Multiscale Simulation Pipeline for ALD & ALE

from Surface Chemistry to Device-Relevant Property Descriptors

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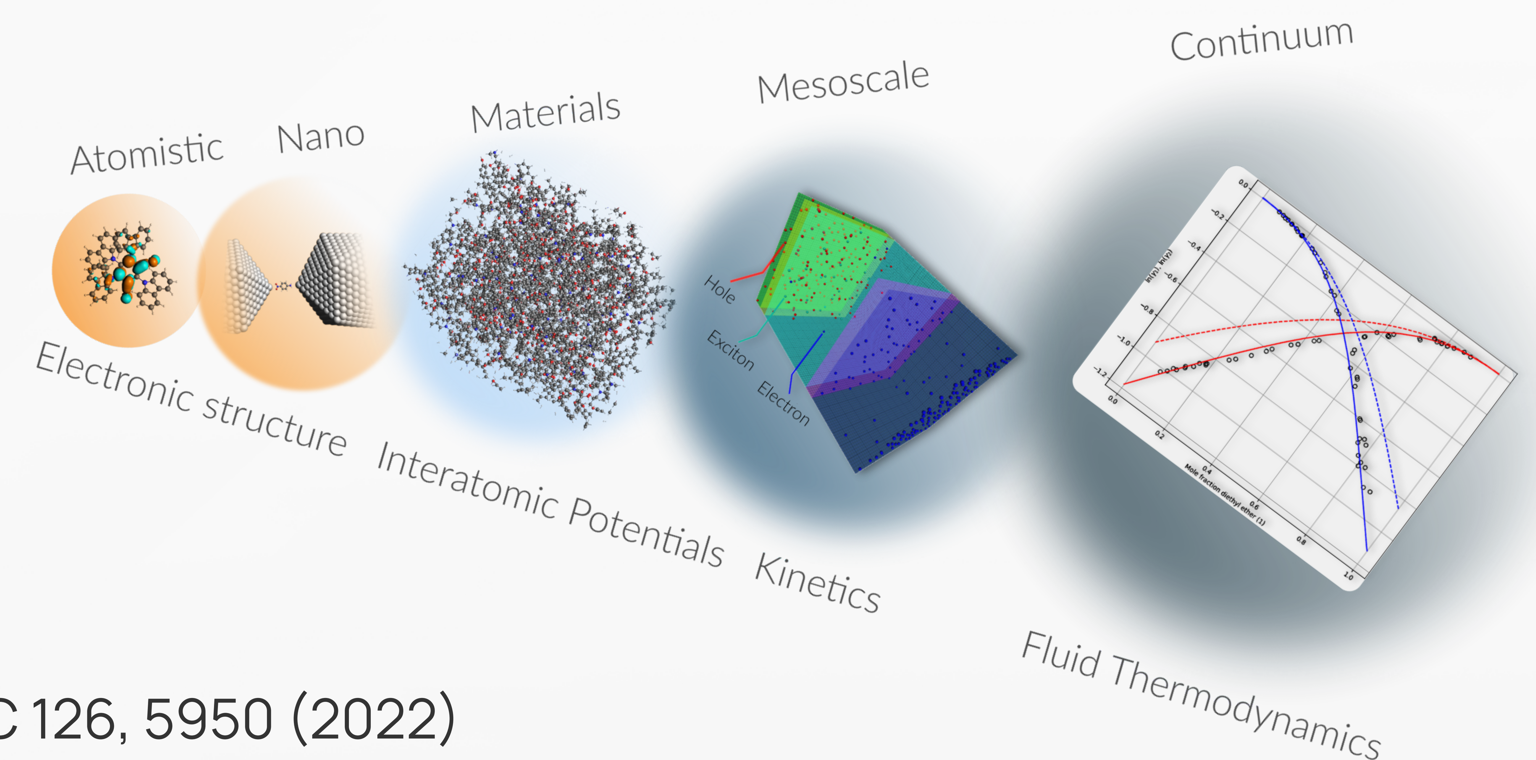
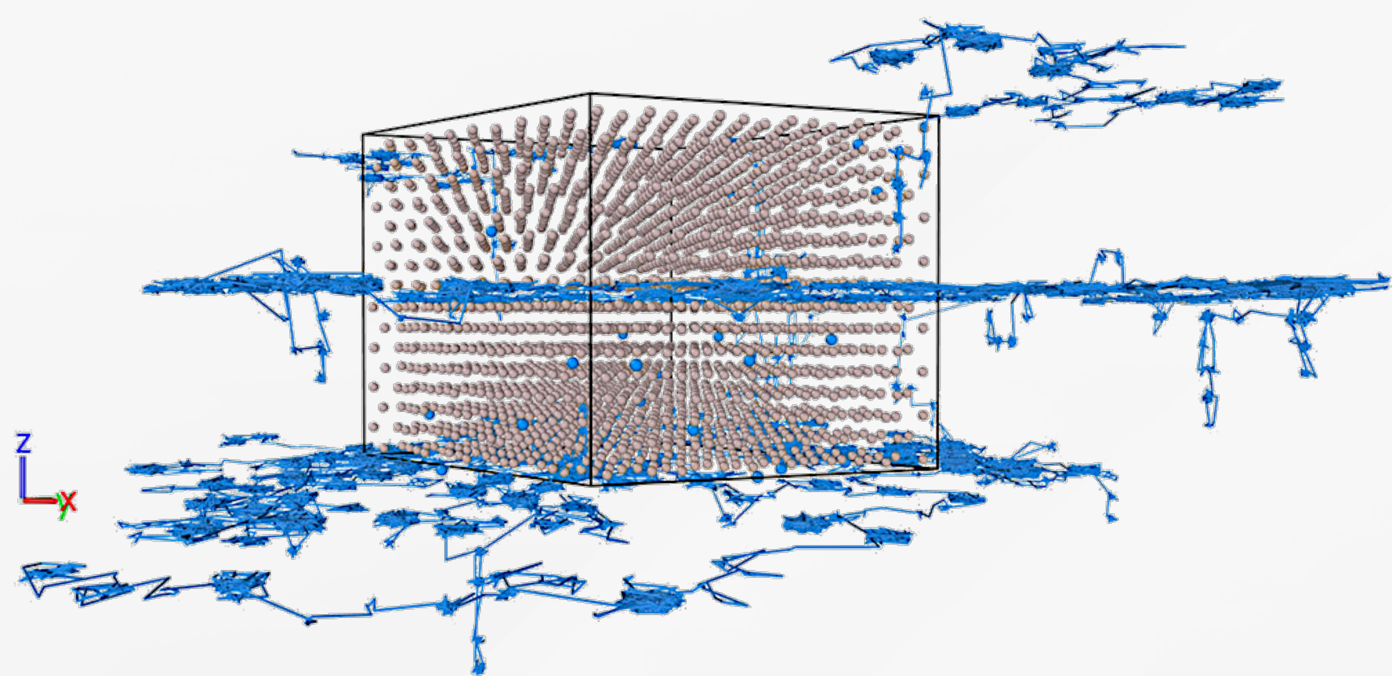
Amsterdam Modeling Suite

