Sean P. Florez

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Research Profile

Computational materials scientist building **AI-accelerated, autonomous workflows** for simulations and interfacial materials. Experience spanning **large-scale MD/DFT campaigns** (LAMMPS, VASP, QE), **ML models for quantum chemistry and experimental data**, and **HPC job orchestration** across DoD and academic clusters. Interested in using generative models, representation learning, Bayesian methods, and agentic systems to close the loop between **simulation, experiment, and scientific decision-making** in materials discovery.

Skills

- **Programming & ML:** Python; scikit-learn, imbalanced-learn; RDKit, Mordred; NumPy, Pandas, Matplotlib; basic PyTorch familiarity.
- **Simulations:** LAMMPS, VASP, Quantum ESPRESSO, NAMD; INTERFACE FF/IFF; VASPsol; Materials Studio; atomistic model building and parameterization.
- **HPC & Automation:** Slurm/PBS, job arrays, shell scripting; workflow design for large MD/DFT campaigns; data lineage, evidence-bundle style post-processing.
- **Domains:** Interfacial MD (MXenes, oxides, MOFs, Pt/NEC), hydration and electrostatics, shear mechanics, solvation models, DAC/CO_2 capture–relevant materials.

Research Experience (Materials & AI/ML)

Computational Chemistry Researcher — Heinz Interfaces Lab, Uni. Colorado 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, and matched experimental surface charge trends.
- Ran atomistic MD of Pt-nanoparticle–catalyzed N-ethylcarbazole (NEC) dehydrogenation in NAMD; parameterized NEC and Pt for site-specific adsorption/dissociation mechanisms relevant to LOHC catalyst design.
- Developed and open-sourced supporting tools (MolSAIC for code-first MD setup; pdb2msi for PDB→Materials Studio conversion) and post-processing scripts for charge, potential, and density profiles.

High-Performance Computing Intern — Air Force Research Laboratory, WPAFB — May 2025 – Aug 2025

- Built a shear-testing MD workflow in LAMMPS for OH-terminated Ti_3C_2 MXenes under controlled hydration; executed 1000+ trajectories on DoD HPC to map stress, hydration, and slip statistics.
- Fit slip probability $p(\tau)$ vs. shear stress using logistic models, revealing 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 strengths by an order of magnitude, defining stress windows and design guidance for EM-shielding composites.

Selected AI/ML for Materials Projects

QM9 Quantum-Chemical Property Prediction (TensorFlow FNNs) — GitHub: qm9-smiles-predictor

- Implemented four fully reproducible pipelines (single-task, multitask, autoencoder, hybrid Mordred+ECFP4) on the QM9 dataset to predict nine quantum-chemical properties for ∼130k molecules.
- Reproduced and critiqued SMILES-FNN literature baselines; showed where multitask learning underperforms and where hybrid descriptors reduce MAE (e.g., for dipole moment and polarizability) relative to Mordred-only models.
- Engineered a modular training/evaluation stack with command-line workflows, tests, and visualization scripts suitable as a starting point for more expressive GNN/equivariant models.

Automated Phase Identification in Experimental pXRD (opXRD Archive) GitHub: opxrd-ml-binary-phase

- Ingested the ∼92k-pattern opXRD archive (∼2.4% labeled) and formulated a binary classification task for the rare As_8O_{12} phase; built an interpolation-based 2θ grid and normalized intensities for ML.
- Trained logistic regression and random forest classifiers; applied SMOTE to address extreme class imbalance and improved minority-phase F1-score to 0.80 with balanced precision/recall on held-out data.
- Positioned the pipeline as a prototype for automated, scalable pXRD analysis in self-driving materials laboratories, emphasizing robustness to heterogeneous experimental conditions.

Optimization of VASPsol Solvation Parameters (DFT + Surrogate)

- Benchmarked the VASPsol implicit solvation model against experimental energies from the Minnesota Solvation Database for neutral and charged solutes in water; explored cavity and screening parameters for implicit solvation.
- Implemented grid search and Nelder–Mead optimization of key VASPsol parameters to reduce RMSE; outlined a surrogate-model-based strategy for future calibrations to avoid high-count parameter sweeps.

Additional Experience

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

- Prioritized propulsion and energy concepts; delivered 8 decision-ready briefs mapping technical readiness, risk, and experimentation paths for TRL 3–5 technologies.
- Coordinated with Service labs and DoD R&D orgs to connect emerging academic research with operational experimentation and transition pipelines.

Technology Commercialization Intern — Idaho National Laboratory (DOE) May 2024 – Aug 2024

- Conducted customer-discovery interviews (Energy I-Corps); led a commercialization plan for a lab-origin technology.
- Supported a DOE proposal (∼$2M awarded) and prototyped AI/NL tools for the technology-transfer team.

Education

University of Colorado Boulder — Ph.D., Materials Science & Engineering Expected May 2028
Focus: atomistic simulations of interfaces; AI/ML-accelerated workflows for materials and interfacial phenomena.

University of Florida — B.S., Materials Science & Engineering (Minor: Chemistry) May 2024

Selected Outputs

- **In preparation:** *Hydration-Tuned Interlayer Shear in OH-Terminated Ti_3C_2 MXenes from Atomistic MD.*
- Open-source: MolSAIC (MD system builder; code-first workflows), pdb2msi (PDB-to-Materials Studio converter).

Leadership

Co-Founder, LabLink Initiative (STEM career access) Aug 2024 – Present

- Built a multi-stakeholder pipeline and AI-enabled matching tools connecting students, labs, and industry for research opportunities.