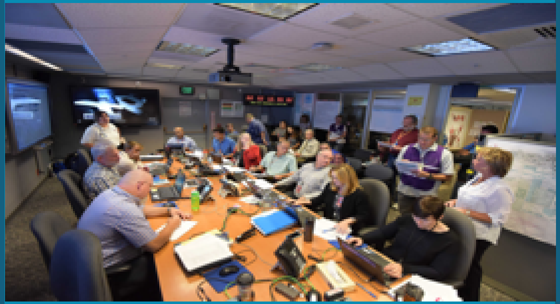
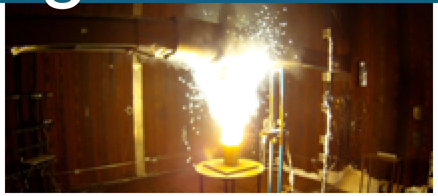
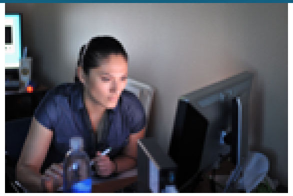
SAND2022-7367C

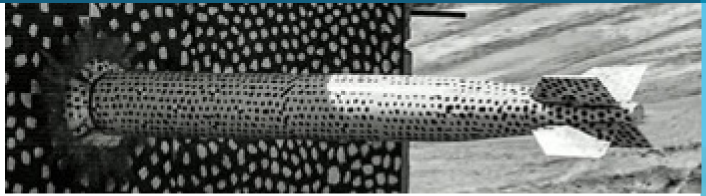
Sandia National Laboratories

Development of SNAP Potentials for Molecular Dynamics Modeling of Hydrogen and Nitrogen Interactions in Tungsten









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2022 PSI Conference

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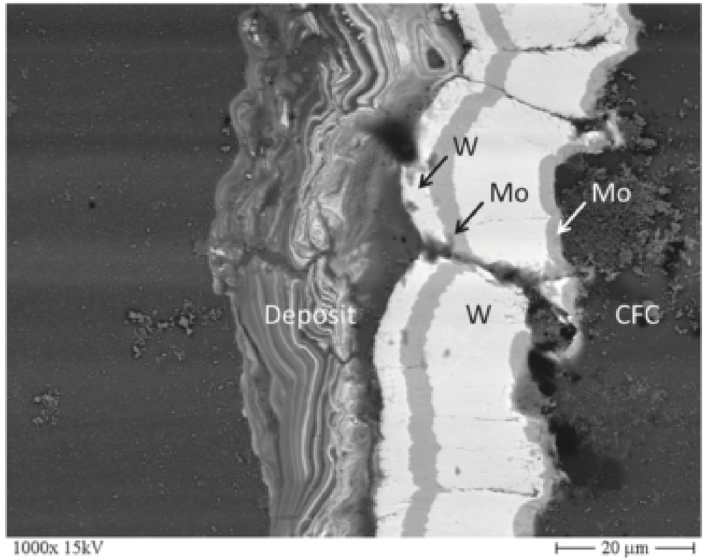
Plasma Material Interactions

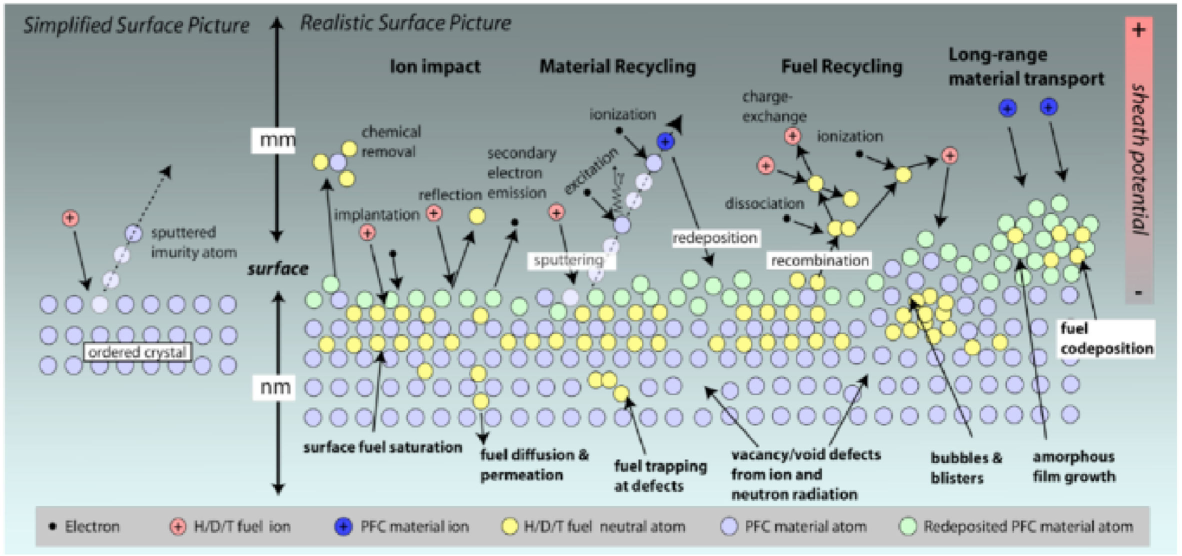
- Important to understand mixed materials effects at divertor surface
  - Material degradation, synergistic effects, implications on hydrogen retention, etc.
- Atomistic modeling will play a critical role but there is a lack of accurate interatomic potentials (IAPs) for modeling these materials especially for multi-component IAPs
- Machine learning interatomic potentials (MLIAPs) have shown to have increased accuracy compared to traditional potentials

