Sean P. Florez

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Security Clearance: Secret (active); Top Secret interim — *investigation initiated 08/2025*
Computational materials & autonomous science. AI/MD/DFT at scale; technology-transition focused.

DoD & National Lab Experience

S&T Scouting Intern *The Joint Staff (J7 / Future Technology Office), Aug–Oct 2025*

- Prioritized propulsion/energy concepts; delivered 8 decision-ready briefs informing J7 concepts and project proposals.
- Coordinated with 4 Service/DoD R&D orgs to map TRL 3–5 capabilities to experimentation and transition paths.
- Advised on integration of academic research into DoD initiatives.

High Perfomance Computing Intern *Air Force Research Laboratory, Wright–Patterson AFB, May–Aug 2025*

- Built a shear-testing MD workflow in LAMMPS for OH-terminated Ti_3C_2 MXenes under controlled hydration; executed 1000+ trajectories using DoD HPC allocations.
- Fit slip probability $p(\tau)$ vs. stress via logistic regression; revealed a non-monotonic hydration effect—low coverage lubricates, high coverage rebuilds strength via water-bridged H-bonds.
- Delivered first MD evidence that hydration tunes MXene interlayer shear by an order of magnitude; defined stress windows and design guidance for EM-shielding composites.

Technology Commercialization Intern *Idaho National Laboratory, May–Aug 2024*

- Conducted 20 customer-discovery interviews (Energy I-Corps); authored a commercialization plan for the PI team.
- Developed AI/LM-driven tech-transfer and compliance workflows for a DOE proposal; resulting in a $2M DOE grant.

Materials Modeling Intern *Air Force Research Laboratory, May–Dec 2023*

- Built and validated an automated DFT workflow (Quantum ESPRESSO + Python/ASE/pymatgen) for high-throughput screening of low-work-function emitters, enabling rapid, reproducible selection for field-emission applications.

Academic Research

Computational Chemistry Researcher *Heinz Interfaces Lab (CU Boulder), Oct 2024–Present*

- Led pH-resolved MD of hydrated α-$Al_2O_3(0001)$ (pH 2–12) using INTERFACE FF; built reproducible pipelines; quantified Na^+/Cl^- layering, and water structuring in agreement with experiment.
- Conducted atomistic MD of Pt-nanoparticle–catalyzed N-ethylcarbazole (NEC) dehydrogenation in NAMD; parameterized NEC and Pt systems for site-specific adsorption/dissociation mechanisms guiding LOHC catalyst design.
- Open-sourced supporting software across projects (MolSAIC; pdb2msi), and post-processing scripts for NEC dehydrogenation and alumina charge/potential profiles.

Computational Materials Research Assistant *Hennig Lab (UF), Oct 2021–May 2024*

- Benchmarked and optimized VASPsol for electrochemical interfaces, developing ML surrogate models that improved solvation energy accuracy by ∼5% across 3000+ DFT calculations spanning diverse solvent–solute systems.

Education

University of Colorado Boulder — Ph.D., Materials Science & Engineering *Expected May 2028*
University of Florida — B.S., Materials Science & Engineering (*Minor: Chemistry*) *May 2024*

Skills

MD/DFT: LAMMPS, NAMD, VASP/VASPsol, Quantum ESPRESSO **FF:** CHARMM, IFF/CVFF
Python: NumPy, pandas, SciPy, MDAnalysis, ASE, pymatgen, matplotlib **HPC:** Slurm/PBS, job arrays
ML/UQ: regression, classification, logistic models, error/uncertainty modeling, feature engineering, scientific NLP
Scale: ∼10k+ core-hours on DoD/academic clusters; 10^6–10^7 MD timesteps; multi-GB trajectory analysis

Leadership & Programs

Co-Founder, LabLink Initiative (Nonprofit) *Aug 2024–Present*

- Built a multi-stakeholder pipeline connecting students to STEM/business roles; led concept for an AI-enabled Career Development Platform aligned to DOE workforce priorities.

Publications / Preprints

- **In preparation (lead author):** *Modeling of MXene Shear Properties via Atomistic Molecular Dynamics Simulations.* Preprint planned 12/2025.