Atomistic & multiscale simulations:
- DFT, train (ML) force fields
- Reactions & rates for kinetics (kMC)
- Mechanical, electronic & thermodynamic properties



H + Ru: penetration, sputtering/etching

ReaxFF parametrization using Amsterdam Modeling Suite (J. Phys. Chem. C 126, 5950 (2022)



H diffusion in Ru grain boundaries

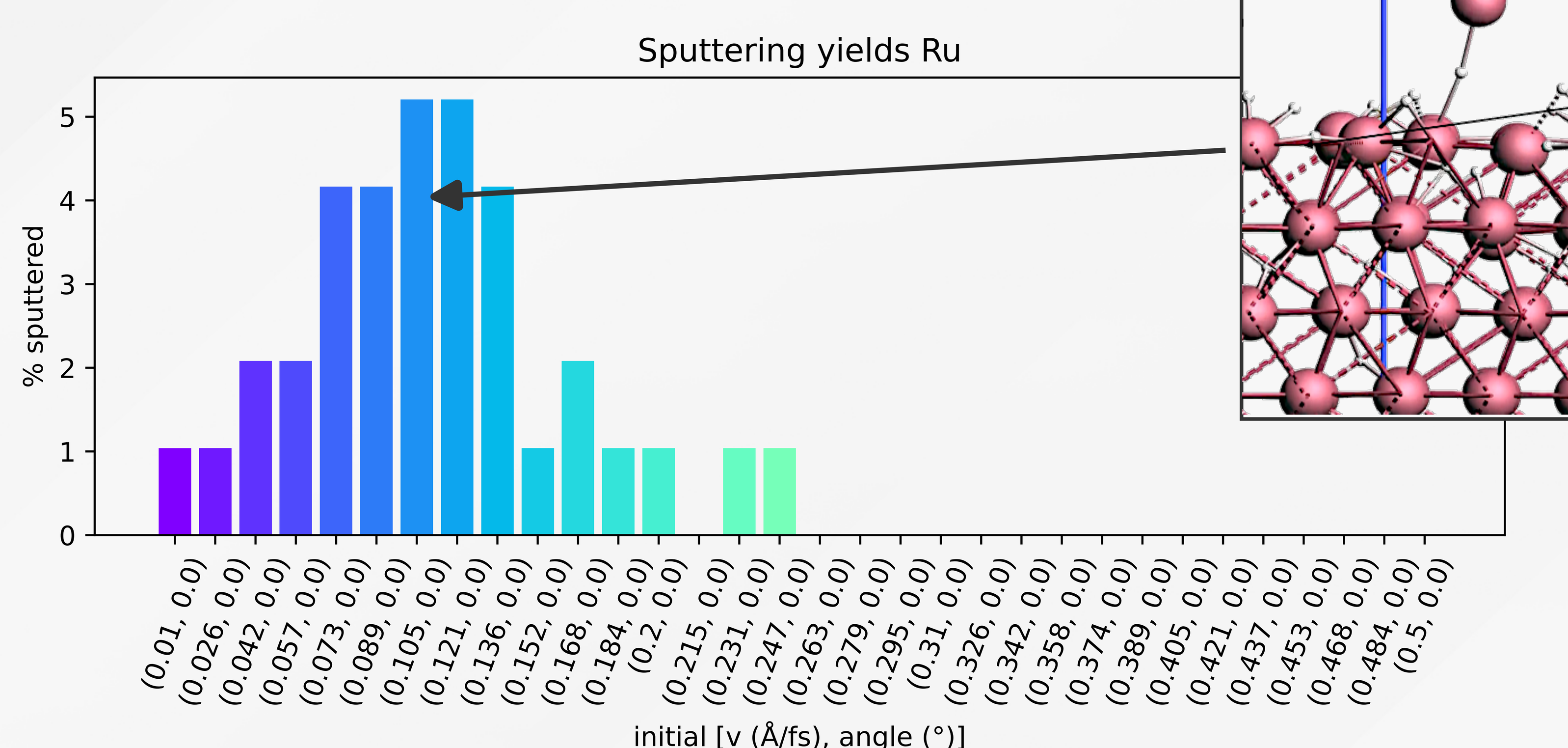
- 1D (tilt), 2D (twist)
- Design rules for Ru morphology → reduced EUV mirror damage

Accuracy improvements
- Automated PES exploration
- Active learning ML potential refinement