Co-Deposit Layer at Divertor Surface

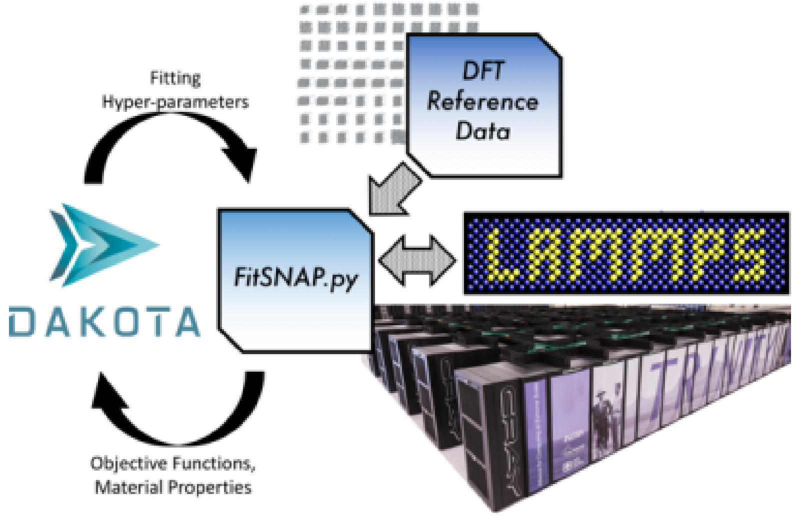


M Mayer *et al* 2016 *Phys. Scr*. **2016** 014051

Complex Physics at Plasma-Material Interface



Wirth, et al. MRS Bulletin 36 (2011) 216-222



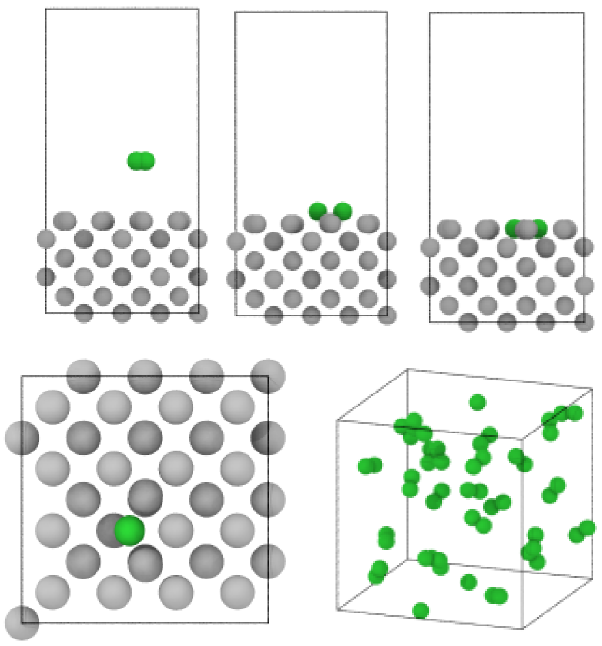
Code available: https://github.com/FitSNAP/FitSNAP

M. A. Wood, M.A. Cusentino, B.D. Wirth and A.P. Thompson, Phys. Rev. B 99, 184305

SNAP Results for W-H

Initial Results

Training Data



Fitted Properties

- Energy/Force errors
- H defect formation energies
- H/H_2 surface binding energies
- H dimer/trimer binding curves

