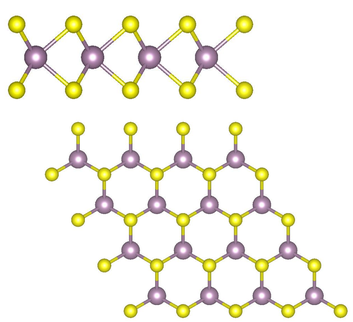
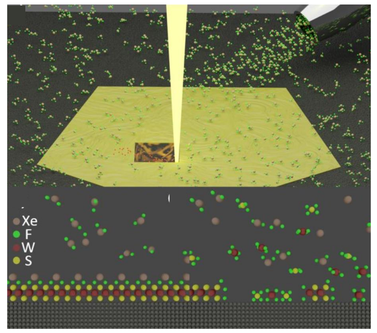
Modeling Gas-Assisted Etching of MoS_2 and WS_2 with Machine-Learned Interatomic Potentials

Samantha Ellis, California State University, Northridge, Northridge, CA 91330
Matthew Lee, Duke University, Durham, NC 27708
Jingsong Huang and Eva Zarkadoula, Oak Ridge National Laboratory, Oak Ridge, TN 37830
Physical Sciences Directorate

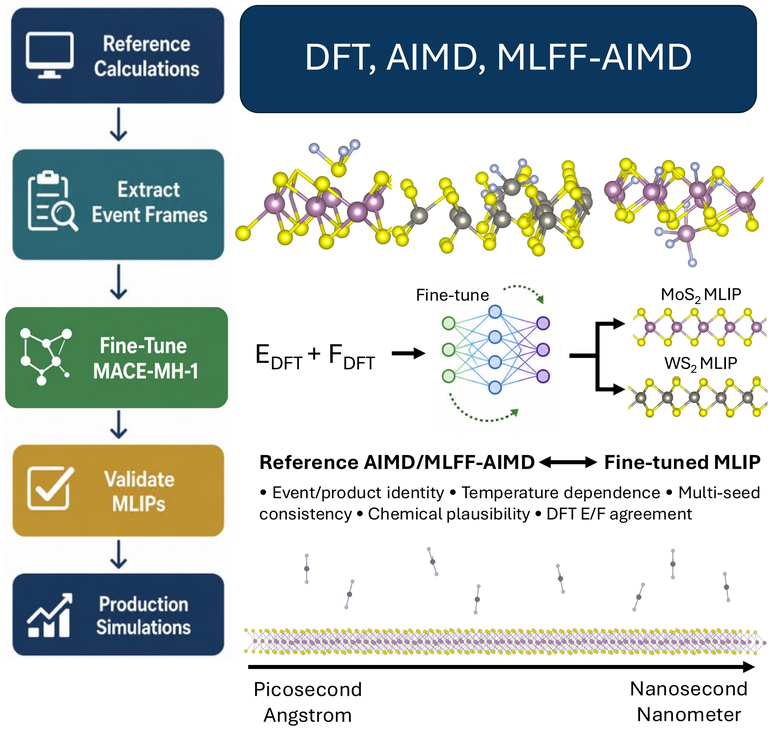
Background & motivation



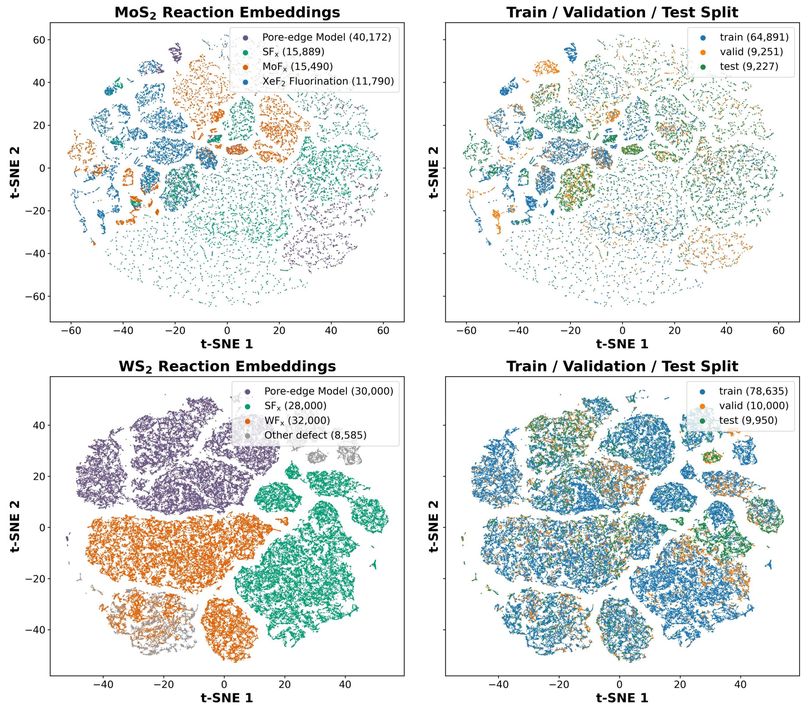


- Atomically thin TMDs offer useful electronic properties but require precise, damage-free patterning.
- XeF_2 etchant assisted FEBIE can etch TMDs with nanoscale precision, but the mechanism remains unclear.
- AIMD captures reactive chemistry but is limited to small length scale and short time scale.
- **Can a fine-tuned MLIP extend etching simulations to larger scales at lower cost?**

