DR. RISHI GURNANI

Email: rishipgurnani@gmail.com | >1200 academic citations | h-index = 9
Personal Website | GitHub Profile

EDUCATION

Georgia Institute of Technology | Atlanta, GA | GPA: 4.00

- Doctor of Philosophy, Materials Science & Engineering (MSE) (2019 2023)
- · Master of Science, Computer Science

University of California, Berkeley | Berkeley, CA

· Bachelor of Science, Materials Science & Engineering (2014 - 2018)

Relevant Courses: Polymer Chemistry, Biomacromolecular Structure, Deep Learning, Semi-Supervised Learning

NOTABLE PUBLICATIONS

(Additional on next page)

- 1. Al-assisted discovery of high-temperature dielectrics for energy storage (Nature). Read online.
 - Discovered a polymer dielectric with energy density >11x any commercially available polymer.
- 2. Design of functional and sustainable polymers assisted by artificial intelligence (Nature). Read online.
- 3. polyGNN: Multitask graph neural networks for polymer informatics (2023). Read online.

WORK EXPERIENCE

Matmerize Inc. | Atlanta, GA

Director of Software Engineering & Algorithms (March 2021 - Present)

- Oversee the development of an enterprise ML software (~2000 commits, ~100k lines of code, 5 languages) serving >1000 users from >20 companies.
- End-to-end experience with ML model development & deployment: data-wrangling, web scraping, ML model prototyping & optimization, graphical user interface, unit testing, end-to-end testing, cloud deployment (AWS).
- · Expert in:
 - Physics-informed ML, Graph Neural Networks,
 Cheminformatics, (Un) supervised Learning,
 Dimensionality Reduction, Clustering, Regression,
 Classification.
- · Deep knowledge of:
 - RDKit, PyTorch, SymPy, Numpy, Pandas, Scikit-learn,
 Selenium, Playwright, BS4, Flask, D3, SQL, PyTest,
 Cypress, Vitest, Full Stack Development.

NOTABLE AWARDS AND INVITED TALKS

(Additional on next page)

- 1. **Keynote address**, Research, Innovation & Science for Engineered Fabrics Conference (2024).
- 2. **Graduate Student Award in Polymer Science (Finalist)**, ACS Division of Polymeric Materials (2024).
- 3. Best Ph.D. Thesis, Georgia Tech Chapter of Sigma Xi (2024).
- 4. **Graduate Student Award**, Materials Research Society (2023).
- 5. **Gold Medal for Best Presentation**, 2nd Energy & Informatics International Forum (2022).
- 6. **Best Talk**, Georgia Tech Student Polymer Network Spring Symposium (2022).

OPEN-SOURCE CODE

- 1. **polyGNN**: Code for training fast and accurate structure-property models.
 - Used for the companion paper polyGNN: Multitask graph neural networks for polymer informatics.
 - View on GitHub (35 stars ☆).

ADDITIONAL PUBLICATIONS / WRITINGS

- polyG2G: Machine learning applied to generative design of polymer dielectrics (2021).
- A Physics-Enforced Neural Network to Predict Polymer Melt Viscosity (2024).
- Gas permeability, diffusivity, and solubility in polymers: Simulationexperiment data fusion and multi-task ML (2024).
- Interpretable ML-based predictions in metal-organic frameworks (2020).
- Machine-learning predictions of polymer properties with Polymer Genome (2020).

Complete publication list on my website.

ADDITIONAL AWARDS AND INVITED TALKS

- 1. **Programs to Predict the Properties of New Polymers**, It's a Material World Podcast (2023). View online.
- 2. **Debugging Neural Networks**, Hands-on Data Science & ML Training Series, nanoHUB (2021). Watch on YouTube.
- 3. polyG2G: ML Algorithm for Generative Design of Polymer Dielectrics, 2nd Energy & Informatics International Forum, Tokyo Institute of Technology (2022). View online.
- 4. Polymer Genome: Accelerating Materials Discovery via Data-Driven Approaches,
 - 76th Annual Meeting & Exhibition, Society of Tribologists and Lubrication Engineers (2022). View online.
 - Materials Machine Learning Symposium, Sandia National Laboratory (2021). View online.