Defect Formation Energies

Bulk Defects	DFT (eV)	SNAP (eV)
E_f^{Tet} (eV)	0.88	0.94
E_f^{Oct} (eV)	1.26	unstable
E_f^{Sub} (eV)	4.08	3.65

Surface Binding Energies

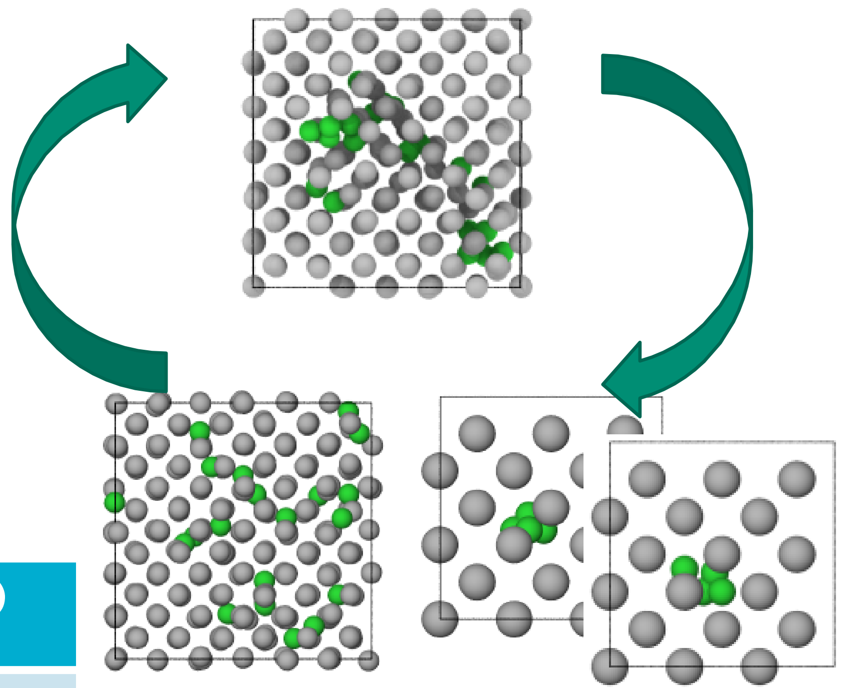
Surface Binding	DFT (eV)	SNAP (eV)
E_B^{H} (eV)	-2.67	-4.02
E_B^{H2} (eV)	-0.53	-0.53

Adsorption Energies

H Ads. (not fitted to)	DFT (eV)	SNAP (eV)
(100) Ads. Site	Bridge	Bridge
(100) Ads. Energy	-0.96	-2.36
(110) Ads. Site	Hollow	Hollow
(110) Ads. Energy	-0.75	-1.80

Introduce Additional Training Data “By Hand” Active Learning

Testing: Poor Behavior



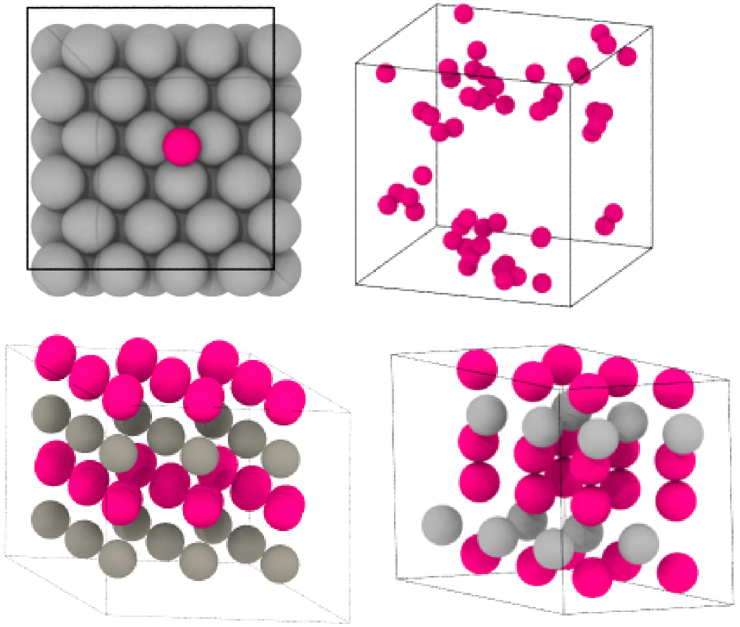
SNAP Refit: Improved Behavior

Run Vasp

W: Grey H: Green N: Pink

SNAP Results for W-N

Training Data



Fitted Properties

- Energy/Force errors
- N defect formation energies
- N adsorption energies
- N dimer/trimer binding curves
- W_xN_y cohesive energies

