Emil I. Jaffal

Research Chemist, ICL Industrial Products
Incoming Ph.D. Student, City University of New York

(914) 382-9929
ejaffal@fordham.edu
emiljaffal.github.io

EDUCATION

City University of New York, Hunter College — Expected 2028
Ph.D., Chemistry
Thesis: TBA
Advisor: Dr. Anton Oliynyk

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

PROFESSIONAL EXPERIENCE

City University of New York, Chemistry Department
Ph.D. Student — Aug 2024 – Present
Advisor: Dr. Anton Oliynyk

Currently 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 (ML) 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 ML 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 ML models in the field of solid-state materials.

ICL Industrial Products
Research Chemist — Sep 2023 – Aug 2024

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.

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

- **Jaffal, E.**; Shiryaev, D.; Vtorov, A.; Lee, S.; Barua, N. K.; Oliynyk, A. O. Simple and effective solid state structure featurizer: a comparative study for explainable and interpretable machine-learning models. **2024**. *Manuscript in preparation.*
- Schneider, J. A.; Johnston, K.; Mikita, E.; **Jaffal, E.** Effect of Backbone Linearity on Mixed-Conductance in New Pyrene Dianhydride-Based Conjugated Ladder Polymers. **2024**. *Manuscript 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

- CUNY Science Scholarship 2024
- Fordham University Dean's List 2023
- NSF Summer Research Funding Grant (DMR-1928882) 2022

LEADERSHIP/SERVICE

- Fordham University Arabic Club
  Vice President Sep 2022 – May 2023
- Fordham University Muslim Students Association
  Treasurer Jan 2022 – Aug 2022
- 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: Proficient in a wide array of synthesis and purification techniques, including distillations, extractions, filtrations and recrystallizations. Skilled in preparing diverse solutions and operating standard laboratory equipment such as hot plates, rotary evaporators, and blast furnaces. Experienced in handling advanced industrial equipment like cone calorimeters, extruders, and various flammability testers, as well as conducting tests using Instron universal testing systems. Possesses expertise in utilizing instrumentation such as flash chromatography, UV-Vis, NMR, fluorescence, and IR spectroscopy, coupled with adept interpretation of analytical results.

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)