DANILA SHIRYAEV

Curriculum Vitae

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EDUCATION

Bachelor of Arts, Chemistry Aug 2023 – Dec 2024

Hunter College, City University of New York, NY, US

Hunter College Foundation scholarship

GPA: 3.9/4.0

Specialist, Chemistry (transferred to Hunter College) Sep 2016 – Mar 2022

Moscow State University (MSU), Moscow, Russia

Full tuition merit-based scholarship with a monthly stipend

GPA: 3.6/4.0

RESEARCH EXPERIENCE

CUNY Research Foundation Jan 2024 – Present

Research associate, Oliynyk's research group

Solid-State and Material Science research

- Work on intermetallics, synthesis and characterization of new compounds and their crystal structures
- Electronic structure calculations
- Using machine learning approaches to predict and systematize crystal structures of solids with classification
- Development of recommendation engine to target novel intermetallics materials

Moscow State University Jan 2019 – Mar 2022

Research assistant, Badun's research group

Radionuclides and Labeled Compounds research

- Preparation of tritium-labeled organic compounds using the thermal activation method
- Investigation by radionuclide methods of adsorption phenomena at liquid/liquid interface

Moscow State University Sep 2016 – Dec 2019

Research assistant, Pankratov's research group

Nuclear Chemical Materials Science research

- Synthesis of compounds of Fe in unstable oxidation states with given functional properties
- Development of materials and methods for reagent and reagent-free water treatment
- Application of absorption and emission Mössbauer spectroscopy to solid state research

PUBLICATIONS

Xhabrahimi B.; Jaffal, E.; **Shiryaev, D.**; …; Oliynyk, A. A Recommendation Engine to Target Novel Intermetallics: Prediction and Synthesis of Novel Neutron Absorber Gd10RuCd3. (*in preparation*)

Selvaratnam, B.; Jaffal, E.; **Shiryaev, D.**; Oliynyk, A. Dataset of Prototype Structures Adopted by Intermetallic Compounds with AB Stacking. Chemistry June 9, 2025. DOI: 10.26434/chemrxiv-2025-smpsh. (*submitted to Data in Brief*)

Shiryaev, D.; Sun, Y.; Jaffal, E.; Oliynyk, A. Exploring Feature Engineering for Crystal Structure Classification: Interactive Applications of PCA and PLS-DA Clustering. Chemistry April 11, 2025. DOI: 10.26434/chemrxiv-2025-235nn. (*submitted Journal of Chemical Education*)

Sethi, S. S.; Dutta, A.; Jaffal, E. I.; Yadav, N.; **Shiryaev, D.**; Hoang, B.; Machathi, A.; Lee, S.; Das, K.; Jana, P. P.; Oliynyk, A. O. Unsupervised Machine Learning Prediction of a Novel 1:3 Intermetallic Phase with

the Synthesis of TbIr3 (PuNi3-Type) as Experimental Validation. *J. Am. Chem. Soc.* 2025, 147 (17), 14739–14755. DOI: 10.1021/jacs.5c03510.

Jaffal, E. I.; Lee, S.; **Shiryaev, D.**; Vtorov, A.; Barua, N. K.; Kleinke, H.; Oliynyk, A. O. Composition and Structure Analyzer/Featurizer for Explainable Machine-Learning Models to Predict Solid State Structures. *Digital Discovery* 2025, 4 (2), 548–560. DOI: 10.1039/D4DD00332B.

Evseeva A, **Shiryaev D**, Ornithofauna of Shokalsky Island, Kara Sea. The Russian Journal of Ornithology. 2015. V. 24, pp. 4490-4494

RELATED WORK EXPERIENCE

Research Foundation CUNY – *New York, US* Oct 2024 – Present

Research Associate

- Mechanical property optimization through defect chemistry of pnictides. Research in enhancing the hardness, wear, and corrosion resistance of tantalum-based materials for oil drilling applications.
- Focus on defect engineering through pnictogen doping to improve durability and performance under extreme conditions, combining experimental synthesis with X-ray diffraction, DFT calculations, and mechanical testing
- Mentoring other undergraduate students in their laboratory investigation

Evotech-Mirai Genomics – *Moscow, Russia* Jul 2021 – Dec 2021

Clinical application manager

- Trained over 100 new customers on device functionality, resulting in a 15% increase in customer satisfaction ratings
- Successfully launched and managed over 20 new laboratories in Russia and Kazakhstan, expanding the market presence by 20%

EuroChem – *Nevinnomyssk, Russia* Jun 2021 – Jul 2021

Absorption operator

- Operated absorption unit, ensuring smooth and efficient operation of critical processes, hourly sampling
- Detailed study of all processes occurring at each unit on NPK fertilizers production

"Archimedes" – *Moscow, Russia* Oct 2020 – May 2021

PCR laboratory assistant

- Responsibilities included the complete testing cycle, from processing samples to analyzing the results
- Conducted a major optimization of work in the laboratory, thereby improving and structuring workflow, reporting, improving conditions for both customers and staff

PRESENTATIONS

ACS Mid-Atlantic Regional Meeting – *South Orange, NJ, US* May 2025

"Visualization and recommendation framework for targeting novel solid-state materials"

POSTERS

Hunter Research Conference – *New York, NY, US* Apr 2025

"Structure type explorer (STEx): visualization and recommendation approach to target novel solid-state materials"

HACKATHONS

SSMC-Collaboration Incubator – *Madison, WI, US* May 2025

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

TEACHING EXPERIENCE

Moscow State University Fall 2021

Teaching Assistant

Radiochemistry lab course with Dr. Badun

STUDENTS MENTORED

Sviatoslav Pisarev (B.A. Chemistry, 2024)

Brook Xhabrahimi (B.A. Chemistry, 2025)

Natalia Poznyakova (B.A. Chemistry, 2025)

Miriam Ismail (B.A. Chemistry, 2025)

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

GRANTS AND SCHOLARHIPS

Scholarship from Hunter College Foundation ($8300)

2024

Scholarship from Hunter College Foundation ($13500)

2023

TECHNICAL SKILLS

Software: Bruker Suite, Topas, Match, VESTA, Diamond, Pearson's Crystal Data, TopSpin, VASP, Microsoft Office.

Programming & markup languages: Python, Bash, HTML/CSS, Markdown.

Languages: Russian (native), English (full professional proficiency), French (elementary)

MEMBERSHIPS

American Chemical Society (ACS) 2024 - present

Material Research Society (MRS) 2024 - present