Enhancing MXene Composite Shear Behavior for Electromagnetic Shielding using Molecular Dynamics Simulations

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.

RESEARCH LOCATION: Wright-Patterson AFB, OH

PROJECT DESCRIPTION:

The proposed effort seeks to leverage knowledge from previous (FY24) HIP internship project to model shear strength properties of MXene-based composites using atomistic molecular dynamics simulations. The specific focus of the effort will be to identify the surface functionalities which significantly improve the shear strength of MXenes composites for their incorporation in structural composites for electromagnetic radiation protection. All simulations will be performed using HPC resources.

Structural performance of MXene composites is predominantly governed by non-covalent bonded interactions either between inter-MXene flakes (due to 2D nature) or MXene-polymer interactions, leading to eventual failure due to limited shear strength. We have developed an atomistic force-field potential for MXenes, geared towards accurate prediction of crystal structure, vibrational properties, surface energies, and mechanical properties. Project plan will involve:

- Building surface functionalized (dopamine and its derivatives) MXene films
- Modeling shear behavior for various surface functionalities via MD simulations
- Predicting the bounds of inter-flake shear strength as a function of surface functionalization
- Modeling shear behavior for surface functionalized MXenes with polymeric interfaces

All simulations will be carried out via LAMMPS MD package using HPC DSRC resources. Modeling outcomes will feed into higher-level finite element modeling, guiding multiscale efforts to understand MXene composite structural properties with the eventual goal of developing structurally sound EM-capable multifunctional composites.

Internship Technical Tasks:

- Build multiple functionalized MXenes systems for MD simulations.
- Utilize HPC resources to model mechanical shear properties of MXenes and MXene Composites.
- Analyze generated data to gain understanding of how different surface functionalities affect the shear properties of MXene flakes, providing valuable guidance to higher scale (FEM) modeling.
- Summarize findings in a technical report and draft journal publications post-internship.
- Present findings in technical meetings and an RX-wide poster session.

Professional Development Opportunities:

- Attend RX101 seminars focusing on Materials and Manufacturing Directorate's importance in the AF mission and AFRL's materials research areas.
- Participate in guided tours of RX and, if arranged, HPC supercomputer facilities.
- Engage in weekly technical research team meetings to understand AFRL current and future research directions.
- Interact and learn from the subject matter experts from various technical fields
- Gain a competitive advantage and improve long-term career opportunities.

ANTICIPATED START DATE:

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

QUALIFICATIONS:

The ideal candidate should be knowledgeable in:

- Molecular dynamics simulations on LAMMPS MD package
- High Performance Computing Resources
- Python for Pre-/Post- processing of data

Willingness to tackle complex problems and independent thinking preferred.

ACADEMIC LEVEL:

Degree received within the last 60 months or currently pursuing:

- Master’s
- Doctoral

DISCIPLINE NEEDED:

- Chemistry and Materials Sciences
- Engineering
- Science & Engineering-related