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

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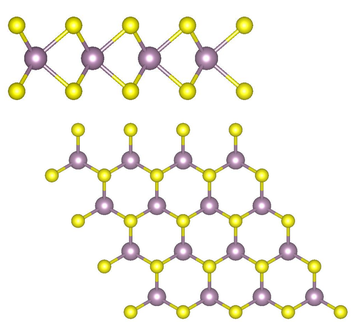
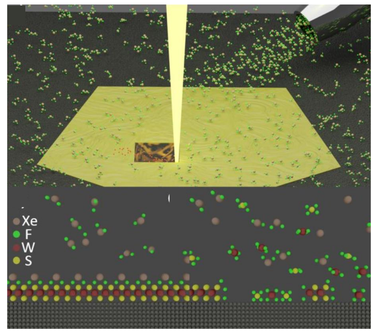
Physical Sciences Directorate

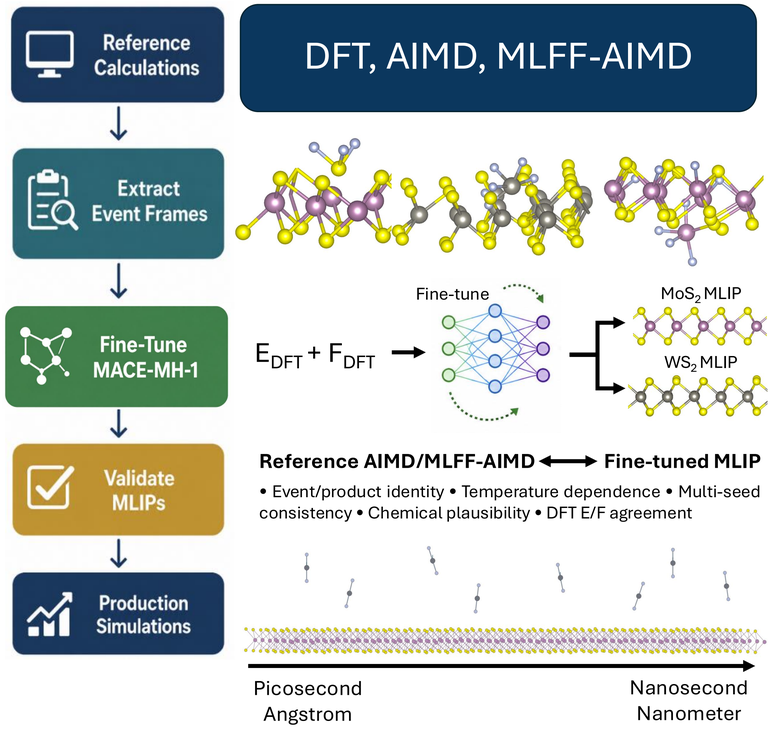
Background & motivation





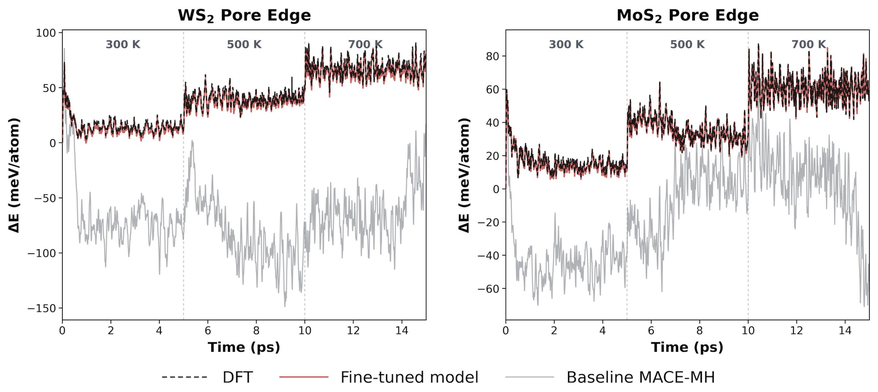
- Atomically thin TMDs offer useful electronic properties but require precise, damage-free patterning.
- XeF_2 etchant assisted FEBIE can etch TMDs with nanoscale precision, but the mechanism remains unclear.
- AIMD captures reactive chemistry but is limited to small length scale and short time scale.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