MD simulations:
sputtering & H penetration

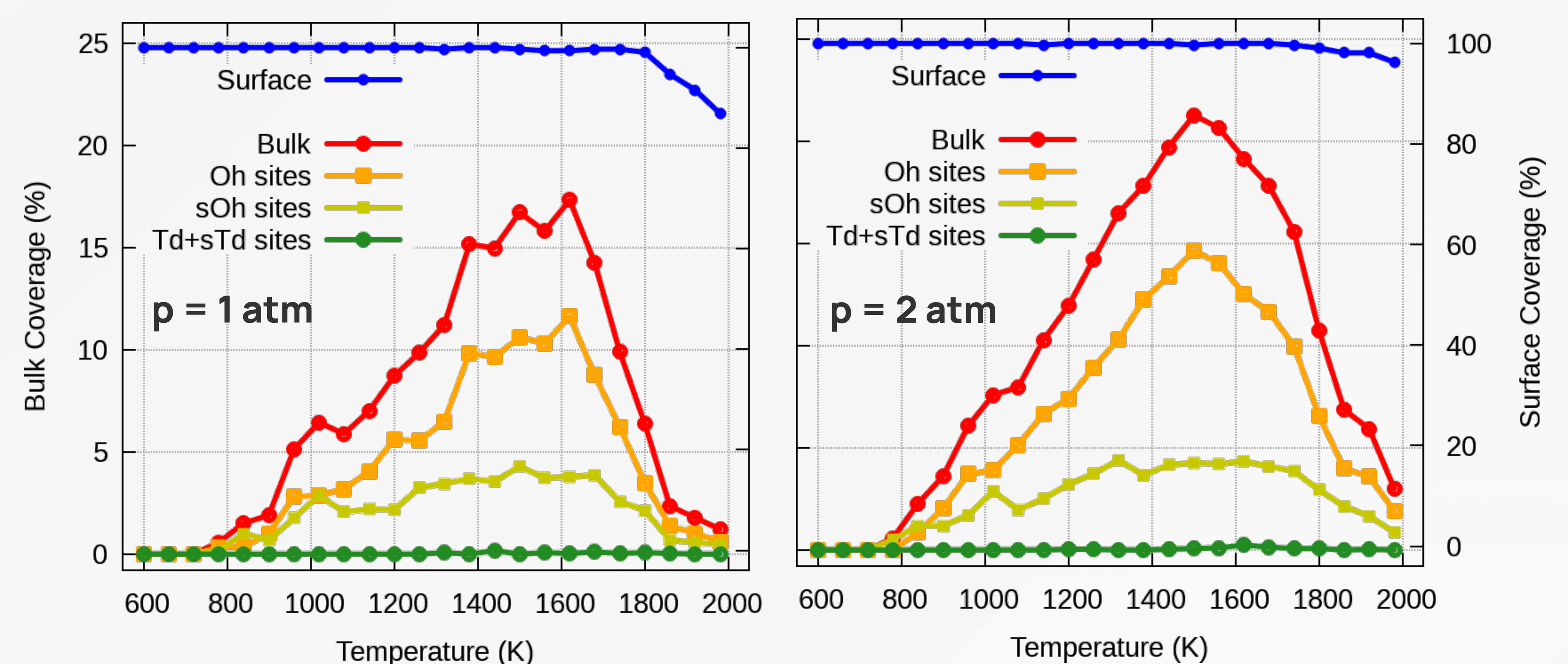
Sputtering Yields

- H incident velocities:
  [0.01 - 0.5] Å/fs -(400-20,000 K)



