

Sina Dehghan Toranposhti

📍 Raleigh, NC ✉ sdegha2@ncsu.edu ☎ 9197580351 in [sina-dehghan](#) 🌐 [Sina-dntp1379](#)

Summary

- Materials scientist with 3 years of experience in conjugated polymer formulation and conformation analysis using data-assisted experiments and machine learning. Built the first conjugated polymer light-scattering dataset and evaluated ML generalizability under out-of-distribution conditions.
- Developed interpretable, physics-based models by integrating experimental metadata into conventional SAM models, improving prediction accuracy and measurement reproducibility.
- Designed hybrid kernels, developed and assessed Gaussian Process models for combining experimental variables and molecular fingerprints for Bayesian optimization in self-driving laboratories.
- Developed automated liquid handling system for multi-solvent formulation and characterization of conjugated polymer solution to study and control aggregation behavior by tailoring intermolecular interactions of solvents in the blend to conjugated polymers.
- Served as chair of Material Science safety committee and Graduate Student Association. Experienced in new lab setup, project leadership, technical writing, lab and safety management, mentoring, and establishing new experimental capabilities.

Education

Ph.D. Material Science & Engineering [North Carolina State University](#) [🔗](#) **Raleigh, NC** 2023-present

M.S. Material Science & Engineering [North Carolina State University](#) [🔗](#) **Raleigh, NC** 2023-2025
CGPA: 3.7/4.0

Professional Experience & Projects

Hybridization of Continuous and Fingerprint features

- Designed hybrid GP models integrating continuous experimental features with molecular fingerprints, via kernel combination (standard GP) and deep kernel learning (MLP-GP, GNN-GP); established kernel design strategies for Bayesian optimization and self-driving laboratory applications in materials discovery.
- Enabled unified uncertainty modeling across structural and experimental spaces, thereby improving Bayesian optimization efficiency and self-driving lab decision-making.
- Assessed prediction accuracy, uncertainty calibration and consistency/stability of feature interpretability across multiple experimental datasets.

Robust Learning from Literature Data: Model Generalizability and Uncertainty for Predicting Conjugated Polymer Solution Conformation

- Built a polymer light scattering dataset to replace one-factor-at-a-time (OFAT) studies, enabling high-throughput candidate discovery and ML-guided insights into structure–processing–property relationships.
- Characterized how solution processing (e.g., temperature) and post-processing parameters affect conjugated polymer conformation.
- Showed that dataset heterogeneity and inconsistent analytical models degrade model performance and uncertainty calibration under distribution shifts, motivating standardized reporting and robust calibration for autonomous discovery of conjugated polymer assemblies.

Metadata Analysis to Reveal Environmental Effects in Large-Area Molecular Tunneling Junctions

- Engineered environmental and temporal features (using splines and trigonometric transformation) by integrating weather data with experimental metadata, enabling interpretable models to reveal how operational and environmental factors affect device performance.

- According to data analysis and feature importance, identified key environmental and temporal factors influencing device performance and variability which can be captured by interpretable models and delta learning.

Stoichiometry-Driven Magnetic Frustration

- Designed of experiment and Bayesian Optimization Campaign (applied to automated pipetting robot) to evaluate to explore structure–synthesis–property of metal (lanthanides)-ligand that can be used in quantum computers.
- Approved **patent application** (63/956,271) based on the synthesis protocol and findings active

Organic Mixed Ionic-Electronic Conductors (OMIECs) Formulation

- Developed an automated platform for multi-solvent formulation and characterization (UV-Vis, four-point probe) of OMIECs to control conformation to improve Organic Electrochemical Transistor performance
- Performed fractionation and purification of conjugated polymers via recycling GPC to minimize dispersity and improve performance

PUBLICATIONS & CONFERENCE PRESENTATION

Orchid: <https://orcid.org/0009-0000-1568-7667>

- Sina Dehghan-Toranposhti, M. Alghamdi, A. Smith, M. Seifrid, Robust Learning from Literature Data: Model Generalizability and Uncertainty for Predicting Conjugated Polymer Solution Conformation, APL Machine Learning, <https://doi.org/10.1063/5.0303721>.
- Sina Dehghan-Toranposhti, A. Martin, C. Du, R. Zmarzlak, M. Thuo, M. Seifrid, Metadata Analysis to Reveal Environmental Effects in Large-Area Molecular Tunneling Junctions, <https://doi.org/10.26434/chemrxiv.15001578/v1> (under review)
- A. Jones, E. Boyce, A. Martin, Sina Toranposhti, F. Amoo, E. Ison, S. Brock, M. Seifrid, M. Thuo, Stoichiometry-Driven Magnetic Frustration. (Submitted to JACS since Oct 1, 2025)
- Dehghan-Toranposhti et al., Fabrication, characterization and evaluating properties of 3D printed PLA-Mn scaffolds <https://doi.org/10.1038/s41598-024-67478-9>.
- Dehghan-Toranposhti et al., "Robust Learning from Literature Data: Model Generalizability and Uncertainty for Predicting Conjugated Polymer Solution Conformation", ACS spring 2025, TSMW Spring 2024-2026

Roles & Responsibility

Research Assistant, Ph.D., ([North Carolina State University](#)) 

NC, USA 2023 - Present

- *President of Graduate Student Association (2025-2026)*
- *Chair of Material Research Safety Meeting (2025-2026)*
- *Safety Officer & Lab manager of DDOMLAB (Since 2023)*

Areas of Expertise/Skills

• Data Science & Coding

Statistical analysis, Feature engineering, Custom kernel design, Uncertainty quantification, Out-of-distribution evaluation, Unsupervised clustering, Bayesian Optimization, Design of Experiment, Active Learning, HMC Sampling, Gaussian Process, Graph Neural Network and GP integration, scikit-learn, PyTorch, RDKit, HSPiP, LSF/Bsub, High Performance Computing, Git, bash scripting

• Experimental

Lab setup, SEC-MALS, recycling GPC, UV-Vis & reflectometry spectroscopy, Dynamic and static light scattering, Automated peptide synthesis, Lab setup & maintenance, OpenTrons liquid handling robots, SiLA2 and Lab Orchestration, Spin coating and deposition, SolidWorks, Additive manufacturing, Differential Scanning Calorimetry, Mechanical Testing, Hot press, MFI

• Soft Skills

Team leadership & initiative, Mentorship and training, Project management, Data-driven decision-making, Experimental design, Safety awareness & compliance