Emil I. Jaffal

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

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EDUCATION

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

Fordham University, Fordham College at Rose Hill — 2023
B.Sc., Chemistry

PROFESSIONAL EXPERIENCE

City University of New York
Ph.D. Student — Aug 2024 – Present

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 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 – July 2024

R&D professional with a strong background in flame retardant (FR) evaluation and formulation in polyurethane foams. My synthetic expertise includes developing various novel FR blends for polyurethane foams with external manufacturer and customer additives while ensuring compliance with various international safety regulations. Led a dynamic team pioneering the integration of polyurethane for battery encapsulation, contributing to cutting-edge advancements in environmentally conscious and technologically innovative materials which led to a patent filing. Communicated across departments with sales, marketing, and our customers to ensure overall satisfaction. Reported performance data and wrote technical reports to upper management. Contributed effectively and proactively in cross-functional teams while

maintaining lab equipment, chemical inventory, and safety procedures to ensure seamless operations.

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

Vinyl Azide Project
Developed novel methods for synthesizing vinyl azides into 7-membered azepine rings for potential use in organic semiconductors. Investigated cyclization reactions under varying conditions, including heat and UV light, employing purification techniques like flash chromatography and NMR spectroscopy for compound analysis. Collaborated with team members to troubleshoot issues, interpret experimental data, and refine the synthetic protocols. Conducted extensive computational work, including transition state searches and density functional theory (DFT) calculations, to gain insights into the reaction mechanisms and explore the energy levels of the synthesized compounds.

Pyrene Project
Synthesized pyrene diimide (PyrDI) monomers with several key steps, including a Friedel-Crafts reaction to separate the isomers, and employed various synthetic techniques such as halogenation, flash vacuum pyrolysis, and oxidation reactions. Performed extensive DFT calculations to investigate the geometric, thermodynamic, electronic, and absorption properties of PyrDI oligomers. I conducted calculations for monomer to pentamer forms and periodic boundary condition calculations for various conformations. By comparing cis and trans isomers in their monomeric and oligomeric forms, I analyzed band gap differences, electron distribution, and other valuable optoelectronic properties. The results were used to gain insight into the conjugation pathways and to extrapolate the oligomer properties to better predict formation qualities of oligomeric PyrDI when 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. *J. Mater. Inform.* **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.*

PATENTS

- Thermal Barrier for Potting Lithium Battery Cells. Inventors: Sergei Levchik, Zhihao Chen, Jeffrey Stowell, **Emil Jaffal**, and Munjal Patel. Filed April 2024. *Provisional patent*.

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

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
  Associate Member

TECHNICAL SKILLS

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

Programming languages: Python, Bash, Wolfram.

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

Laboratory: Proficient in a wide array of synthesis and purification techniques, including distillations, extractions, filtrations, and recrystallizations. Skilled in preparing diverse solutions and operating 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. Have expertise in utilizing instrumentation such as flash chromatography, UV-Vis, NMR, fluorescence, and IR spectroscopy, coupled with adept interpretation of analytical results.

LANGUAGES

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