Defect Formation Energies

Bulk Defects	DFT (eV)	SNAP (eV)
E_f^{Tet}(eV)	1.85	1.92
E_f^{Oct}(eV)	1.11	1.17
E_f^{Sub}(eV)	4.72	4.59

Surface Adsorption Energies

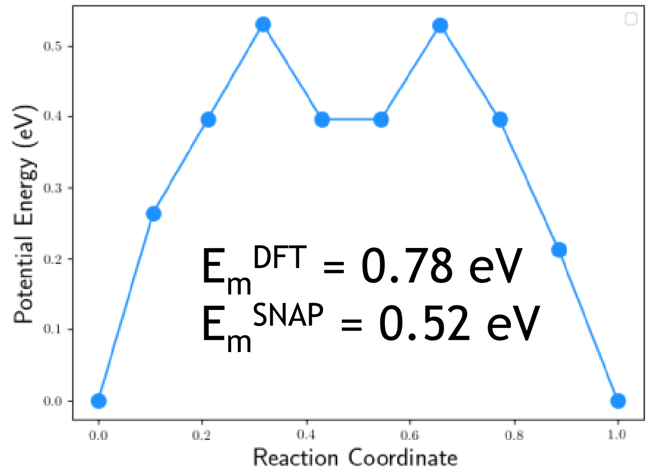
(100) Surface	DFT (eV)	SNAP (eV)
Ads. Site	Hollow	Hollow
Ads. Energy	-3.52	-3.94

W_xN_y Formation Energies

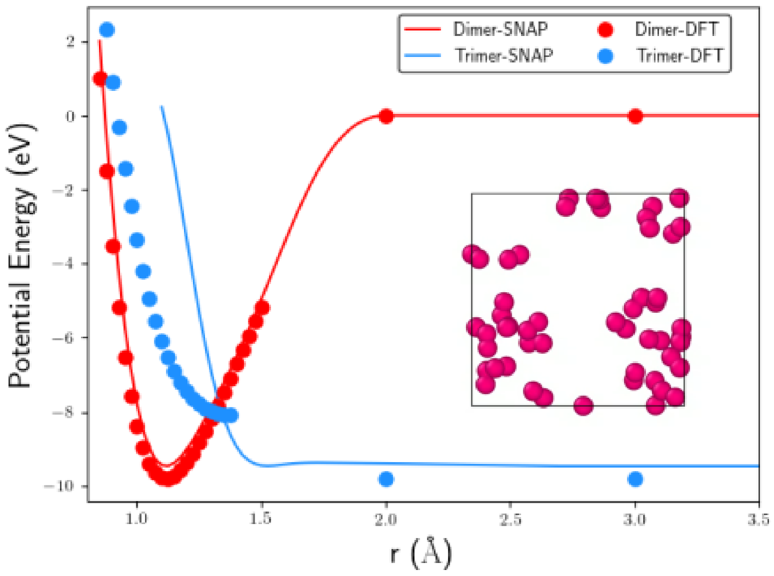
	DFT (eV)	SNAP (eV)
WN_2- P62mmc	-1.82	-2.13
WN_2- P6m2	-0.91	-1.45
WN - NiAs	-0.84	-0.46
WN - WC	-0.23	-1.15
W_2N	-0.03	0.35

