KATERINA VRIZA

Email: avriza@anl.gov | **Google Scholar:** Katerina Vriza | **Github:** github.com/katerinavr | **Phone:** +44 07858504744

EDUCATION

- PhD, Machine learning in Chemistry, Materials Innovation Factory, University of Liverpool & Cambridge Structural Datacenter, Cambridge, 2022. **Academic advisors**: Dr Matthew Dyer, Prof Vitaly Kurlin, Dr Peter Wood, Prof Matthew Rosseinsky.
- MSc, Green Chemistry and Sustainable Industrial Technology, University of York, Green Chemistry Center of Excellence , 2018 . **Academic advisor**: Prof James Clark
- BS, Chemistry, University of Patras, 2016 (top 5%)
- BEng, Electronics and Telecommunication Engineering in Aviation Science, 2012 (honors)

PROFESSIONAL EXPERIENCE

Argonne National Laboratory, USA
Research Staff Scientist *April 2024 to current*

- Design and operate a user facility with integrated robotic equipment to enable the high-throughput synthesis of sustainable materials (https://cnm.anl.gov/pages/polybot).
- Lead organizer and tutor at the physical science summer school: Reaching a New Energy Sciences Workforce (RENEW). Students get experience with experimental techniques, coding in scientific applications, autonomous laboratories and hands-on discovery. Over the past two years, I have dedicated over 150 hours to the preparation and teaching of more than 40 students.
- Collaborating with scientists of other departments on building an Argonne facility context-aware Chatbot - AI research assistant, that can help users with the proposal applications and equipment operation.
- Management and supervision of user proposals for using the Polybot self-driving laboratory for polymer electronics and biosensor design and fabrication. I oversee four user projects per year.
- Writing research proposals to acquire DOE funding.

Postdoctoral Appointee *September 2022 to April 2024*

- Building a self-driving laboratory targeted to the synthesis of sustainable materials.
- Quantum Chemistry simulations for photo responsive polymers.
- Building a network to connect the automated lab equipment with the high performance computing facilities in Argonne National Lab (LCRC, Carbon).
- Developing data mining techniques incorporating Large Language Models and image processing for creating materials databases.
- Training and finetuning foundation models for text-to-image and image-to-image search realated to microscopy images.

Atinary Technologies Inc, Lausanne/Remote
part-time Data Scientist *July 2021 to February 2022*

- Developing an AI/ML platform to digitize R&D operations and enable self-driving labs that accelerate materials discovery.
- Research regarding optimization techniques targeted for experimental chemistry, e.g. incorporating chemical knowledge to the optimizer, effectively searching a constrained chemical space.
- Collaborating with IBM Zurich for enabling the acceleration of organic reactions.
- Grand applications for start-up funding.

Materials Innovation Factory, Liverpool, UK
Postgraduate researcher *Sept 2018 to April 2022*

- Performed VASP simulations and Crystal Structure Prediction for organic crystals and metal-intercalated systems in search for electronic properties.
- Developed predictive ML models for co-crystal design and discovery as part of the Cambridge Structural Datacenter toolkit.

JB Morrell Library, York, UK
Customer service-IT *Sept 2017 to August 2018*

- Providing IT advice regarding the University resources to the students of the University of York.
- Weekend job during my MSc studies.

Hellenic Air force, 117 Andravida Military Airbase, Greece
Aviation Engineer *July 2012 to Sept 2017*

- Served in the Hellenic Military Airforce as an Inspector Electronics Engineer in charge of the electronic department within the 338 squadron, being in charge and leading a technical team of 15 people working on the electronic system of the aircraft F-4E.
- Data analysis and anomaly detection for the aircraft avionics system.
- Maintained and updated the databases regarding the regular aircraft maintenance procedures.
- Aircraft accident investigator. Detected an important materials fault in the aircraft's engine.
- Knowledge and application of quality standards and control processes in the domain of aircraft system maintenance.

ACADEMIC SERVICE

- Reviewing DOE funding proposals across National Laboratories in the USA.
- Reviewer for the journals: Digital Discovery, Chemistry of Materials, APL Machine Learning and Nature Machine Intelligence.

TEACHING, MENTORING AND OUTREACH EXPERIENCE

- RENEW summer school 2023 & 2024: Pathways in Physical Science - Argonne National laboratory. Leading the educational modules for introduction to AI/ML, polymer science, data processing and laboratory automation by combining computer vision algorithms and robotic platforms (Opentrons North Robotics).
- June 2018: Introducing the concept of green chemistry and sustainability at schools in the UK as part of my MSc studies. Mentored students in the synthesis and characterization of bio-plastics.
- 2022 to present - Co-supervising and mentoring summer students from technical schools in Chicago area (SULI stundents).
- 2022 to present - Mentoring young girls and minority groups in the Chicago area to pursue a career in STEAM.
- 2018 to present - Mentoring aviation engineers to pursue a research career abroad.
- 2017 to 2021 - Teaching Assistant at the University of Liverpool for the modules Introduction to Spectroscopy(CHEM170), Physical Chemistry (CHEM152) and Molecular Modelling (CHEM280). Incuding both delivering lessons, marking and assessing student work.

