

PROFESSIONAL EXPERIENCE

Functional Materials Lead

Cambridge Crystallographic Data Centre

2025 – Present

- Developed a strategic initiative to expand into the functional materials market.
- Performed market research to assess customer needs, inform product development, and position offerings.
- Directed the development of new scientific research and product features to address technical challenges and meet emerging customer demands.
- Delivered technical demonstrations to customers and provided hands-on support to the sales team.
- Collaborated cross-functionally with internal teams to align product development, marketing, research, and sales.
- Reported monthly progress and strategic recommendations to the Executive Leadership Team (ELT), contributing directly to high-level decision-making processes.
- Operated autonomously to build a foundation for long-term commercial success, laying the groundwork for measurable revenue growth in a new market segment.

PROFESSIONAL EXPERIENCE CONTINUED

Research & Applications Scientist

Cambridge Crystallographic Data Centre

2019 – 2025

- Worked with remote US and UK teams.
- Collaborated with Pfizer scientists, providing data-driven analyses of pharmaceutical molecule stability. Key contributions include work on nirmatrelvir (Paxlovid), and work on a drug targeting MPO, with a publication under review.
- Led a cross-functional team to expand into the functional materials market by developing marketing materials, repackaging existing features, and designing new software functionality.
- Developed a transformer neural network model for generating and ranking molecules in multi-component pharmaceutical systems. This work was presented at scientific conferences and integrated into commercial consultancy.
- Supported commercial activities by creating marketing content, providing scientific support, leading client training and demos, and conducting feedback sessions with potential and existing customers.

PROFESSIONAL EXPERIENCE CONTINUED

Research Assistant

Florida State University

2013 – 2018

- Successfully defended a dissertation titled "Dielectric and Magnetic Properties of Hydrogen Bonded Molecular Co-crystals."
- Maintained and operated complex scientific instrumentation, while training new students on their use.
- Co-authored the high-impact publication "Crystal Structure Prediction via Deep Learning," featured on the cover of Journal of the American Chemical Society and cited over 250 times. This work was highlighted in Chemistry World.
- Secured over \$490,000 in funding from the university and NSF to support the group's research.
- Contributed to 10 peer-reviewed manuscripts, including two as primary author, accumulating 486 citations to date.
- Authored a successful proposal to conduct experiments using the TOPAZ instrument at Oak Ridge National Laboratory.
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Teaching Assistant

Florida State University

2013 – 2019

- **Recitation.** General Chemistry II (1046)
- **Laboratory.** Advanced Physical Chemistry (4411L), Organic Chemistry (2211L), General Chemistry I (1045L), General Chemistry II (1046L)

Research Assistant

Kent State University

2009 – 2013

- Synthesized low-coordinate transition metal complexes and characterized them using single-crystal X-ray diffraction.
- Secured three months of funding from the research experience for undergraduates (REU) program sponsored by the NSF.

Teaching Assistant

Kent State University

2011

- **Laboratory.** Chemistry in our World (10030)

EDUCATION

Materials Chemistry (Ph.D.)

Received 2019

Florida State University

- **Dissertation.** *Dielectric and Magnetic Properties of Hydrogen Bonded Molecular Co-crystals.*
- Conducted single-crystal neutron diffraction measurements using the TOPAZ instrument at Oak Ridge National Laboratory (ORNL).
- Jointly advised by Prof. Naresh Dalal and Prof. Michael Shatruk.

Chemistry (B.S.)

Received 2013

Kent State University

- **Honors Thesis.** *The Synthesis, Characterization, and Reactivity of Low-Coordinate, Metal Amides.*
- Advised by Prof. Scott Bunge.
- Awarded scholarships from the Honors College and Choose Ohio First for academic achievements.

RESEARCH GRANTS

- **Light-Induced Magnetic Switching as a Trigger for Phase Transitions in Molecular Materials**
Michael Shatruk (PI), Naresh Dalal (Co-PI)
Funded by National Science Foundation (1464955)
Total award \$477,169 (September 2015 – April 2019)
I was one of the graduate students participating in this NSF-funded research project.
- **Planning Grant. Toward Rational Design and Discovery of Organic Ferroelectrics**
Michael Shatruk (PI), Naresh Dalal (Co-PI)
Funded by Florida State University Council on Research and Creativity
Total award \$13,000 (December 2016 – December 2017)
I was the sole graduate student who worked on this seed research grant.

MENTORING EXPERIENCE

- **Chuming Wang.** Undergraduate student research experience (2018)
- **Jasmine Zou.** High-school student research experience (2016)
- **Emily Case.** High-school student research experience (2015)
- **Gary Soza.** Undergraduate student research experience (2014)

AWARDS & HONORS

- **Cover Art.** Produced a piece of original artwork intended to convey the scientific content of Ryan et. al. 2018. This artwork was selected as the August 2018 cover of the *Journal of the American Chemical Society*.
- **Media Appearances.** Interviewed by WTXL, Florida State University Department of Media Relations and Chemistry World regarding Ryan et. al. 2018.
- **Travel Grants.** Received an award of \$400 from the Department of Chemistry & Biochemistry at Florida State University to apply toward conference travel expenses and award of \$250 from the Gordon Research Conference on Conductivity and Magnetism in Molecular Materials.