Methods



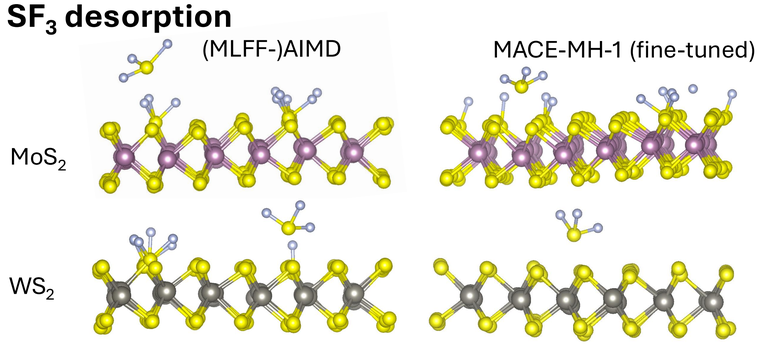
Model improvement on system

Material	Model	Aligned Energy MAE (meV/atom)	Force MAE (meV/Å)	Force RMSE (meV/Å)
MoS_2	Baseline MACE-MH-1	66.0	398.9	695.4
MoS_2	Fine-tuned MACE-MH-1	3.7	46.3	71.6
WS_2	Baseline MACE-MH-1	154.3	589.1	1029.8
WS_2	Fine-tuned MACE-MH-1	8.7	57.1	88.1

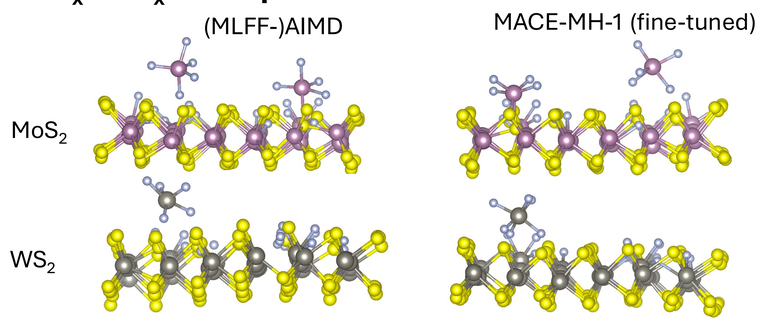


Expected etching events can be observed

SF_3 desorption

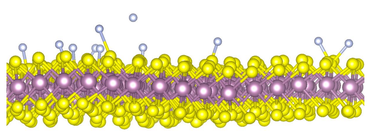


MoF_x /WF_x desorption

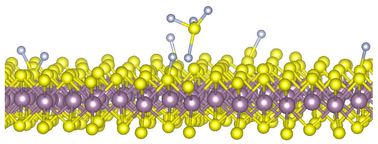


Progressive etching simulation @ 900K

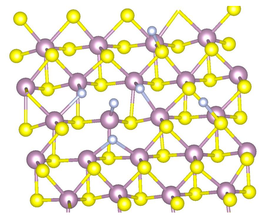
MoS_2 1H, 432 atoms (3.8 x 3.8 nm), 1.4 ns



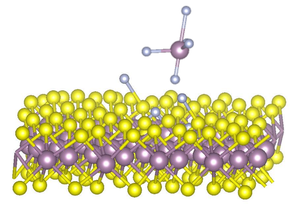
a) Fluorination by F atoms with directed velocity (0.256 ns)



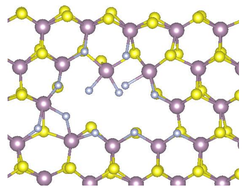
b) SF_3 forms and desorbs (0.265 ns)



c) MoF_4 intermediate (0.367 ns)



d) MoF_5 desorption (0.409 ns)



e) Pore formation via 9 V_S and 2 V_{Mo} (1.394 ns)

- The MLIP can connect individual etching events to progressive nanoscale pore growth

Future Outlook: Comparing MoS_2 and WS_2

- Use matched MLIP ensembles to compare removal pathways, relative event rates, and pore growth in MoS_2 and WS_2.
- Connect these trends to completed DFT/CI-NEB energy barriers to identify material-dependent etching bottlenecks.

Acknowledgments

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