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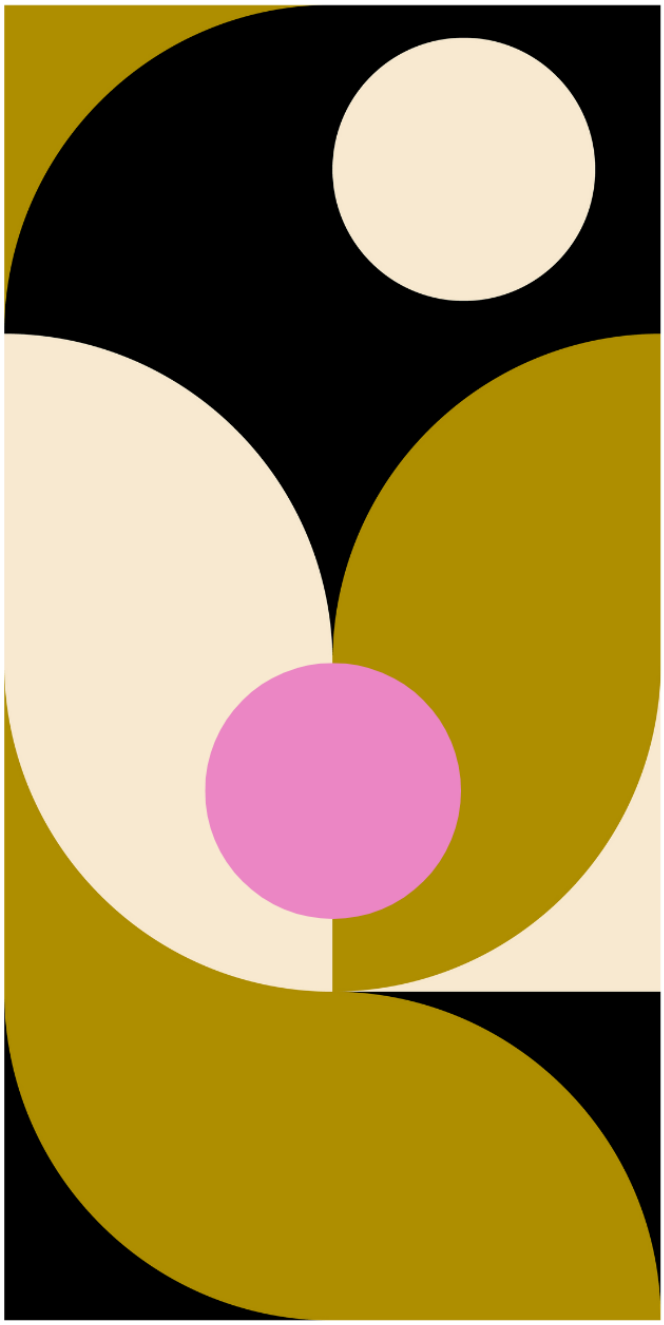

SUMMER 2024

A P/NP-Complete Classification of the Tait-Rolfsen Knot Table

Karomat Alimova, Renata Karpenko, Nyla Lawrence, Fatima Rahimi, Bermet Sultangazieva, and Tamana Sultani
Advisor: Robert McGrail

The goal of this project is to determine the nature of the CSPs over the Tait-Rolfsen knot table, the first 250 knots. At this time the only known polynomial time knot is the Unknot. Most of the rest of the knots of this table have been shown to be NP-Complete. This was achieved for each of these knots by coloring by an NP-Complete quandle. The quandle used are a set of so-called Sharac quandles.

