HIGH PERFORMANCE COMPUTING MODERNIZATION PROGRAM

RESEARCH PROJECT #: HIP-25-009

Unveiling Solvent-Driven Exfoliation of MoS2 for Enhanced Aerospace Applications

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:

This project leverages advanced computational modeling to understand how different solvents influence the exfoliation of MoS2, a promising 2D material with diverse aerospace applications, such as high refractive index with low loss in the Infrared for large area optical coatings. By simulating the complex interactions between MoS2 and various solvents, we aim to uncover the key mechanisms driving exfoliation. This will pave the way for optimized techniques to produce single or few-layer MoS2, a crucial step to manufacturing large area films via solution processing. The project will construct atomistic models of MoS2 in different solvents, employ AIMD simulations to analyze exfoliation dynamics, and calculate band structures to identify experimentally verifiable signatures to optimize processing media to ensure stability/shelf life of the inks, develop metrology and measurements techniques to quantify colloidal structure within the processing media, and establish the impact of the media on optical properties via doping.

This project aims to elucidate the solvent-dependent exfoliation mechanisms of MoS2, a crucial step in harnessing its potential for various applications. Through advanced computational modeling, we will investigate the intricate interactions between MoS2 and solvents of varying polarity, providing valuable insights to guide experimental efforts in controlled and efficient exfoliation. The project plan will involve:

- Construct atomistic models of multi-layered MoS2 interacting with diverse solvents, including benzene (non-polar), DMSO (aprotic polar), and DMF (aprotic polar).
- Employ AIMD simulations using the CP2K MD package on HPC DSRC resources to capture the dynamic behavior of MoS2 in different solvent environments. Cleavage and surface energies of MoS2 in each solvent system will be calculated to elucidate key interactions that may influence exfoliation.
- Compute the band structures of multilayered MoS2 in different solvent systems and pinpoint differences that could be experimentally validated through spectroscopic techniques.

Internship Technical Research:

- Create MoS2 - Solvent systems with various types of solvents
- Utilize HPC resources to model surface energies, cleavage energies, and band structure of MoS2
- Analyze generated data to understand the effect of polarity of solvents on MoS2 band structure, cleavage energy, & surface energy.
- Present findings in technical meetings in summer HIP symposium and an RX-wide poster session
- Summarize findings in a technical report and draft journal publications post-internship

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.

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:

- Fundamentals of ab-initio calculations (VASP, CP2K, Quantum Espresso).
- Fundamentals of ab-initio calculations (VASP, CP2K, Quantum Espresso.)
- High Performance Computing Resources and how to run simulations on HPC.
- Python for Pre-/Post- processing of data.

ACADEMIC LEVEL:

Degree received within the last 60 months or currently pursuing:

- Bachelor’s
- Master’s
- Doctoral

DISCIPLINE NEEDED:

- Chemistry and Materials Sciences
- Computer, Information, and Data Sciences
- Engineering