Research Summary Samuel J. Dawley

Platform for the Accelerated Realization, Analysis, and Discovery of Interface Materials

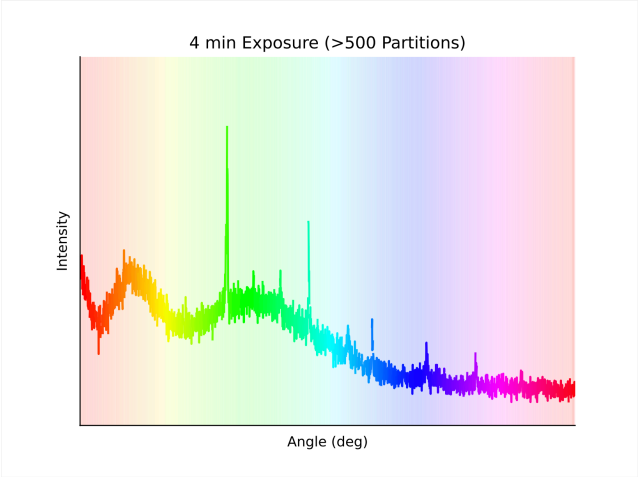
Research Intern

Dr. David Elbert, Dr. Apurva Mehta, and Dr. Tyrel McQueen *June - August 2022*

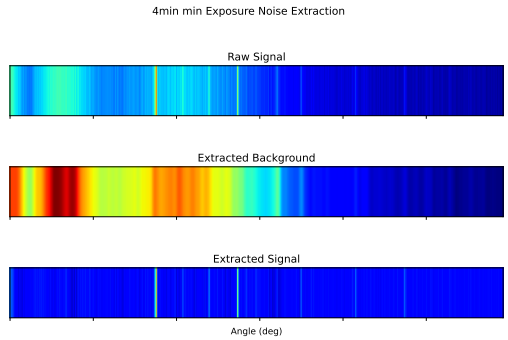
The Platform for the Accelerated Realization, Analysis, and Discovery of Interface Materials (PARADIM) is an NSF-funded materials innovation platform intended to help create and design new interface materials for use in the next generation of electronic devices. With PARADIM I studied methods for on-the-fly data analysis as a means of accelerating the materials discovery process and ultimately designing strategies for autonomous materials discovery. In particular, my research focused on extracting information from noisy signals (e.g., X-ray diffraction patterns) to elucidate the structure and onset of phase changes, i.e., spectral peaks. The crux of the algorithm, written in Python, relies on testing for common coefficients of variation across adjacent partitions of the data. Some highlights of my accomplishments include:

- Development and programmatic implementation of an algorithm for automatic peak detection; utilizes statistical analysis of and partitioning of local variation within noisy signals and spectra to determine the onset of phase changes. An example of such partitioning can be found in Figure 1a.
- Creation of Python program for live-streaming data directly from collection instrument. Streaming done using Apache Kafka and cloud-based storage.
- Collaboration with scientists at the SLAC National Accelerator Laboratory for applying machine learning methods to develop further methods of signal extraction from noisy signals (Figure 1b). The data shared between groups includes both one-dimensional and two-dimensional diffraction patterns, the latter collected from the Stanford Synchrotron Radiation Lightsource at SLAC, allowing for greater generalization of analysis tools and application.
- Preparation, collection, and analysis of samples for powder X-ray diffraction experiments.

A full research report, poster, and recording of my presentation can be found on the PARADIM website linked below.



(a) Partitioning of spectral data sets prior to analysis of local variation. The optimal number of partitions is typically dependent on the data set; a good first approximation to the best partition size is the full-width half-maximum of the most intense observed peak.



(b) Machine learning analysis of X-ray diffraction patterns collected from a synchrotron for extraction of signals from background noise. The code to reproduce the output can be found on GitHub.

Figure 1: Methods for data analysis and some results for my research performed at PARADIM. A full research report, poster, and recorded oral presentation can be found on the PARADIM website, under my name: *paradim.org/reu_participants*

Johns Hopkins University Department of Chemistry Research Assistant

Dr. Lan Cheng *February 2022 - Present*

The overarching goal of my research with Prof. Lan Cheng involves investigating the properties of ionic and molecular diatoms in laser-cooled, ultracold opto-electronic traps. We have used coupled-cluster methods with the CFOUR computational suite to calculate the polarizabilities and lifetimes of such compounds and collaborated with experimentalists in the Doyle Group at Harvard to corroborate results. The strong agreement between our results and those determined experimentally comes from our treatment of relativistic effects, which grow increasingly important as the trapped atoms grow heavier. Some achievements of my research include:

- A publication being prepared for peer review:

  C. Hallas, N. B. Vilas, L. Anderegg, P. Robichaud, A. Winnicki, **S. Dawley**, C. Zhang, L. Cheng, J. M. Doyle "Lifetimes for polyatomic molecules in an optical dipole trap" *in preparation*, Phys. Rev. A (2022).

- Benchmark calculations of spin-orbit coupling in heavy-element molecules comparing perturbative and variational treatments. This work is currently submitted for presentation at the meeting of the American Chemical Society in the Spring:

  S. Dawley; C. Zhang; X. Zheng; L. Cheng. "Benchmark calculations of spin-orbit coupling within exact two-component theory: Comparison of perturbative and variational treatments." *in preparation for* the National Meeting of the ACS , Indianapolis, IN, 2023.