Scattered Light in Gravitational-wave Detectors: The Good, the Bad, and the Noisy

Kincade Avery, Emma Derrick, Belén Gutiérrez-Peña, Prottoy Samir, Hank Zhang, Danielle Darling, and Caden Hubbell
Advisor: Antonios Kontos

The Laser Interferometer Gravitational-Wave Observatory (LIGO) uses a technique known as laser interferometry to detect gravitational-waves (GW) produced by astrophysical events such as black hole mergers and binary neutron star systems. These GW detectors require optical coatings that produce very little noise from both optical and mechanical losses. Our research focused on a) developing an improved experimental setup and procedure for characterizing small defects within mirror coatings using scattered light, b) running complementary measurements using a set-up at California Institute of Technology (CalTech), c) using a Spatial Light Modulator (SLM) to aid in laser beam tracking, and d) running light simulations for use in the future Cosmic Explorer GW interferometer.

Shedding Light on C-N Bond Formation: Visible Light Photocatalysis of N-Aminopyridinium Ylides

Zachary P. Burmeister, Asher Longdon-Stewart, and Olivia Nguyen

Advisor: Emily McLaughlin

Carbon-nitrogen (C-N) bonds are ever-present in both natural and unnatural small molecules. Our research group is interested in developing new synthetic methods to create two C-N bonds, simultaneously, to produce substituted aziridine products. The feasibility, scope, and evidence of a photocatalytic energy transfer mechanism for aziridination of alkenes using bench-stable, N-aminopyridinium ylides are studied. Our group uses a visible light-driven process where a metal photocatalyst alongside blue LED light promotes the direct aziridination of substituted alkenes (C=C) with N-aminopyridinium ylides. Previous literature reports, along with data collected from our lab suggest that highly reactive nitrenes can be generated from both azidoformates and N-aminopyridinium ylides using visible light catalysis, leading to the formation of aziridines in the presence of alkenes.To better understand the nature of the potential nitrene intermediate, the effects of substitution and stereochemistry of the alkene and resulting aziridine products are observed through NMR studies.

Inhibition of DHFR Enzyme by Ruthenium Metal Complexes

William Chang, Freddy Coronel, and Luke Collins
Advisor: Swapan Jain

Cancer treatment has long targeted the folic acid pathway, where dihydrofolate reductase (DHFR) catalyzes the reduction of dihydrofolate to tetrahydrofolate using NADPH, a critical process for DNA synthesis and cell proliferation. In our research, we explored the potential of ruthenium-based complexes (Ru79, Ru80, Ru81), synthesized by the Anderson Lab, to inhibit DHFR activity, aiming to identify novel chemotherapeutic agents with reduced cytotoxicity. To achieve this, we synthesized the DHFR enzyme through protein overexpression and purification, followed by DHFR activity assays to evaluate binding affinity and enzymatic effects. Additionally, we conducted fluorescence quenching and isothermal titration calorimetry (ITC) to assess the strength of the interaction between DHFR and the ruthenium-based compounds. Ru79, Ru80, and Ru81 showed promise as inhibitors of DHFR enzymatic activity, significantly reducing enzyme activity, suggesting strong binding affinity and potential therapeutic efficacy. Other ruthenium-based complexes, including Ru-cymene, Ru-imidazole, and Ru-benzene, were also tested but showed minimal inhibition, confirming the drug's role in enzyme inhibition. Methotrexate was used as a positive control, effectively inhibiting DHFR activity and validating our experimental design. These findings highlight the potential of ruthenium-based compounds in cancer

therapy, warranting further investigation into their inhibitory mechanisms and therapeutic viability. Future work will focus on testing additional ruthenium complexes and replicating these studies to confirm our results.

Enhancing Direct Laser Writing: Innovations in Fluorescent Resins, Circuitry, and Stage Control Software

Sophie Cherif, Sahil Husaini, Jacqueline Lagunes, Katie Lowney, and Harper Serringer
Advisor: Christopher LaFratta

Two-Photon Polymerization (TPP), or direct laser writing, occurs when a molecule absorbs two photons simultaneously, initiating a polymerization reaction. We use near IR light, at 800 nm from a Ti-sapphire laser and an inverted optical microscope. The beam is focused into a drop of resin in between two pieces of glass. The sample is moved on a computer-controlled stage enabling 3D patterning with sub-micron resolution. The system was used for an ongoing metrology project and for a new project involving microneedles for drug delivery. For the benefit of both projects we worked to make technical improvements to the system. The four most significant improvements to the process were: a program to convert CAD structures, using fluorescently doped resins for easier sample imaging, and incorporating a GaAsP Photodiode to monitor the laser power, and creating a program to account for the unevenness of the stage.