Initial Results

Bulk Migration Barrier



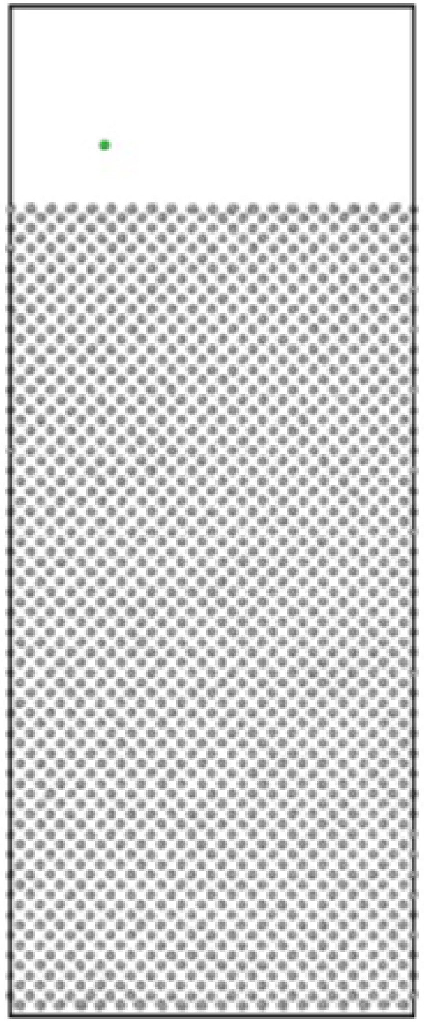
Nitrogen Binding Curves

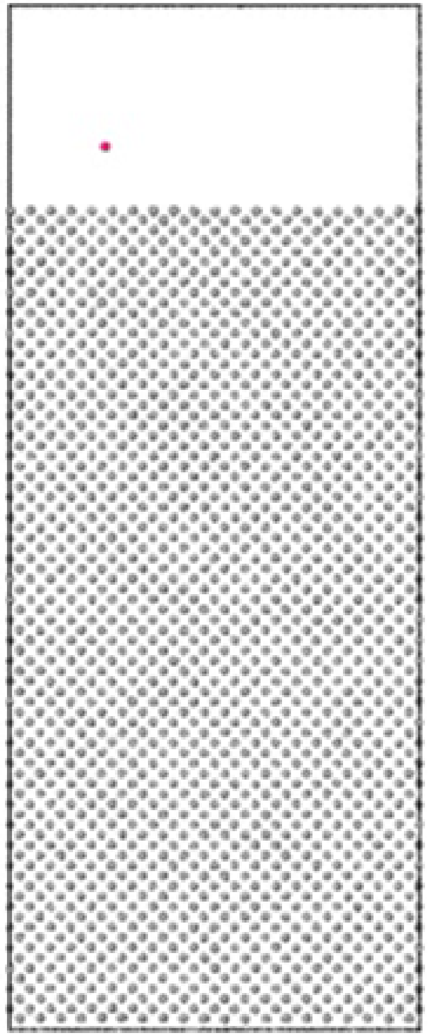


W: Grey H: Green N: Pink

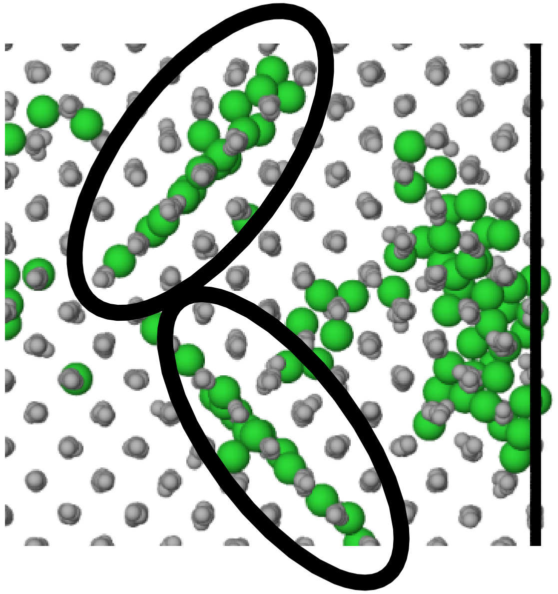
Production Implantation Simulations

- 75 eV hydrogen (left) or nitrogen (right) into (100) tungsten at 1000 K
- Atoms implanted every 10 ps
- Hydrogen:
  - Diffuses throughout the material
  - Forms oriented platelets that were similarly observed with other potentials at high H concentrations
- Nitrogen
  - Remains very close to the surface, within first ~2 nm
  - Surface becomes disordered and the beginning of ordered W-N structures emerge that are similar to NiAs structure