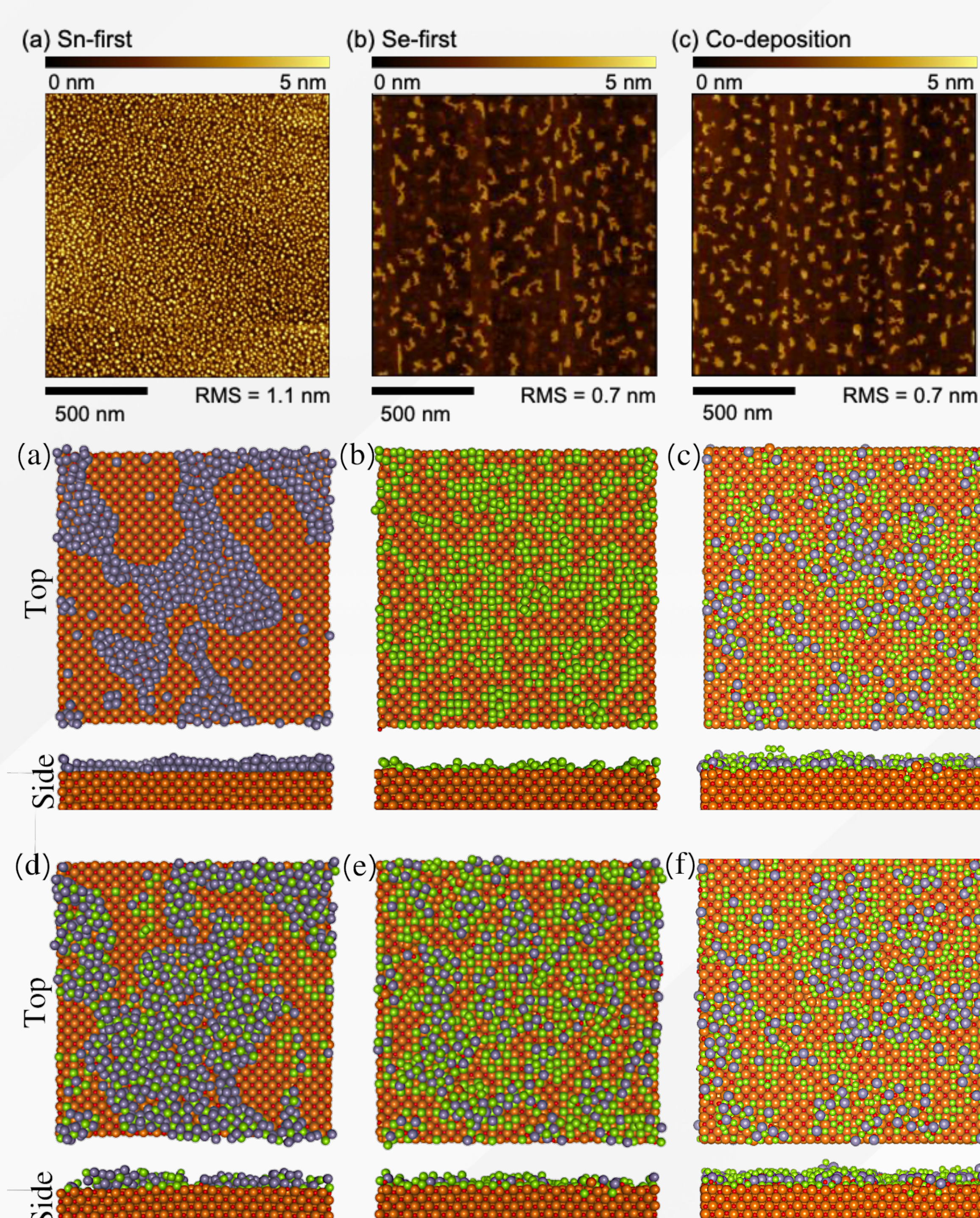
Temperature/Pressure Dependent Coverage

- Auto-extracted H migration rates
  → 3D kinetic Monte Carlo penetration simulations