Community Sciences Lab: The Story of Benner Road

Glorianne Couey, Shirley Dong, Bisan Safi, Albright Tuah, and Fuhua Feng Wu
Advisors: Elias Dueker & Gabriel Perron

The present study investigated the potential factors of damage to the backyard of residents living on Benner Road, Red Hook, and provided them with actual scientific data from our research. The surveyed residents have reported increased backyard flooding, persistent sewage odor, and unstable ground near the stream at site 6 of the Saw Kill. The Saw Kill is a tributary of the Hudson River and a source of drinking water for Bard College. We, the Bard Community Sciences Lab (CSL), have researched across the Saw Kill watershed and collaborated with the community to answer the question: Has climate (precipitation changes), or the increased wastewater treatment by the town of Red Hook changed the water quality at site 6 or affected the reported backyard issues. We analyzed local historical weather datasets and tested for temperature, conductivity, and dissolved oxygen weekly throughout the summer. We discovered changes in water quality at site 6 and through the Sawkill watershed data from 2016 to present. As a result, we perceived and predicted that the increased wastewater treatment effluent is related to the backyard issues. At present, we are continuing to conduct both biological and chemistry analysis of the water samples both above and below site 6 and the Red Hook Wastewater treatment effluent area to gather more scientific evidence of

water quality and support the local community in addressing any potential or future water issues.

Equational Unification over the Theory of the Involutory Quandles

Volodymir Didur, Renata Karpenko, and Tamana Sultani
Advisor: Robert McGrail

This poster explores the unification problem over involuntary quandles. First, we demonstrate that unification can be reduced to matching. Second, we have some partial results which determine certain terms that cause this problem to be solvable. In particular, we show that the relative number of variables vs constants in an ex- pression may determine whether the matching is possible. If the number of variables present in expression exceeds the number of constants then there is a matching.

Nanolab

Zainab Hashimi, Jiyu Kwon, Lauren Mendoza, Ethan Young, and Swati Kanojia
Advisor: Paul Cadden-Zimansky

Graphene, a 2D material just one atom thick, is renowned for its strength, lightness, high electrical and thermal conductivity, flexibility, large surface area, and unique quantum effects. These properties have led to extensive research. Our study aims to explore how adding structural features to flat graphene affects its electric properties by using laser writing to create resin structures on a flat substrate and suspending graphene over them to observe the changes.

Atomic Pair Distribution Function Analysis of the Structural Evolution during CsPbX3 Nanocrystal Halide Exchange

Meherin Hossain

Advisor: Matthew Greenberg

Halide exchange is a popular strategy to tune the photophysical properties of CsPbX 3 perovskite nanocrystals after synthesis. In this research, we model the atomic structural changes during halide exchange reactions using atomic pair distribution function (PDF) analysis for Br - → Cl - , Br - → I - halide exchange reactions. Real space modeling of the PDF provides insights into the structural stability of mixed-halide phases and the structural evolution during halide exchange. Our results reveal varying degrees of atomic disorder and phase stability as a function of halide composition.

Equipartitioned Colored Tverberg Tuples

Emily Huang, Jasper Miller, and Daniel Rose-Levine
Advisor: Steven Simon

This project expands on known results in Discrete Geometry using unexpected connections with Equivariant Topology. Problems regarding points and shapes in affine space can be reframed through the lens of continuous maps from simplicial complexes to $\mathbb{R}^d$, a surprisingly fruitful approach which allows for the application of an array of useful topological theorems.

The central result this project revolves around is known as Tverberg's Theorem, a result regarding the convex hull of points in $\mathbb{R}^d$, or the "simplest" shape that includes all the points.