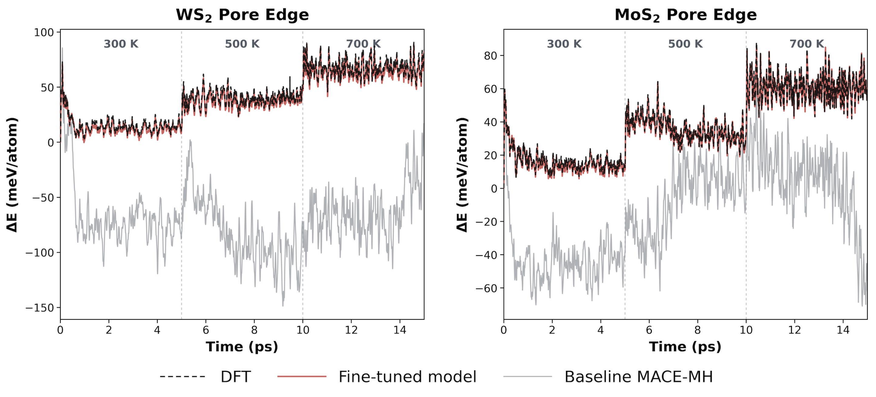
Methods



Training data split for fine-tuning MACE-MH-1



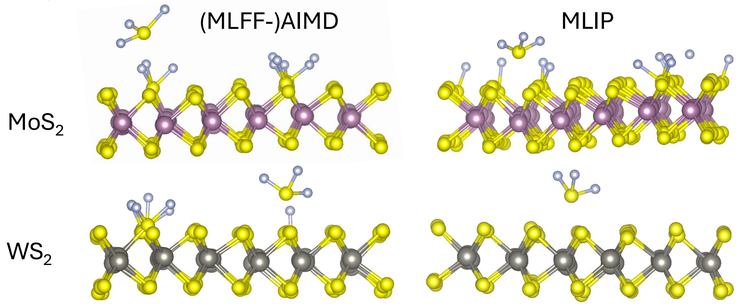
Model improvement on system



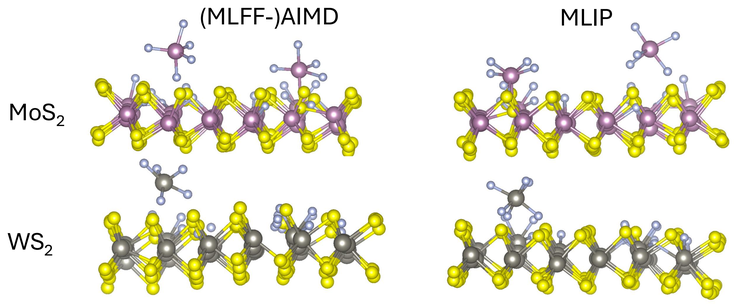
Material	Model	Energy MAE (meV/atom)	Force MAE (meV/Å)	Force RMSE (eV/Å)
MoS_2	Baseline MACE-MH	4304.5	210.6	0.2851
MoS_2	Fine-tuned MoS_2	8.5	46.3	0.0716
WS_2	Baseline MACE-MH	4933.4	214.3	0.2893
WS_2	Fine-tuned WS_2	9.1	57.1	0.0881

Expected etching events can be observed

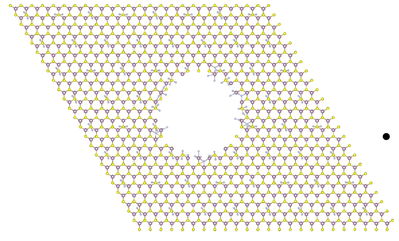
SF_3 desorption



MoF_x /WF_x desorption



Modeling etching at long length/time scale



Constructed large-pore MoS_2 model for future MLIP simulations of progressive etching.

- MLIPs enable nanometer-scale etching simulations over substantially longer times than AIMD.
- A large-cell MoS_2 trajectory captured a candidate pathway from an initially bare S site: S → SF → SF_2 → SF_3, followed by SF_3 detachment.
- Key MLIP-generated events will be evaluated using DFT and targeted AIMD.
- Future simulations will model progressive fluorination and pore growth and compare etching in MoS_2 and WS_2.

Acknowledgments

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