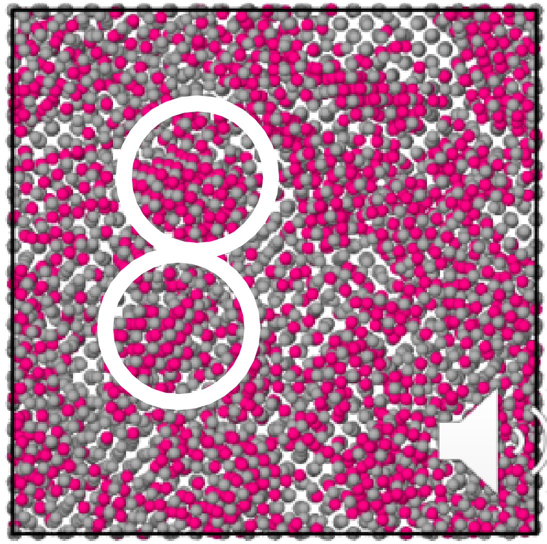




H Platelet Formation

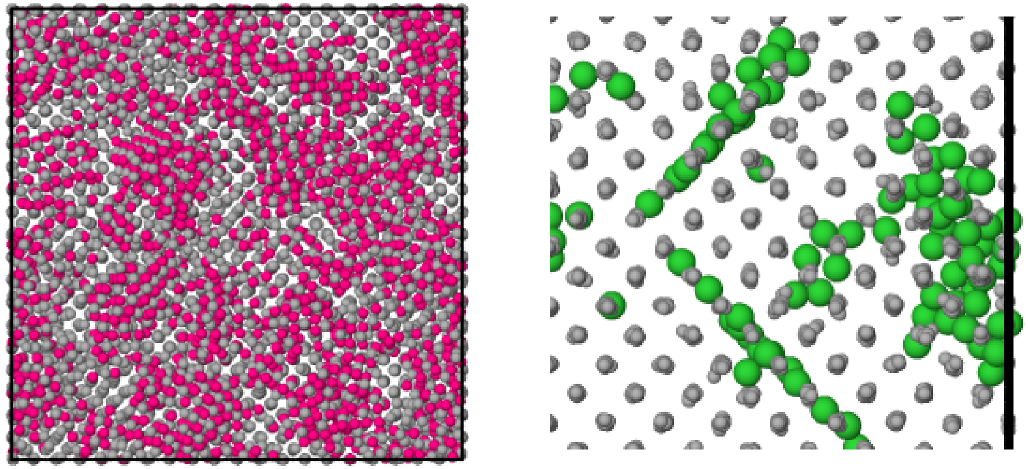


W_xN_x Formation

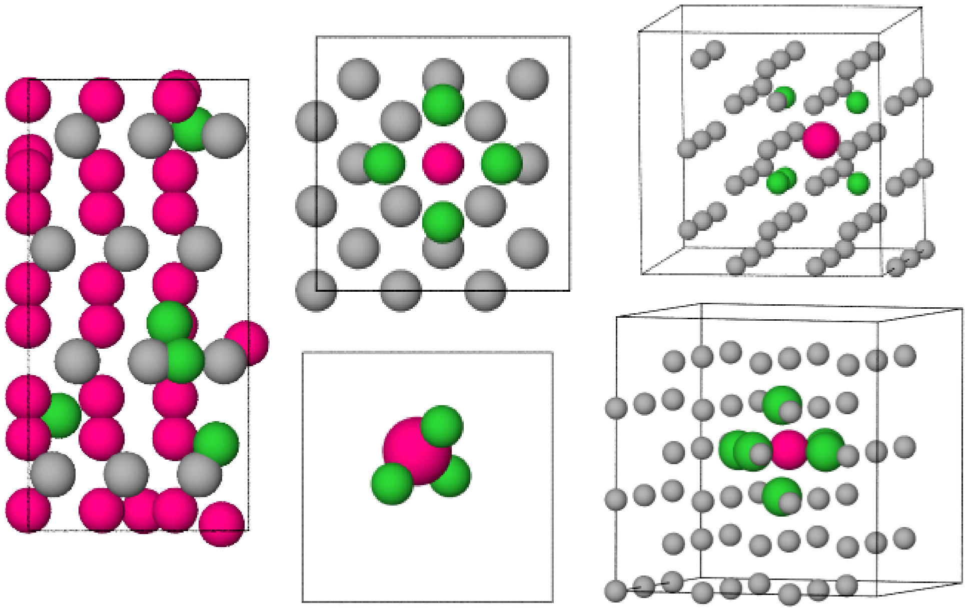


Summary/Future Work

- MD modeling of complex mixed materials at the divertor surface is needed but there is a lack of potentials for these types of material systems
- A SNAP potential for W-H and W-N and SNAP can reproduce key material properties for gas-metal interactions
- The W-H and W-N SNAP potentials have been used to perform production implantation simulations
- Future work entails further refining of potentials and expansion to full W-N-H SNAP potential



Future Work: W-N-H Potential



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