# 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

New York, NY Ph.D. Student

City University of New York, Hunter College

Jul 2024 - Present

# Solid-State 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.
- o Directly mentoring a handful of students, providing guidance in their research projects with both experimental and computational techniques.

## Undergraduate Researcher

Bronx, NY

Fordham University

Sep 2021 – May 2023

#### Organic/Materials 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.
- o 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 Laboratory – Dr. Joshua Schrier

- Identified probable transition states of novel syntheses as part of an NSF-funded collaboration within the chemistry department.
- o 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

- Developed novel flame retardant (FR) blends for polyurethane foams in collaboration with external manufacturers and customers, ensuring compliance with international safety regulations.
- Pioneered the integration of polyurethane for battery encapsulation, contributing to advancements in sustainable and high-performance materials, leading to a patent application.
- Led application efforts for VeriQuel® F series, a proprietary phosphorus-based FR for flexible foams,

- conducting iterative testing with customers and scaling toll production for MT quantities, with early sales reaching \$800K.
- Executed laboratory experiments, standardized flammability tests, and physical property assessments to support new product development and market-driven innovations in halogenated and non-halogenated FRs.

# **Publications**

Improving Mechanical Properties Through Defect Chemistry in Hard Material Ta <sub>3</sub> P. <i>In preparation</i> .	l July 2025
Jaffal E.I., Shiryaev D., Selvaratnam B. & Oliynyk A.O.	
Quaternary Germanide Structures and Their Properties. In preparation.	July 2025
Pozdnyakova N., <b>Jaffal E.I.</b> , & Oliynyk A.O.	
Explainable Recommendation Engines to Predict Complex Intermetallic Synthesis and Characterization of $Gd_{10}RuCd_3$ , a Neutron Absorption Material. In revision, J. Am. Chem. Soc.  Xhabrahimi B., Jaffal E.I., & Oliynyk A.O.	·
Dataset of Prototype Structures Adopted by Intermetallic Compounds with AB Stacking. Preprint submitted to Data Brief. Selvaratnam B., Jaffal E.I., Shiryaev D. & Oliynyk A.O.	June 2025
Exploring Feature Engineering for Crystal Structure Classification: Interactive Applications of PCA and PLS-DA Clustering. <i>In revision, J Chem. Ed.</i>	
Shiryaev D., <b>Jaffal E.I.</b> , Selvaratnam B., Sun Y. & Oliynyk A.O.	
Materials Informatics Tools to Analyze Crystal Structures: Crystal Structure of the Novel Ternary Indide ErCo <sub>2</sub> In. Integr. Mater. Manuf. Innov.	<b>c-</b> June 2025
Tyvanchuk Y., Lee S.,, <b>Jaffal E.I.</b> , Selvaratnam B. & Oliynyk A.O.	
Unsupervised ML Prediction of Novel 1:3 Intermetallic with Synthesis of TbIr <sub>3</sub> (PuNi <sub>3</sub> -type) as Experimental Validation. J. Am. Chem. Soc. Sethi S.S., Dutta A., Jaffal E.I., & Oliynyk A.O.	Feb 2025
Composition and Structure Analyzer/Featurizer for Explainable MI Models to Predict Solid State Structures. Digit. Discov.  Jaffal E.I., & Oliynyk A.O.	Jan 2025
Synthesis of PyrDi Isomers with Tunable Excimer Formation. Org. Lett	Jan 2025
Johnston K., McCostis A., Mikita E., <b>Jaffal E.</b> & Schneider J.A.	
Guest Lectures	
Solid-State Chemistry: Introduction to Thermoelectrics – Hunter College, NY	May 2025
Courses Taught	
General Chemistry Lab (10600) – Hunter College, NY	Aug 2025 – June 2026

#### Presentations

Brookhaven Lab Nuclear Chemistry Summer School – New York, NY	Jul 2025
Using explainable recommendation engines for the discovery of $\mathrm{Gd}_{10}\mathrm{RuCd}_3$	
ACS Mid-Atlantic Regional Meeting – South Orange, NJ	May 2025
Quaternary Intermetallic Germanides: Structure, Properties, and Potential Applications	
Fordham University Jean Dreyfus Lectureship – Bronx, NY	Apr 2023
The Schneider Lab	
Brookhaven Lab Nuclear Chemistry Summer School – New York, NY	Jul 2024
The Oliynyk Lab	
MAPS: Research at Fordham – Bronx, NY	Nov 2022
Vinyl Azide Cyclization: Where Organic and Computational Chemistry Meet	

#### Posters

# North American Solid State Chemistry Conference – Ames, IA Quaternary Intermetallic Germanides: Structure, Properties, and Potential Applications

#### Hackathons

### SSMC-Collaboration Incubator - Madison, WI

May 2025

Selected participant for national hackathon-style research workshop. Collaborated on the *Rational Design* of *Thermoelectrics* with an interdisciplinary cohort of PhD students and professors.

# **Selected Projects**

See the full suite of apps on the Oliynyk lab website, both developed myself here.

# XRD Comparison & Matching Tools

Mar 2025

Contributed to the development and deployment of GUIs, allowing novice users to compare multiple '.xy' files from X-ray diffraction (XRD) data with .cif files. These help identify impurities, match phases, and visualize differences in crystal structure XRD patterns with ease.

## 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 for machine learning models 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 & Munjal Patel.

#### **Honors and Grants**

CUNY Certificate of Achievement	2025
Awarded \$3,000 in recognition of outstanding success as a first-year student, includ-	
ing the acceptance of my first-author publication during the Fall 2024 semester.	
CUNY Science Scholarship	2024
Fordham University Dean's List	2023
NSF Summer Research Funding Grant (DMR-1928882)	2022

#### Service

Materials Today Physics – Reviewer	Aug 2025 – Present
Fordham University Muslim Students Association – Treasurer	Sep 2022 - May 2023
Fordham University Arabic Club – Vice President	${ m Jan} \ 2022 - { m Aug} \ 2022$
Fordham Undergraduate Research Journal – Peer Editor	Sep 2022 - May 2023

# Students Mentored

Brook Xhabrahimi (B.Sc. Chemistry, 2025)

Natalia Poznyakova (B.Sc. Chemistry, 2025)

Miriam Ismail (B.Sc. Chemistry, 2025)

Riya Upadhyay (B.A. Human Biology, 2024)

Alex Vtorov (B.Sc. Chemistry, 2025)

Joseph Oziel (The Bronx High School of Science, 2025)

Yujing Sun (The Bronx High School of Science, 2025)

Brandon Lin (The Bronx High School of Science, 2025)

# Memberships

Sigma Xi, The Scientific Research Honor Society –  $Associate\ Member$ 

Mar 2023 – Present

#### Technical skills

**Software:** Adobe Illustrator, Bluehill, ChemOffice, Gaussian16, Mathematica, Maestro, Microsoft Suite, Signals Notebook, TopSpin, VASP, WebMO.

Programming & markup languages: Python, Bash, HTML, Wolfram (Mathematica).

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

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