AWARDS

- Award for outstanding postdoctoral performance for the year 2023 in Argonne National Laboratory.
- Travel award to present my research at the Women in ML NeurIPS 2023 symposium.
- Argonne Impact Award for notable achievement in Innovation, August 2023, for organizing the summer school outreach activities in Argonne National Laboratory.
- Competitive state scholarship from the highest research organization in Greece, the Academy of Athens,for Postgraduate studies in Chemistry, covering all my expenses for studying abroad.
- Post graduate research studentship from the Leverhulme Research Center for Functional Materials Design and Cambridge Crystallographic Datacenter.
- York University Scholarship to undertake the Master in Green Chemistry and Sustainable Industrial Technology.

CONFERENCE PRESENTATIONS

- Microscopy and Microanalysis 2024: Foundational models for microscopy datasets, speaker
- ACS Spring 2024: Extracting and utilizing multimodal datasets of images and text with large language models, speaker
- ACS Fall 2023: Harnessing the Power of Data, speaker best talk award
- 4th RSC-BMCS / RSC-CICAG Artificial Intelligence in Chemistry 2021, remote, speaker

REPRESENTATIVE PUBLICATIONS

- C. Wang*, Y. Kim*, **A. Vriza***, H. Chan, J. Xu, et al, Autonomous Platform for Solution Processing of Electronic Polymers, 2024, under review Nature Communications.
- A. Nyayachavadi*, C. Wang*, **A. Vriza***, H. Chan, J. Xu, S. Rondeau-Gagné et al, Tunable Solid-State Properties and Anisotropic Charge Mobility in Hydrogen-Bonded Diketopyrolopyrrole Polymers via Automated Device Fabrication and Characterization, Adv. Funct. Mater. 2024, 2403612.
- **A. Vriza**, H. Chan, J. Xu, Self-Driving Laboratory for polymer electronics, Chem. Mater. 2023, 35, 8, 3046−3056.
- M. H. Prince, H. Chan, **A. Vriza**, T. Zhou, V. K. Sastry, M. T. Dearing, R. J. Harder, R. K. Vasudevan, M. J. Cherukara, Opportunities for Retrieval and Tool Augmented Large Language Models in Science (under review)
- W. Liu, Y.Wu, **A. Vriza**, J. Xu et al, Depolymerizable and recyclable luminescent polymers with high light-emitting efficiencies, Nat Sustain (2024).
- Q. Yang, **A. Vriza**, H. Chan, J. Xu et al, Artificial Intelligence for conjugated polymers, Chem. Mater. 2024, 36, 6, 2602−2622.
- R. Vescovi, T. Ginsburg, K. Hippe, D. Ozgulbas, C. Stone, A. Stroka, R, Butler, B. Blaiszik, T. Brettin, K. Chard, M. Hereld, A. Ramanathan, R. Stevens, **A. Vriza**, J. Xu, Q. Zhang, I. Foster, Towards a Modular Architecture for Science Factories, 2023, arXiv preprint arXiv:2308.09793.
- **A. Vriza**, I. Sovago, D.Widdowson, P. A. Wood, V. Kurlin, N., M. S. Dyer, Molecular Set Transformer: Attending to the co-crystals of the Cambridge Structural Datacenter, Digital Discovery 2022. https://doi.org/10.1039/D2DD00068G.
- **A. Vriza**,A. B. Canaj, R. Vismara, L. J. K. Cook, T. D. Manning, M. W. Gaultois, P. A. Wood, V. Kurlin, N. Berry, M. S. Dyer, M. J. Rosseinsky, One class classification as a practical approach for accelerating $\pi - \pi$ co-crystal discovery, Chem. Sci, 2021, 00, 1−3.
- Pia Mueller, **A. Vriza**, Adam D Clayton, Oliver S May, Norman Govan, Stuart Notman, Steven V Ley, Thomas W Chamberlain, Richard A Bourne, Exploring the chemical space of phenyl sulfide oxidation by automated optimization, React. Chem. Eng., 2023, 8, 538-542.

OTHER SKILLS

Organize Organizing and coordinating seminars for AI in materials science in the Materials Innovation Factory, Program planing in international military exercises

Languages English: professional proficiency. German: conversational. Greek:native

Activities Yoga, Dancing Swing, Hiking in the mountains, Rafting, Paddling