Massachusetts General Hospital Research Intern

Dr. Benjamin Medoff and Dr. Tristan Kooistra *June - August 2021*

Within the Medoff Lab at the Massachusetts General Hospital (MGH), I researched methods of data collection and visualization for studying the mechanisms involved with the inflammation of airway epithelium cells due to idiopathic pulmonary fibrosis (IPF). In particular, a coculture of basal cells and murine immune cells with IPF was created, maintained, and monitored to measure the heterogeneity of cell patterning as a function of time. I was responsible for culturing cells and recording the resultant patterning at different intervals. My primary contribution to the research project included a data visualization method and consequent method of analysis; I developed a Python program for determining cell-to-cell distances using a Delaunay triangulation and subsequent visualization using a Voronoi tessellation. All of the code for the project can be found on GitHub. Some results can be seen in Figure 2.

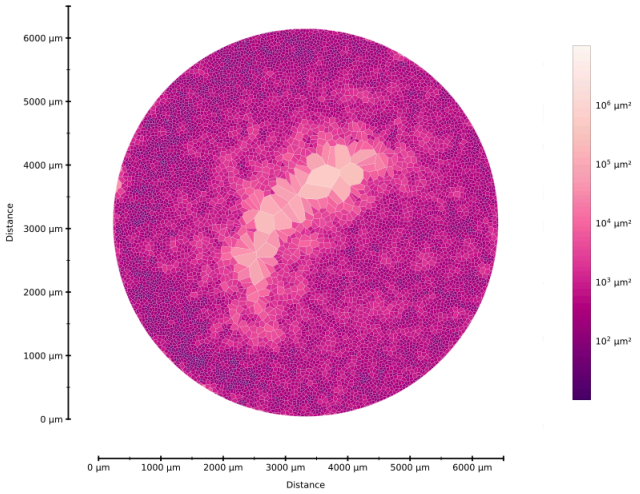


Figure 2: Voronoi tessellation of patterning for coculture of basal and murine immune cells. Coloring is done on a logarithmic scale.

Johns Hopkins University Department of Chemistry RESEARCH ASSISTANT

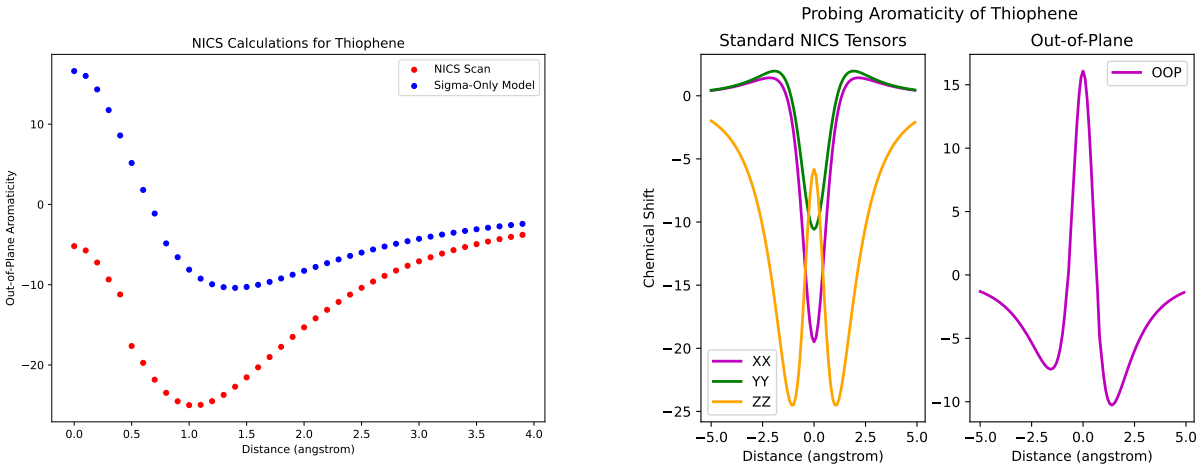
Dr. John Dayton Tovar *January 2020 - Present*

My original research project in the Tovar lab involved cycloparaphenylenes (CPPs), macrocyclic aromatic compounds exhibiting hybrid linear and radial conjugation. The goals of the project ranged from optimization of synthetic conditions to molecular orbital characterization, both of which I accomplished while leaving behind promising research directions for future students. During this time, I gained expertise in fundamental techniques in organic synthesis, purification, and characterization, including NMR analysis and mass spectrometry. Some key accomplishments of my project include:

- Synthesis of functionalized [8]CPPs and optimized synthetic schemes for total synthesis. In the process, I synthesized a novel aromatic compound that may act as scaffolding for functionalized CPP precursors in the future.
- Molecular orbital characterization with density functional theory using Gaussian on high-powered computing clusters at the Maryland Advanced Research Computing Center (MARCC). In tandem, I wrote a Python script that communicates with the SSH client of MARCC for automatic submission of jobs on computing clusters.

The second research project I adopted and am currently working on concerns the aromaticity of functionalized borepins and their derivatives. Probing aromaticity is done with the Aroma package for Gaussian, a computational plug-in that measures aromaticity using the nucleus-independent chemical shift (NICS) method. Results from a successful calculation for thiophene are shown in Figure 3. The primary accomplishments of my computational work include:

- Updating the Aroma package to work with Gaussian16. Involved updating Python version on high-power computing clusters.
- Determination of aromaticity for functionalized borepins.



(a) Probing aromaticity of thiophene with and without contributions from π-bonding (NICS scan and Sigma-Only Model, respectively). Distance is measured as the radial distance from the center of the ring along the plane of the molecule.

(b) Chemical shift tensors of in each of the Cartesian directions for thiophene as well as the out-of-plane (OOP) chemical shift. Distance is measured the same as in Figure 3a.

Figure 3: Results from Aroma for calculating nucleus-independent chemical shifts of thiophene.