Accelerating Polymer Network Design with Molecular Simulation and Machine Learning

About AFRL:

The Air Force Research Laboratory (AFRL) is the primary scientific research and development center for the Department of the Air Force. AFRL plays an integral role in leading the discovery, development, and integration of affordable warfighting technologies for our air, space, and cyberspace force. AFRL's Materials and Manufacturing Directorate develops materials, processes, and advanced manufacturing technologies for aircraft, spacecraft, missiles, rockets, and ground-based systems and their structural, electronic, and optical components.

RESEARCH LOCATION: Wright-Patterson AFB, OH

PROJECT DESCRIPTION:

Polymer resins and thermosets have a variety of applications such as aerospace composites, coatings, and tough self-healing materials due to their manufacturability and tough mechanical properties. Tuning the topology of the network structure in these materials offers unique pathway to controlling the macroscopic properties (elastic modulus, toughness, etc.) but the complete space of accessible topologies has yet to be observed. This project aims to combine molecular simulations (Monte Carlo, Molecular Dynamics, etc.) with generative machine learning algorithms to sample and explore a vast topology space for controlling the design of new materials for air and space applications.

Polymer networks formed through molecular dynamics (using LAMMPS) will be used to train an efficient graph generative model to learn all-particle and coarse-grained network topologies. This model will then efficiently generate a large set of realistic topologies for networks synthesized for training. Metrics for graph characterization such as chain length dispersity, characteristic loop size, and topological feature concentration will provide insight into the types of topologies that could be realistic targets for polymer scientists.

In light of the graph characterization, a micromechanical model will be developed to account for the combined effect of the topological features present. The resulting analysis pipeline can then be re-trained for new chemistries, giving polymer scientists the ability to pre-screen the space of feasible network topologies and associated bulk material properties without exhaustive experimentation.

The intern will gain familiarity with graph representations of polymer network topologies, as well as experience with connecting their graph to bulk behaviors. Transferable skills will be gained by researching with our code workflow on a local cluster, on the Google Cloud Platform, and on the HPC. The intern will also gain experience with Python packages that are popular across disciplines, including TensorFlow, Numpy, Matplotlib, and Scikit-learn. The structure of the internship will provide a balance of concrete research and open-ended research questions to best ensure an experience that is both productive and challenging.

In addition to these project-specific activities, the AFRL Materials and Manufacturing Directorate (AFRL/RX) provides several opportunities for interns to learn about STEM research areas and career pathways. For example, the directorate organizes the weekly RX101 technical seminar series where the mission and technical overview of each research team is presented. RX also has a machine learning working group and seminar series, called "MIrACLE", that the intern will be encouraged to attend. The AFRL/RX summer student poster session also provides an opportunity for the student intern to interact with AFRL researchers and showcase their summer research activities.

Week 1-2: Introduction to DSRC, Python, and the AFRL graph analysis.

Weeks 3-5: Evaluation of polymer topologies using metrics from graph theory.

Weeks 6-8: Generate new polymer networks and validate their behavior in LAMMPS.

Weeks 9-10: Prepare final report, RX poster, HIP presentation, and archive code.

ANTICIPATED START DATE:

May 2025 – Exact start dates will be determined at the time of selection and in coordination with the selected candidate.

QUALIFICATIONS:

Preferred qualifications include:

- Pursuing a BS, MS or Ph.D. in Material Science, Mechanical Engineering, Computer Science, or Physics.
- Knowledge of either 1) machine learning algorithms, 2) polymer physics and/or 3) LAMMPS.
- Knowledge and coursework in polymer physics and molecular dynamics.
- Knowledge of programming such as MATLAB, Python, C++, and/or Julia is preferred.

ACADEMIC LEVEL:

Degree received within the last 60 months or currently pursuing:

- Bachelor's
- Master's
- Doctoral

DISCIPLINE NEEDED:

- Computer, Information, and Data Sciences
- Engineering
- Chemistry and Material Sciences
- Physics
- Science & Engineering-related