Our work involves generalizing this result and other related results using tools of Equivariant
Topology.

Using Geometric Shapes to Count and Classify Types of Quads

Diba Imran, Yueer Lin, Husna Manalai, and Zifan Xu
Advisor: Lauren Rose

Quads is a card game similar to SET, with 64 cards. Each card displays one of 4 symbols appearing 1-4 times, in one of four colors. Players try to find “quads” – sets of 4 cards where the symbols either have the same number, color or shape, different numbers, colors or shapes, or a pair of numbers, colors or shapes. This structure allows for various types of quads and a certain layout of the deck allows for various shapes to form. We used Geometric shapes to visualize types of quads and then combinatorics formulas to classify quads of each type.

RASCALL:
Approximating Spectral Data for Molecules

Yashar Khan
Advisor: Clara Sousa-Silva

RASCALL (Rapid Approximate Spectral Calculations for All) is a computational approach to approximating spectra for any given molecule. It uses experimental measurements and structural chemistry to provide the spectra for the prompted molecules. It relies on the predictability of specific functional groups and simulates spectra based on the estimated contribution that the particular functional groups make to the molecule's spectrum. While RASCALL has numerous applications, its functionality was restricted to the command line and within a Python virtual environment. To improve usability, I focussed on creating a web application for RASCALL, ensuring that a user would not have to be familiar with the intricacies of git or the command line to use the software. This involved improving RASCALL's existing codebase and creating an entirely new plotting and spectral analysis algorithm that would work when implemented directly onto a web server. A Flask application was then created, where users can easily prompt and generate spectra for any molecule almost instantly, while also being able to find information about any molecule in RASCALL's database.

Unification Problem for Idempotent, Right Quasi Groups Is Decideable

Nyla Lawrence and Fatima Rahimi

Advisor: Robert McGrail

This poster presents a computer program in SWI-Prolog which performs equation unification on two terms over the theory of idempotent right quasi groups. Moreover, it provides all substitutions that support this process, as well as the computed answer substitution. It uses a term rewriting system (TRS) for idempotent right quasi groups in order to support the narrowing approach to unification. This approach to narrowing is terminating and hence always produces a unifier if it exists and reaches failure when it does not exist. Hence, it demonstrates that equation unification of right idempotent quasi groups is decidable. Moreover, SWI-Prolog's backtracking will ensure that all possible unifiers can be found.

Visible Light Photocatalysis for the [2 +2] Cycloaddition of Indole Derivatives and Olefins

Amirat Maiyegun and Max Schultz

Advisor: Emily McLaughlin

Photocatalysis is a chemical reaction that uses light to activate a substance. Photocatalysis replicates the natural photosynthesis process by transforming solar energy into required chemical energy, making it a viable alternative and sustainable approach to dealing with the worldwide environmental issue (Fujishima et al., 2007). A [2+2] photocycloaddition refers to a reaction where two double bonds from different molecules directly add together to form a ring made up of four carbon atoms (called a cyclobutane ring), essentially turning the two double bonds into connected four single bonds. In our experiment, we used photocatalysis to perform a [2+2] cycloaddition involving a compound called 3-acetyl-1-benzoylindole, mixed with various alkenes (a type of molecule), solvents, and different ingredient ratios. We also used an iridium-based catalyst to help the reaction along, all under regular visible light. The goal was to find the best combination to produce the most product efficiently.

Exploring the Catalytic Power of Acyltransferase from *Mycobacterium Smegmatis*

Gwenn Malick

Advisors: Swapan Jain & Emily McLaughlin

New biocatalytic enzymes are being discovered and celebrated for their ability to lower reaction rates and yield high enantiomeric excess. Traditional chemical catalysis in synthetic chemistry often employs metals, many of which are dwindling on our planet, whereas enzymes and biological organisms, which are regenerative and accessible, are worthy alternatives to metal catalysis. In this work, we focus on the acyltransferase enzyme from *Mycobacterium smegmatis* (MsAct). MsAct has been shown to favor condensation reactions over hydrolysis in aqueous conditions due to its hydrophobic pocket, making it a promising candidate for a wide range of industrial applications. The enzyme has been previously reported to perform trans-esterification, amidation, trans-amidation, and per hydrolysis reactions exceptionally well, and can withstand a wide range of pH (6-10) environments compared to that of other known biocatalysts. Herein we report our research on broadening the substrate scope of amide and ester formation with wild-type MsAct, exploring its enantioselectivity and its activity towards more polar substrates.