ALD/MBE + ReaxFF

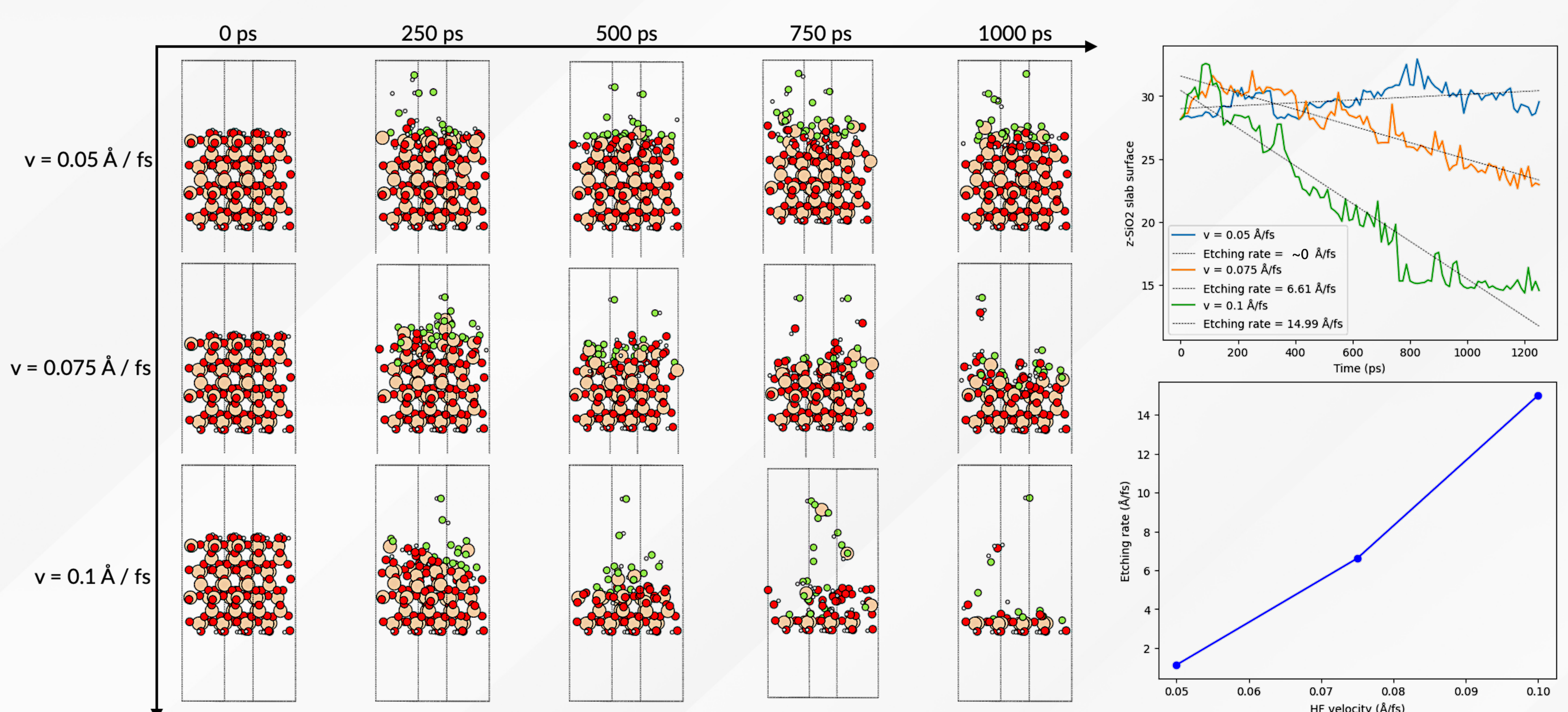
- Graphene masking & flux sequencing control nucleation



(J. Phys. Chem. C 128, 14924 (2024); Mater. Today Adv. 28, 100640 (2025))

Etching rates

- Newly parametrized ReaxFF reproduces etching rates
  (ACS Omega 6, 16009 (2021))



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