Emil I. Jaffal

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Education

City University of New York, The Graduate Center — Expected 2028
Ph.D., Chemistry
Advisor: Dr. Anton Oliynyk

Fordham University, Fordham College at Rose Hill — Aug 2019 – May 2023
B.Sc., Chemistry

Research experience

Ph.D. Student — *New York, NY*
City University of New York, Hunter College — Jul 2024 – Present

Solid-State Chemistry Laboratory, Dr. Anton Oliynyk

- Conducting exploratory syntheses of novel intermetallic materials with corresponding analyses using powder X-ray diffraction and scanning electron microscopy.
- Enhancing machine learning applications to predict properties of up various binary and ternary compounds, focusing on improving interpretability and predictive capabilities of models in solid-state materials by incorporating detailed structural information.
- Mentored a handful of students in the lab, providing guidance in research projects and experimental/computational techniques.

Undergraduate Researcher — *Bronx, NY*
Fordham University — Sep 2021 – May 2023

Organic/Materials Chemistry Laboratory, Dr. Julia Schneider

- Steered materials research involving various reactions as part of a novel multi-step synthesis to create organic semiconductors (OSCs) with tunable conjugated heterocycles to improve conductivity.
- Instrumentation experience includes handling UV-Vis, NMR, fluorescence, and IR spectroscopy with respective machinery and analytic interpretations. General synthesis and purification skills include distillations, extractions, filtrations, and recrystallizations.

Computational Chemistry Laboratory, Dr. Joshua Schrier

- Identified probable transition states of novel syntheses as part of a collaboration within the chemistry department.
- Performed numerous Gaussian ab initio calculations of internal energies, electronic structures, and geometric data using density functional theory to analyze reaction thermodynamics and predict isomer formations of OSCs.

Professional experience

Research chemist — *Tarrytown, NY*
ICL Industrial Products — Sep 2023 – Jul 2024

- Synthetic expertise includes developing various novel flame retardant blends for polyurethane foams with external manufacturers and customer additives while ensuring compliance with international safety regulations.
- Pioneered the integration of polyurethane for battery encapsulation, contributing to cutting-edge advancements in environmentally conscious and technologically innovative materials, leading to a

patent application.

- Executed laboratory experiments aligning with market support and new product development objectives.
- Conducted standardized flammability and physical property tests to assess the performance of various halogenated and nonhalogenated flame retardant products.

Publications

Composition and Structure Analyzer/Featurizer for Explainable ML Models to Predict Solid State Structures. *Preprint.*   Oct 2024

Jaffal E.I., Shiryaev D., Vtorov A., Lee S., Barua N.K., and Oliynyk A.O.

10.26434/chemrxiv-2024-rrbhc

Synthesis of Pyrene Diimide Isomers with Tunable Excimer Formation. Organic Letters. *Accepted.*   Oct 2024

Johnston K., McCostis A., Mikita E., **Jaffal E.**, Schneider J.A..

Presentations

Brookhaven Nat'l Lab Nuclear Chem Summer School – *New York, NY*   Jul 2024
The Oliynyk Lab

Materials Research Society Meeting and Exhibit – *Boston, MA*   Nov 2023
Effect of Backbone Linearity on Mixed-Conductance in New Pyrene Dianhydride-Based Conjugated Ladder Polymers

Fordham University Jean Dreyfus Lectureship – *Bronx, NY*   Apr 2023
The Schneider Lab

MAPS: Research at Fordham – *Bronx, NY*   Nov 2022
Vinyl Azide Cyclization: Where Organic and Computational Chemistry Meet

Posters

Gordon Research Conference – *Newry, ME*   Jul 2024
Materials Informatics: Binary/Ternary Composition and Structure Featurizer for ML Models

Projects

Composition Analyzer/Featurizer (CAF)

Developed an interactive Python script that generates chemical compositional features and provides tools for filtering, sorting, and merging data. Aids novice solid-state chemists and materials scientists in generating compositional training data ranging from dozens to tens of thousands of compounds.

Patents

Heat Resistant Semi-Rigid Polyurethane Foams. *Provisional patent 63/680,764.*   Aug 2024

Emil Jaffal, Sergei Levchik, Zhihao Chen, Jeffrey Stowell, and Munjal Patel.

Honors and Grants

CUNY Science Scholarship	2024
Fordham University Dean's List	2023

NSF Summer Research Funding Grant (DMR-1928882)   2022

Service

Fordham University Muslim Students Association – *Treasurer*	Sep 2022 – May 2023
Fordham University Arabic Club – *Vice President*	Jan 2022 – Aug 2022
Fordham Undergraduate Research Journal – *Peer Editor*	Sep 2022 – May 2023

Memberships

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

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.
Languages: Arabic (native), English (native), Spanish (conversational).