Orienting of Attention is Location-Based for Both Arrows and Eye-Gaze Cues

Aida Malikova, Polina Rafailova, and Rebecca Wintjen
Advisor: Thomas Hutcheon

Humans reflexively follow the gaze of others, a phenomenon demonstrated in the lab using the gaze-cueing paradigm (Driver et al., 1999; Hutcheon et al., 2024). These joint attention mechanisms are essential for developmental, social and cognitive processes. The shared attention is crucial for language acquisition in children, social interaction, and social learning. Research in the area will allow to improve current educational practices, provide insights into social cognition, and enhance human-computer interaction.

Marotta et al. (2012) investigated whether arrow or eye-gaze cues drive different types of attentional selection in a gaze cueing paradigm. They found a double dissociation within the same task with arrow cues producing a pure object-based effect, and eye-gaze cues triggering a specific location-based effect. We attempted to replicate Marotta et al. (2012) findings and extend them to real-life contexts, using schematic faces and real-life objects (Christmas tree).

Three within-subjects experiments using the gaze-cueing paradigm were conducted. Participants had 16 practice trials and 256 experimental trials. The SOA between the cue and

target onset was 300 msec. Cue type (arrow, face) and target location (up, down, right, left) were randomized within each block of trials.

We found a statistically significant specific location-based effect for both eye-gaze and arrow cues in all three experiments. In Experiments 1 and 3, an object-based effect was found for arrows as cues. This effect was not replicated in Experiment 2, where schematic faces were employed as stimuli. It suggests that while faces may be processed as holistic objects, the presence of an atypical target, such as an 'X' on a face, may attract greater attentional resources, resulting in a specific location-based effect.

Our findings suggest distinct attentional mechanisms for arrow cues. It seems that an individual’s attention is first directed at a specific location pointed at by an arrowhead before spreading across the entire object. This mechanism highlights the dynamic nature of attentional selection when processing directional cues. Future studies could further explore this process using eye-tracking technology to capture more detailed patterns of attentional shifts.

Venus: A Spectral Mystery

Lauren Mendoza
Advisor: Clara Sousa-Silva

Claims of the detection of phosphine in the atmosphere of Venus have recently sparked interest in and ignited debate around its atmosphere because of phosphine's status as a biosignature. These claims also motivated a proposal to use the TEXES spectrograph mounted on the NASA Infrared Telescope Facility located on Hawaii's Mauna Kea mountain to produce an infrared spectrum of the clouds of Venus from wavenumbers 1115 cm-1 to 1123 cm-1 on June 30th and July 2nd, 2021. This wavenumber range has not been studied prior and is distinct for its lack of CO2 transitions, increasing the likelihood of detecting less abundant molecules in Venus's atmosphere such as phosphine, ozone, and ammonia which are relatively active in this infrared region. Here, we present the null results from spectral analysis of the TEXES observation data via both the unprocessed, Level 2 FITS and an average of the aforementioned spectra after sky-division.

