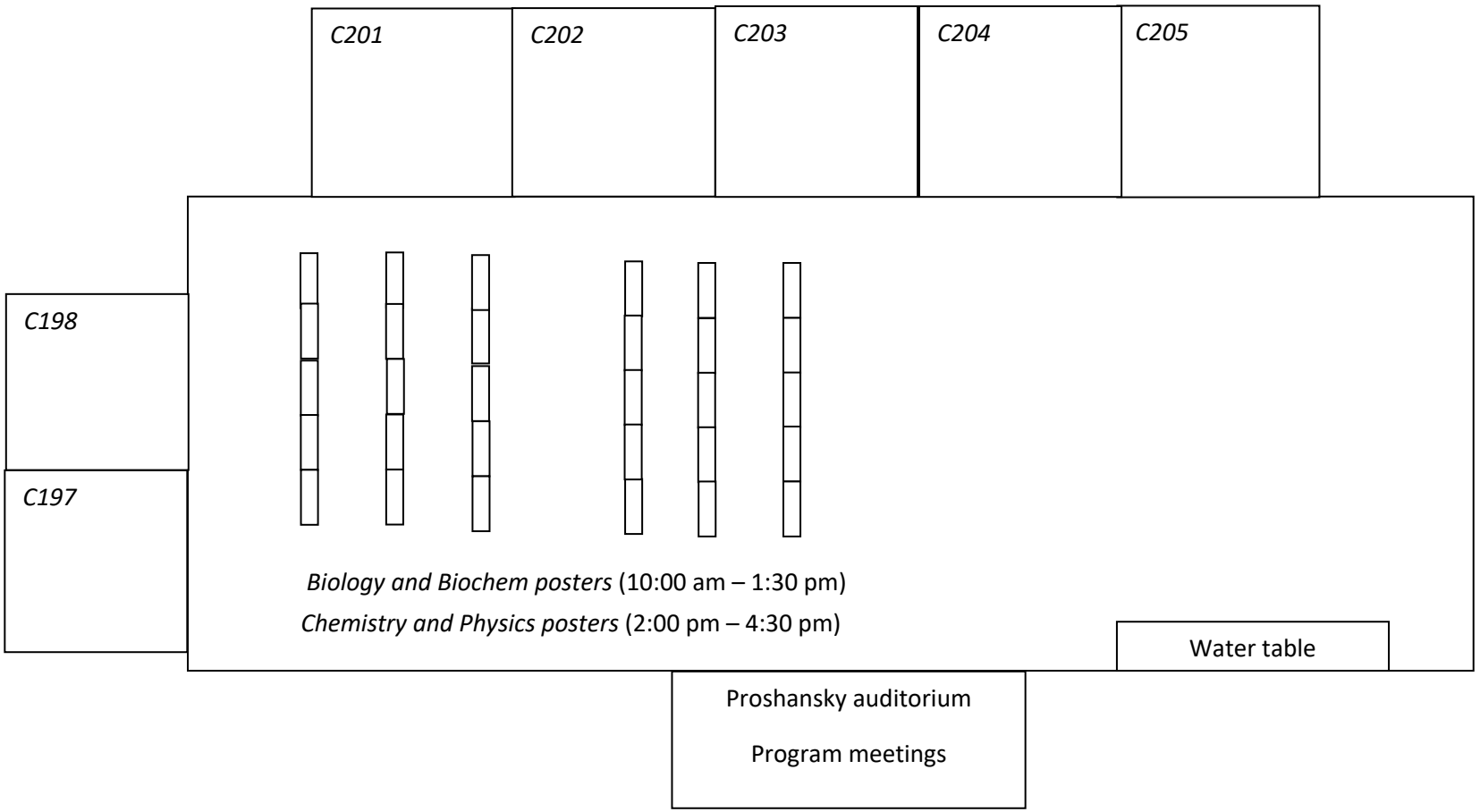
**Poster Session 2, Chemistry and Physics**

| Faculty Member | | Poster Number |
|---|---|---|
| Alfano | Robert R. | 24 |
| Almeida | Euclides | 16 |
| Alù | Andrea | 22, 23 |
| Bell | Keaton | 16 |
| Benseman | Timothy | 16 |
| Bergou | Janos | 21 |
| Bongiorno | Angelo | 8, 14 |
| Braunschweig | Adam | 13 |
| Choi | Jun Yong | 9 |
| Contel | Maria | 5 |
| Deych | Lev | 16 |
| Gayen | Swapan K. | 28 |
| Genack | Azriel | 17 |
| Giovambattista | Nicolas | 29 |
| Greer | Alexander | 1 |
| Grosso | Gabriele | 22, 23 |
| Gumbs | Godfrey | 19 |
| Gunner | Marilyn | 12 |
| Gupta | Rupal | 14 |
| Harding | Wayne | 15 |
| Hu | Qiao-Sheng | 7 |
| Jin | Shi | 7 |
| Kabat | Dan | 31, 32 |
| Kawamura | Akira | 15 |
| Kruk | Michal | 7 |
| Krusin-Elbaum | Lia | 25 |
| Kuskovsky | Igor | 17 |
| Loverde | Sharon | 8 |

**Poster Session 2, Chemistry and Physics**

| Faculty Member | | Poster Number |
|---|---|---|
| Lyons | Alan | 8 |
| Makse | Hernan | 27 |
| Menon | Vinod | 26 |
| Miri | Mohammad-Ali | 17 |
| Mirkin | Michael | 10 |
| Mootoo | David R. | 15 |
| Murelli | Ryan | 6 |
| Peet | Ralf | 7 |
| Poget | Sebastian | 4 |
| Popp | James | 18 |
| Ra'di | Younes | 23 |
| Raja | Krishnaswami | 7 |
| Sfeir | Matthew | 22, 23 |
| Shew | Chwen-Yang | 8 |
| Stark | Ruth E. | 2, 3 |
| Suarez | Sophia | 30 |
| Takei | So | 17 |
| Wang | Chen | 11 |
| Xu | Min | 20 |
| Zheng | Shengping | 15 |
| Zhou | Shuiqin | 8 |
| Zimmer | Manuel | 27 |

# Floor Plan


C201
C202
C203
C204
C205
C198
C197
Biology and Biochem posters (10:00 am – 1:30 pm)
Chemistry and Physics posters (2:00 pm – 4:30 pm)
Water table
Proshansky auditorium
Program meetings