TECHNICAL SKILLS

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| <ul style="list-style-type: none"> ▪ Crystallization techniques (organic molecules and metal-complexes) ▪ Inert atmosphere synthesis (glovebox and Schlenk line) ▪ Crystallography (single crystal and powder X-ray and TOPAZ neutron) ▪ Magnetometry (SQUID) ▪ Capacitance measurements for dielectric properties | <ul style="list-style-type: none"> ▪ Differential scanning calorimetry (DSC) and thermogravimetric analysis (TGA) ▪ Infrared and UV-vis spectroscopy, including variable-temperature measurements. ▪ Standard laboratory and chemical safety ▪ Data-driven informatics analysis of pharmaceutical small-molecule solid forms |
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SOFTWARE AND COMPUTATIONAL SKILLS

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| <ul style="list-style-type: none"> ▪ Data Visualization. Origin, Microsoft Excel, Matplotlib ▪ Crystallography. Bruker and Rigaku data collection and Olex2 refinement ▪ Databases. SciFinder, Reaxsys, Cambridge Structural Database | <ul style="list-style-type: none"> ▪ Image Editing. Adobe products (Photoshop and Illustrator), Affinity, and Canva ▪ Languages. Python, HTML, CSS, JavaScript ▪ Frameworks. Tensorflow, Pytorch, HuggingFace, Cuda ▪ Computing. Putty, SSH, GPU computing |
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NON-TECHNICAL SKILLS

- Leadership and team management
- Providing scientific and technical training to internal and external users of varying skill levels
- Scientific writing and communication
- Production of scientific reports and data analysis
- Experience working and leading in highly cross-functional environments

LANGUAGE PROFICIENCY

- **English.** Native in speaking, writing and reading.
- **French.** Intermediate in speaking, writing and reading.

CONFERENCES & WORKSHOPS

- **CCDC at Crystallographic Schools (Oral Presentation)**
American Crystallographic Association National Meeting 2024
Denver, CO
- **Generative Transformer for Scoring Pharmaceutical Coformers (Oral Presentation)**
Bio-IT World Conference & Expo 2024
Boston, MA (Virtual)
- **Using a Transformer Neural Network to Prioritize and Suggest Coformers (Poster Presentation)**
Gordon Research Conference & Symposium – Crystal Engineering 2024
Newry, ME
- **Developing a Transformer Neural Network for Scoring Pharmaceutical Coformers (Oral Presentation)**
American Chemical Society Spring National Meeting 2024
New Orleans, LA (Virtual)
- **Utilizing Data-Driven Tools to Investigate the Relative Stability of Solid Forms: CSD-Enabled Solid-Form Informatics “Healthchecks” (Oral Presentation)**
American Crystallographic Association National Meeting 2023
Baltimore, MD
- **Utilizing Structural Databases for Crystallography (Workshop Instructor)**
American Crystallographic Association Summer School 2023
Evanston, IL
- **Exploring Structural Database Use in Crystallography (Workshop Instructor)**
American Crystallographic Association Summer School 2022
West Lafayette, IN
- **Learning from a Million Structures (Oral Presentation)**
Bio-IT World Conference & Expo 2021
Boston, MA (Virtual)
- **CSD Workshop (Workshop Instructor)**
Rigaku School for Practical Crystallography 2021
Virtual
- **CSD Workshop (Workshop Instructor)**
Rigaku Symposium Series 2019
Yale - New Haven, CT
- **AI Meets Cheminformatics Learning from a Million Structures: Data Mining, Machine Learning, AI and the Cambridge Structural Database (Oral Presentation)**

American Chemical Society Spring National Meeting 2021

Virtual

- **Anti-Ferroelectricity in an Organic Acid-Base Salt (Oral Presentation)**
Florida Inorganic and Materials Symposium 2018
University of Florida - Gainesville, FL
- **Anti-Ferroelectric Transition in an Organic Acid-Base Salt (Poster Presentation)**
Gordon Research Conference & Symposium – Conductivity & Magnetism in Molecular Materials 2018
Bryant University - Smithfield, RI
- **Small Molecule Crystallography School 2018 (Workshop Attendee)**
University of Southern Florida - Tampa, Florida
- **Spin-Frustration in a Hexanuclear Iron(III) Complex (Poster Presentation)**
Gordon Research Conference & Symposium, Conductivity & Magnetism in Molecular Materials 2016
Mount Holyoke - South Hadley, MA
- **NMR Training Workshop 2016 (Workshop Attendee)**
Florida State University - Tallahassee, Florida
- **Spin-Crossover Complexes & Hydrogen Bonding Motifs (Poster Presentation)**
Florida Annual Meeting and Exposition 2015
Tampa, FL
- **Molecular Ferroelectrics (Poster Presentation)**
Florida Inorganic and Materials Symposium 2015
University of Florida - Gainesville, FL
- **Multifunctional Molecules: Combining Spin Crossover and Dielectric Anomalies (Poster Presentation)**
North American Solid-State Chemistry Conference 2015
Florida State University - Tallahassee, FL
- **Molecular Analogues to Multiferroics: Coupling Ferroelectricity to Spin-Transitions (Poster Presentation)**
Florida Annual Meeting and Exposition 2014
Tampa, FL
- **Molecule Based Multiferroics (Poster Presentation)**
Florida Inorganic and Materials Symposium 2014
University of Florida - Gainesville, FL

