# Emil I. Jaffal

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# Education

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

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

#### **Research** experience

#### Ph.D. Student

City University of New York, Hunter College

# 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 various binary and ternary compounds, focusing on improving interpretability and predictive capabilities of models in solid-state materials by incorporating detailed structural information.
- Mentoring a handful of students in the lab, providing guidance in research projects and experimental/computational techniques.

#### Undergraduate Researcher

Fordham University

# 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**

ICL Industrial Products

- 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

Expected 2028

Aug 2019 – May 2023

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New York, NY Jul 2024 – Present

Bronx, NY

Sep 2021 – May 2023

Tarrytown, NY Sep 2023 – Jul 2024

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patent application.

- $\circ~$  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<br>Models to Predict Solid State Structures. Digital Discovery. DOI: 10.1039/D4DD00332B<br>Jaffal E.I., Shiryaev D., Vtorov A., Lee S., Barua N.K. & Oliynyk A.O. | Jan 2025  |
|--|-----------|
| Synthesis of Pyrene Diimide Isomers with Tunable Excimer Formation.<br>Organic Letters. DOI: 10.1021/acs.orglett.4c03523   | Jan 2025  |
| Johnston K., McCostis A., Mikita E., <b>Jaffal E.</b> & Schneider J.A.   |           |
| Presentations  |           |
| <b>Brookhaven Lab Nuclear Chemistry Summer School</b> – <i>New York, NY</i><br>The Olivnyk Lab   | Jul 2024  |
| 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  |           |
| Contributed presentations  |           |
| *indicates an upcoming presentation  |           |
| *Canadian Chemistry Conference & Exhibition – Ottawa, ON   | June 2025 |
| Excimer formation and anti-Kasha emission in new pyrene diimide isomers  |           |
| Materials Research Society Meeting and Exhibit – Boston, MA  | Nov 2023  |
| Effect of Backbone Linearity on Mixed-Conductance in New Pyrene Dianhydride-<br>Based Conjugated Ladder Polymers   |           |
| Posters  |           |
| Gordon Research Conference – Newry, ME   | Jul 2024  |
| Materials Informatics: Binary/Ternary Composition and Structure Featurizer for ML Models   |           |
| Projects   |           |
| Composition Analyzer/Featurizer (CAF)  | Jun 2024  |

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 2024Emil Jaffal, Sergei Levchik, Zhihao Chen, Jeffrey Stowell & Munjal Patel.Aug 2024

# Honors and Grants

| CUNY Certificate of Achievement   | 2025                  |
|---|-----------------------|
| Recognized for outstanding success as a first year graduate student and subm<br>my first publication during the Fall 2024 semester. | itting                |
| 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).