Emil I. Jaffal

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EDUCATION

Fordham University, Fordham College at Rose Hill May 2023
Bachelor of Science, Chemistry

PROFESSIONAL EXPERIENCE

ICL Industrial Products
Research Chemist Sep 2023 – Present

R&D professional with a strong background in flame retardant product evaluation and formulation. My expertise includes conducting laboratory experiments, standardized tests with polyurethane foams, and developing correlating methods. My synthetic experience includes developing various polyurethane foams with manufacturer-based additives and ensuring compliance with various international safety regulations. Leading a dynamic team in formulating novel blends, aligning with the latest restrictions on halogenated flame retardants. Pioneering the integration of polyurethane for battery encapsulation, contributing to cutting-edge advancements in environmentally conscious and technologically innovative materials. Communicating with sales, marketing, and customers to ensure overall satisfaction. Reporting performance data and writing technical reports to upper management. Contributing effectively and proactively in cross-functional teams while maintaining lab equipment, chemical inventory, and safety procedures to ensure seamless operations.

City University of New York, Chemistry Department
Graduate Research Assistant Jan 2024 – Present
Advisor: Dr. Anton Oliynyk

Focused on developing an open-source Python tool for high-throughput extraction of crystal structure features. This tool systematically processes Crystallographic Information Files (CIF) to construct supercells and extract descriptors tailored to a material's specific structure. The project demonstrated the featurizer's robustness by processing binary and ternary files. The tool aims to enhance the relevance of machine learning applications for predicting properties of binary and ternary compounds, providing a promising avenue for material property optimization. Introduction to the project highlighted the challenges of traditional machine learning models in solid-state materials, which often lack structural information. The goal was to address this gap by creating a tool that generates various elemental and structural-based features, to improve the

interpretability and predictive capabilities of machine learning models in the field of solid-state materials.

Fordham University, Chemistry Department
Undergraduate Research Assistant Sep 2021 – May 2023
Advisors: Dr. Julia Schneider and Dr. Joshua Schrier

Vinyl Azide Project
Helped to develop novel methods to synthesize vinyl azides into 7-membered azepine rings as potential organic semiconductors. Investigated the cyclization reactions under different conditions, including heat and UV light. Employed purification techniques like flash chromatography and rotary evaporation to isolate and purify the synthesized compounds. Utilized HNMR and CNMR spectroscopy to analyze the chemical structure and confirm the formation of the cyclization products. Employed various analytical instruments such as NMR to obtain accurate and precise data for characterization. Maintained comprehensive laboratory records and documented experimental procedures, observations, and results in meticulous laboratory notebooks. Collaborated with team members to troubleshoot issues, interpret experimental data, and refine the synthetic protocols. Conducted extensive computational work, including transition state searches and DFT calculations, to gain insights into the reaction mechanisms and explore the energy levels of the synthesized compounds.

Pyrene Project
While involved in the pyrene project, I actively synthesized pyrene diimide monomers. The synthesis involved several key steps, including a Friedel Crafts reaction to separate the isomers. Various synthetic techniques were employed, including halogenation, flash vacuum pyrolysis, and oxidation reactions. I performed extensive density functional theory (DFT) calculations to investigate the geometric, thermodynamic, electronic, and absorption properties of pyrene diimide oligomers. I conducted calculations for monomer to pentamer forms and periodic boundary conditions (PBC) calculations for different conformations. By comparing the cis and trans isomers in their monomeric and oligomeric forms, I analyzed band gap differences, HOMO/LUMO distribution, and other valuable optoelectronic properties. The results were used to gain insights into the conjugation pathways and to extrapolate the oligomer properties to predict the formation qualities of pyrene diimide better when it was synthesized.

PUBLICATIONS

- E. Jaffal, D. Shiryaev, A. Vtorov, S. Lee, N. K. Barua, A. O. Oliynyk, "Simple and effective solid state structure featurizer: a comparative study for explainable and interpretable machine-learning models," *in preparation*.

- J.A. Schneider, K. Johnston, E. Mikita, E. Jaffal, "Effect of Backbone Linearity on Mixed-Conductance in New Pyrene Dianhydride-Based Conjugated Ladder Polymers," *in preparation.*

PRESENTATIONS

- Materials Research Society Meeting & Exhibit – Boston, MA (Presentation) Nov 2023
  Effect of Backbone Linearity on Mixed-Conductance in New Pyrene Dianhydride-Based Conjugated Ladder Polymers
- Fordham University Jean Dreyfus Lectureship – Bronx, NY (Presentation) Apr 2023
  The Schneider Lab
- MAPS: Research at Fordham – Bronx, NY (Presentation) Nov 2022
  Vinyl Azide Cyclization: Where Organic & Computational Chemistry Meet

HONORS AND GRANTS

- NSF Summer Research Funding Grant (DMR-1928882) May 2022
- Fordham University Dean's List May 2023

LEADERSHIP/SERVICE

Fordham University Arabic Club
Vice President Sep 2022 – May 2023

Assisted the president in preparing financial reports, bureaucratic paperwork, and campaigning for outreach. Aided in organizing club meetings and programs alongside the Club President to engage members and potential members in participating and guiding them through the Arabic major and minor.

Fordham University Muslim Students Association
Treasurer Jan 2022 – Aug 2022

Managed finances for one of the largest religious organizations on campus. Maintained accurate records of financial transactions to prepare for end-of-year reports, operation packages, analyses for budget breakdowns and developments, and E-board reviews.

Fordham Undergraduate Research Journal
Peer Editor Sep 2022 – May 2023

MEMBERSHIPS

Sigma Xi, The Scientific Research Honor Society Mar 2023 – Present

TECHNICAL SKILLS

Software: Bluehill, ChemOffice, Gaussian16, Mathematica, Maestro, Microsoft Office, Signals Notebook, TopSpin, WebMO.

Programming languages: Wolfram, Python, Bash.

Packages: NumPy, SciPy, Scikit-Learn, Pandas, Matplotlib, Jupyter Notebook.

Wet Laboratory: General synthesis and purification skills include distillations, extractions, filtrations, recrystallizations, pH measurements, and making various solutions. This includes operating basic laboratory equipment such as hot plates, rotary evaporators, and blast furnaces. More advanced industrial equipment experience includes cone calorimeters, extruders, various flammability testers, and Instron universal testing systems. Instrumentation experience includes flash chromatography, UV-Vis, NMR, fluorescence, and IR spectroscopy with respective analytic interpretations.

PROJECTS

Machine Learning Ensemble for Bandgap Prediction of Organic Compounds

Using Python and various libraries, I developed a stacked ensemble ML algorithm to predict the bandgap of organic compounds, finding that it significantly underperformed our baseline. This algorithm used an optoelectronic dataset of 24,000 unique molecular band gap calculations from OCELOT (Organic Crystals in Electronic and Light-Oriented Technologies), an open-source database containing a descriptor-based schema for high-throughput calculations. Analyzed various molecular features to deploy a successful and simple algorithm and found that it outperformed the meta-learner MAE by 198%, expediting the time it would have taken to do first-principles DFT calculations.

LANGUAGES

English (native)
Arabic (native)
Spanish (conversational)