REFEREED JOURNAL ARTICLES

1. Pait, M., Shatruck, M., [Lengyel, J.](#), Gómez-Coca, S., Bauzá, A., Frontera, A., Bertolasi, V., Ray, D. Two types of nitrito support for μ_4 -oxido-bridged $[\text{Cu}_4]$ complexes: synthesis, crystal structures, magnetic properties and DFT analysis. *Dalton Trans.* **2015**, 44, 6107–6117.
2. Singha Mahapatra, T., Basak, D., Chand, S., [Lengyel, J.](#), Shatruck, M., Bertolasi, V., Ray, D. Competitive coordination aggregation for V-shaped $[\text{Co}_3]$ and disc-like $[\text{Co}_7]$ complexes: synthesis, magnetic properties and catechol oxidase activity. *Dalton Trans.* **2016**, 45, 13576–13589.
3. Yergeshbayeva, S., Hrudka, J. J., [Lengyel, J.](#), Erkasov, R., Stoian, S. A., Dragulescu-Andrasi, A., Shatruck, M. *Inorg.* Heteroleptic Fe(II) complexes with N_4S_2 coordination as a platform for designing of spin-crossover materials. *Inorg. Chem.* **2017**, 56, 11096–11103.
4. Hrudka, J. J., Phan, H., [Lengyel, J.](#), Rogachev, A. Y.; Shatruck, M. The power of three: Incremental increase in the ligand field strength of n-alkylated 2,2'-biimidazoles leads to spin crossover in homoleptic Fe(II) complexes. *Inorg. Chem.* **2018**, 57, 5183–5193.
5. Ryan, K., [Lengyel, J.](#), Shatruck, M. Crystal structure prediction via deep learning. *J. Am. Chem. Soc.* **2018**, 140, 10158–10168.
6. [Lengyel, J.](#), Stoian, S. A., Dalal, N., Shatruck, M. Directed synthesis and magnetic properties of a hexanuclear ferric cluster. *Polyhedron* **2018**, 151, 446–451.
7. Han, H.; Zhou, Z.; Carozza, J.; [Lengyel, J.](#); Yao, Y.; Wei, Z.; Dikarev, E.V. From lithium to sodium: Design of heterometallic molecular precursors for the NaMO_2 cathode materials. *ChemComm* **2019**, 55, 7243–7246.
8. [Lengyel, J.](#); Wang, X.; Choi, E.S.; Besara, T.; Schönemann, R.U.; Ramakrishna, S.K.; Holleman, J.; Blockmon, A.L.; Hughey, K.D.; Liu, T.; Hudis, J.; Beery, D.; Balicas, L.; McGill, S.A.; Hanson, K.; Mufeldt, J.L.; Siegrist, T.; Dalal, N.; Shatruck, M. An antiferroelectric phase transition in a squaric acid and 2,3-dimethylpyrazine co-crystal. *J. Am. Chem. Soc.* **2019**, 141, 41, 16279–16287
9. Dragulescu-Andrasi, A.; Filatov, A.S.; Oakley, R.T.; Li, X.; Legin, K.; Huq, A.; Pak, C.; Greer, S.M.; McKay, J.; Jo, M.; [Lengyel, J.](#); Hung, I.; Maradzike, E.; DePrince, A.E.; Stoian, S.A.; Hill, S.; Hu, Y.; Shatruck, M. Radical Dimerization in Plastic Organic Crystal Leads to Structural and Magnetic Bistability with Wide Thermal Hysteresis. *J. Am. Chem. Soc.* **2019**, 141, 45, 17989–17994.
10. Singha Mahapatra, T.; Roy, B.C.; Dutta, B.; [Lengyel, J.](#); Shatruck, M.; Ray, D. Structures and magnetic properties of a trinuclear angular $[\text{Ni}_3]$ and a heptanuclear wheel-like $[\text{Ni}_7]$ complexes with a Schiff base ligand. *Polyhedron* **2024**, 249, 116782.
11. Sadiq, G.; Sharma, S.; Stevens, J.S.; Martinez-Bulit, P.; Hunnisett, L.M.; Cameron, C.; Samas, B.; Hawking, E.; Francia, N.; Lengyel, J.; Pidcock, E.; Rahman, S.; Nisbet, M.; Back, K.; Doherty, C.; Basford, P.; Cooper, T.G.; O'Conner, G; Bhardwaj, R.M. An integrated approach combining

experimental, informatics and energetic methods for solid form derisking of PF-06282999. *J. Pharm. Sci.* **2024**, In Press.