Synthesis, Structures, and Photophysical Properties of Pt(II) and Pt(IV) Compounds with Bis-chelate N^S Thioureate Ligands

Ben Murray

Advisor: Matthew Greenberg

Platinum(II) and platinum(IV) compounds with bis-chelate N^S thioureate ligands were prepared by the reaction of N,N,N'-trisubstituted thioureas (N,N=methyl, N'=aryl) with Pt(SMe2)2Cl2 and [Pt2Me4(μ-SMe2)2]. Newly synthesized platinum compounds were characterized by NMR spectroscopy, elemental analysis, high resolution mass spectrometry, and single crystal X-ray diffraction. UV-vis absorbance and photoluminescence measurements were performed on newly synthesized complexes, as well as structurally related ligands. DFT and TD-DFT calculations were performed, and results compared to the observed spectroscopic properties of the newly synthesized complexes. The high temperature thermolysis of Pt(II) and Pt(IV) complexes to nanoparticles in oleylamine was characterized by SEM and X-ray scattering measurements

Synthesis and Characterization of Pt(II) Compounds with Isocyanide Ligands

Everest Oppenheimer, Teeka Duplessis, Ryan H. Lum, and Zainab Aleem

Advisor: Craig Anderson

Cyclometalated Pt(II) compounds with various isocyanide ligands were synthesized and characterized. Two C^N chelate imine ligands were utilized in order to facilitate C-H orthometalation with the tetramethyl platinum precursor Pt2Me4(μ-SMe2)2. Sequentially, the dimethylsulfide ligand was easily substituted with various isocyanides. The target Pt(II) compounds thus contain one chelate C^N imine ligand, a methyl ligand, and an isocyanide in the coordination sphere. The compounds' photophysical properties (absorbance, emission, excited state lifetimes, and photoluminescence quantum yields) were measured and studied as a function of their ligand architecture.

Decision Support Tool for the Anaerobic Digester

Izzi Popolizio
Advisor: Beate Liepert

My research during Bard Summer Research Institute was to examine the feasibility of the implementation of anaerobic digestion (AD) at Bard College, in order to improve food waste management with the potential to generate renewable energy. Bard College seeks sustainable solutions to many environmental problems, one of the most important being the challenge of food waste. Understanding the AD system, with its practical challenges and potential huge positives are crucial for this goal. During the course of my work, I assessed the current composting system, along with the potential benefits of adding AD to the current system. I then addressed the key challenges during the implementation process. Methods included analyzing energy and methane data, creating a cost-benefit analysis, and formalizing a total repair list for the Bard College AD system. Though the project shows potential for positive environmental impacts, there are many challenges that stand in our way in order for the system to be operational, including lack of expertise at Bard College, safety concerns, and uncertainty regarding biogas usage. The people with the expertise that we need in order to fix and maintain the complex system all live in Washington State, with limited resources to help us consistently on the ground here in New York. My research has contributed to the understanding of small scale AD on a college campus, highlighting the potential and the challenges that still face

similar projects. Successful operation would require further investment into the system, more than was already used. Before being operational we need expertise on the ground, development of extensive plans for biogas, day to day operations, and fertilizer application plans. My research has concluded that there is a positive outlook of the project, but moving forward the responsibility is in the hands of the company to maintain and aid in implementation of their older anaerobic digestion systems.

Progress Towards Synthesis of a Chelating Diisocyanide Ligand

Alleisha Romain

Advisor: Matthew Greenberg

Strong field ligands are essential to the rational design of luminescent transition metal complexes. Among strong field ligands, chelating ligands which form two coordination bonds to a single metal ion enhance the stability and rigidity of the complex. This can reduce non-radiative decay pathways responsible for deactivating the excited state, resulting in more efficient light emission. Here, we pursued the synthesis of a m-terphenyl based chelating diisocyanide ligand for use in the preparation of luminescent transition metal complexes.

The 1930s Kazakh Famine: Intergenerational Trauma in the 2nd and 3rd Generations of Survivor Families

