# Molecular Simulation and Design of Polymers for Electrically Assisted Processing Flows

**About AFRL:**

Air Force Research Laboratory (AFRL) is a scientific research organization operated by the United States Air Force Materiel Command. AFRL is dedicated to leading the discovery, development, and integration of aerospace warfighting technologies, planning, and executing the Air Force science and technology program, and providing warfighting capabilities to United States air, space, and cyberspace forces.

The Air Force Research Laboratory Materials and Manufacturing Directorate uses a combination of novel and high-impact experiments, in-house high-fidelity HPC simulation software, and machine learning to characterize and predict the performance of current and emerging materials.

**RESEARCH LOCATION:** Wright-Patterson AFB, OH

**PROJECT DESCRIPTION:**

The project aims to use molecular dynamics simulations to investigate the relationship between polymer structure and electrohydrodynamic properties. By studying the behavior of polymers in electromagnetic fields, we can develop new materials with enhanced properties for applications in electronics, sensors, and aerospace. The project will focus on understanding how charge distribution and molecular weight influence polymer flow and electrorheological properties.

The team will advance our understanding of structure-electrohydrodynamic property relationships through molecular dynamics (MD) modeling (using LAMMPS) of different resin flows in electric fields. We aim to answer the research questions: how does charge sequencing along the polymer backbone modulate its electrorheological properties? In particular, its viscosity and shear- thinning, both orthogonal and along the electric field directions? What is the coupling between shear flow and polarization? What are the prospects for enhanced energy dissipation (for dampers, adhesives, etc.)? Resins with different molecular weights and charge distributions will be tested. Time permitting, the influence of liquid crystals along the backbone will also be considered. MD simulations will be compared with analytical solutions obtained from nonequilibrium statistical mechanics theory.

High-end computing (HEC) will play an indispensable role. Large scale MD simulations are expensive and due to the long-range nature of electrostatics, numerous particle interactions must be resolved.

To achieve the goals of the project, the intern will:

- Familiarize with the project and AFRL. Literature review on electromagnetic interactions in polymer flows. Participate in networking activities (e.g. RX 101).
- Develop LAMMPs-based framework for simulating electromagnetic flows of polymer resins with different molecular weights, charge distributions, and with different electric field magnitudes, frequencies, and directions. Validate the model against literature data.
- Analyze trends in polymer structure-electrohydrodynamic property relationships. Use dimensional reduction (e.g. PCA, UMAP) to probe (latent) polymer structural properties which are driving changes in electrohydrodynamic responses.

- Use computational algebra systems (e.g. Mathematica) and nonequilibrium statistical mechanics formalisms, like the Langevin equation, to derive closed-form approximations for electrorheological behaviors. Compare with simulation data.
- Time permitting, extend framework to allow for liquid crystals along the backbone of the polymer. Repeat studies with an emphasis on understanding the prospects for giant energy dissipation for super-tough, electromagnetically switchable adhesives.
- Final deliverables. Participation in the AFRL poster session, the HIP presentation, and documentation ensure knowledge transfer and research continuity.

MD is broadly applicable in engineering and science, especially in making connections between molecular scale features and bulk properties. Beyond technical tasks, the intern will learn about AFRL, network, attend talks and seminars (e.g. "MIrACLE Forum" on machine learning), and enhance communication skills.

**ANTICIPATED START DATE:**

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

**QUALIFICATIONS:**

Preferred qualifications include:

- Degree obtained or sought in Mechanical Engineering, Chemical Engineering, Physics, or Chemistry.
- Advanced undergraduate or graduate student, or post-doctoral.
- Knowledge of molecular dynamics and/or statistical mechanics.
- Knowledge and coursework in electromagnetism are a plus (but not required).
- Some 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 Materials Sciences
- Physics
- Science and Engineering related