Alua Samat

Advisors: Regatta Bilali and Michelle Twali

The 1930s Kazakh Famine, also known as Asharshylyq, was one of the most disastrous man-made famines in Kazakh, and Soviet, history. It unfolded between 1931-1933 due to the forced collectivization and sedentarization policies towards the pastoral nomadic Kazakh population, and captured the entire region of Kazakh SSR. It was silenced during the following 60 years and had caused an identity shift in the Kazakh population that had to become fully sedentary within 2 years. Even to this day, the effects of the famine remain understudied. Drawing on the previous historical, psychological, and regional studies findings, this proposal aims to address the research gap in the potential psychological effects that the famine had on the 2nd and 3rd generations of the Kazakh famine survivor families, in relation to intergenerational trauma. Using the Historical Intergenerational Trauma Transmission model by Bekes & Starrs (2024), I propose that a study would reveal that the older second & third generation representatives would score higher on family and offspring vulnerability than younger third generation members; however, family & offspring vulnerability will be higher in the generations whose families migrated and live outside of the USSR, compared to those who stayed in the

USSR, due to the suppression of the famine recall in the Soviet Union.

Spirographs, Knots, and Complex Hypersurfaces

Sebastian Sargenti, Niko Singband, and Thanasis Kostikas
Advisor: Charles Doran

The Spirograph is a toy that allows users to create elaborate spiral patterns using a combination of two gears which spin around each other. The resulting curves are examples of epitrochoidal and hypotrochoidal curves.

These curves have a long history dating back to 225 BCE and a well known parametric form. However, information other than this is difficult to find and spread out. Our goal was to better study these curves and collect this information into one source. It turns out, that Spirograph curves are algebraic objects — ie they can be represented as the zero set of polynomials, always of relatively high degree. We examined these trochoidal curves from the viewpoint that they are fundamentally algebraic objects and the resulting consequences of this.

An Automated Approach to Nanocrystal Structure Solution and Refinement Using the Real-Space Atomic Pair Distribution Function

Farman Hossain Sayem and Nadia Mehjabin
Advisor: Matthew Greenberg

This research aims to automate the process of nanocrystal structure solution and refinement from X-ray atomic Pair Distribution Function measurements (PDF). Traditional phase analysis using XRD in reciprocal space is complicated by the broad peak shapes for nanocrystalline materials. A comprehensive algorithm has been developed to retrieve CIF data from the Materials Project online structural database, calculate real space PDFs from these structures, and refine them to best fit experimental data. The algorithm is implemented in Python, utilizing Pymatgen and DiffPy-CMI libraries for atomic structure manipulation and PDF calculations. Initial sorting of candidate structures by their Pearson correlation coefficients with the experimental data was found to be a highly efficient method for identifying the correct nanocrystal structure.

Halide Exchange in Pb-Free CsMnX3 Perovskites with Trimethylsilyl Halide Reagents

Timofey Semenov and Sasha Fraser

Advisor: Matthew Greenberg

The design of non-toxic, earth abundant metal halide nanocrystals with tunable photophysical properties is a major goal in nanomaterials synthesis given the toxicity of Pb 2+ . While halide exchange has been extensively studied in Pb based perovskite nanomaterials, similar studies for other Pb free perovskites are underexplored. Here we show halide exchange between molecular trimethylsilyl bromide and cesium manganese chloride nanocrystals. Unlike halide exchange in cesium lead halide perovskites, which occurs rapidly, the kinetics of this reaction are far slower allowing direct measurement of the process with NMR, PLE, and in situ X-ray total scattering.

Inventing the UV: Experimental Constraints for Improving Terrestrial Exoplanet Photochemical Models

Vera Topcik

Advisor: Clara Sousa-Silva

The ExCITE_PM project is a collaboration that aims to produce photochemical models that will help predict the molecular composition of the surface and atmosphere of rocky, temperate exoplanets. In order to do this, the spectra of certain molecules are needed to create these models. This summer, I was tasked with providing the UV spectra of two molecules that are believed to be detected on these exoplanets: HNO (Nitroxyl) and HSO. However, both molecules have very limited, if not no existing spectral data. HNO has very limited spectral data in the infrared wavelengths. Given these limitations, my task became to find good proxy molecules with spectra in the UV that can be given to the modelists and experimentalists in this collaboration. There have been suggested proxy molecules used for both molecules (Hu et al 2012, 2013), however this summer, I have been working to find a better proxy choice for these molecules.