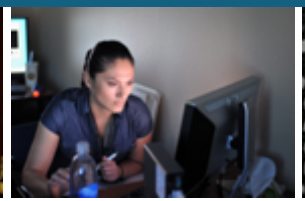
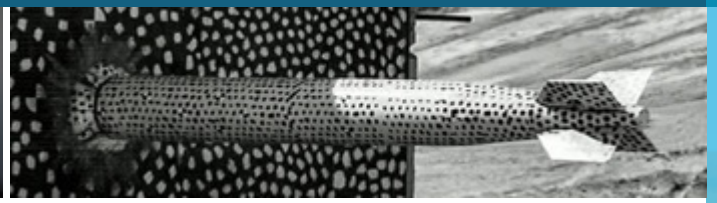
SAND2022-1994C

Sandia National Laboratories

Development of SNAP Interatomic Potentials for Gas-Metal Interactions for Fusion Energy Materials





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[2] Center for Computing Research

2022 APS March Meeting
March 16 2022

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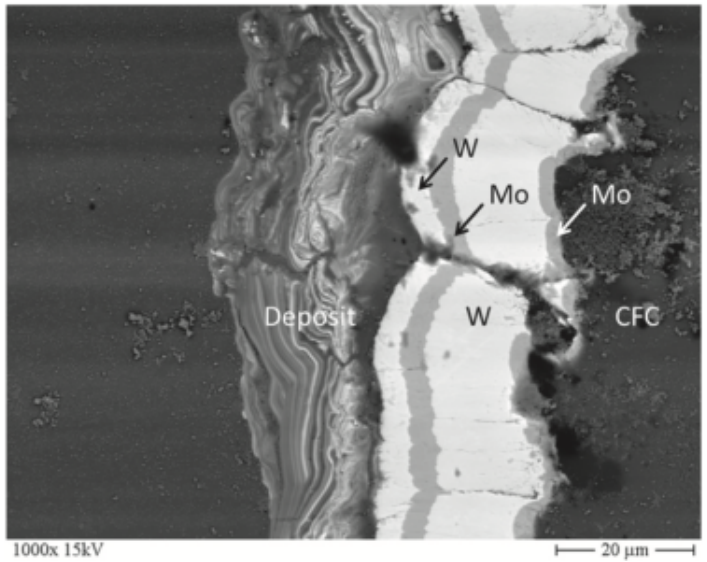
Plasma Material Interactions

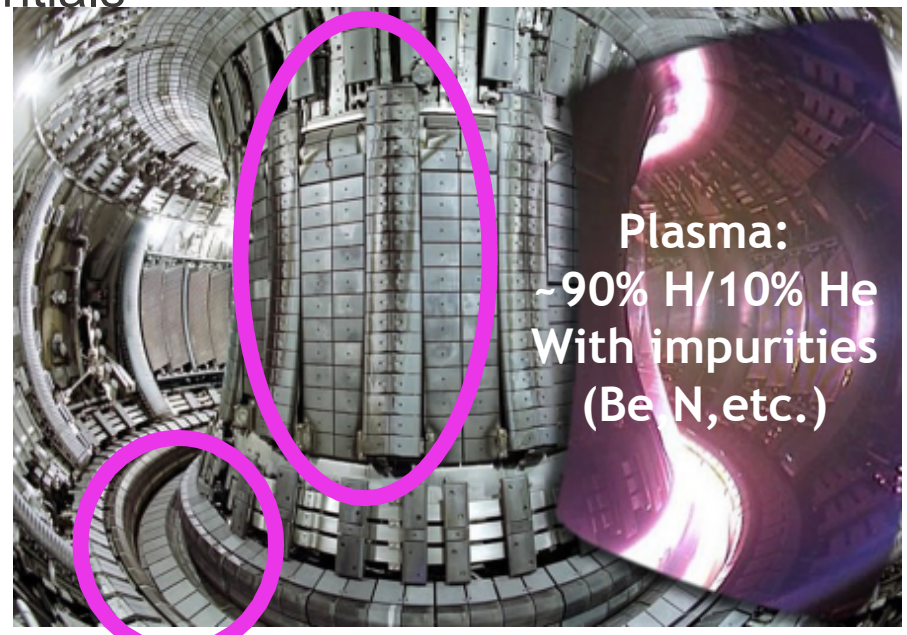
- Important to understand mixed materials effects at divertor surface
  - Material degradation, synergistic effects, implications on hydrogen retention, etc.
- Atomistic modeling will play a critical role but there is a lack of accurate interatomic potentials (IAPs) for modeling these materials especially 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



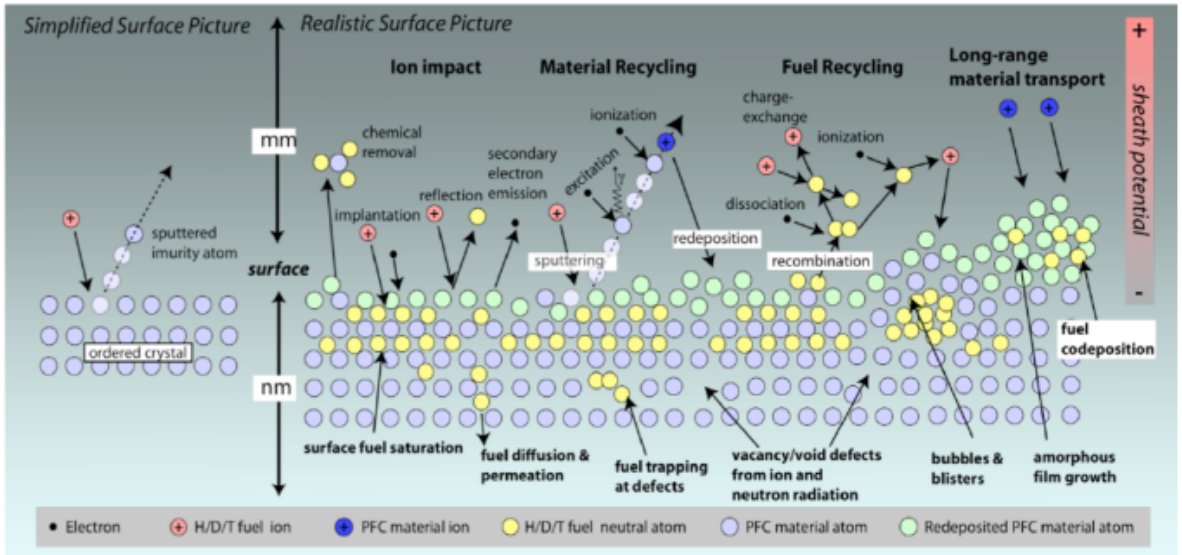
M Mayer *et al* 2016 *Phys. Scr.* **2016** 014051

Beryllium First Wall



Tungsten Divertor

Complex Physics at Plasma-Material Interface



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

SNAP Definition and Work Flow

Model Form

- Energy of atom i expressed as a basis expansion over K components of the bispectrum (B_k^i)

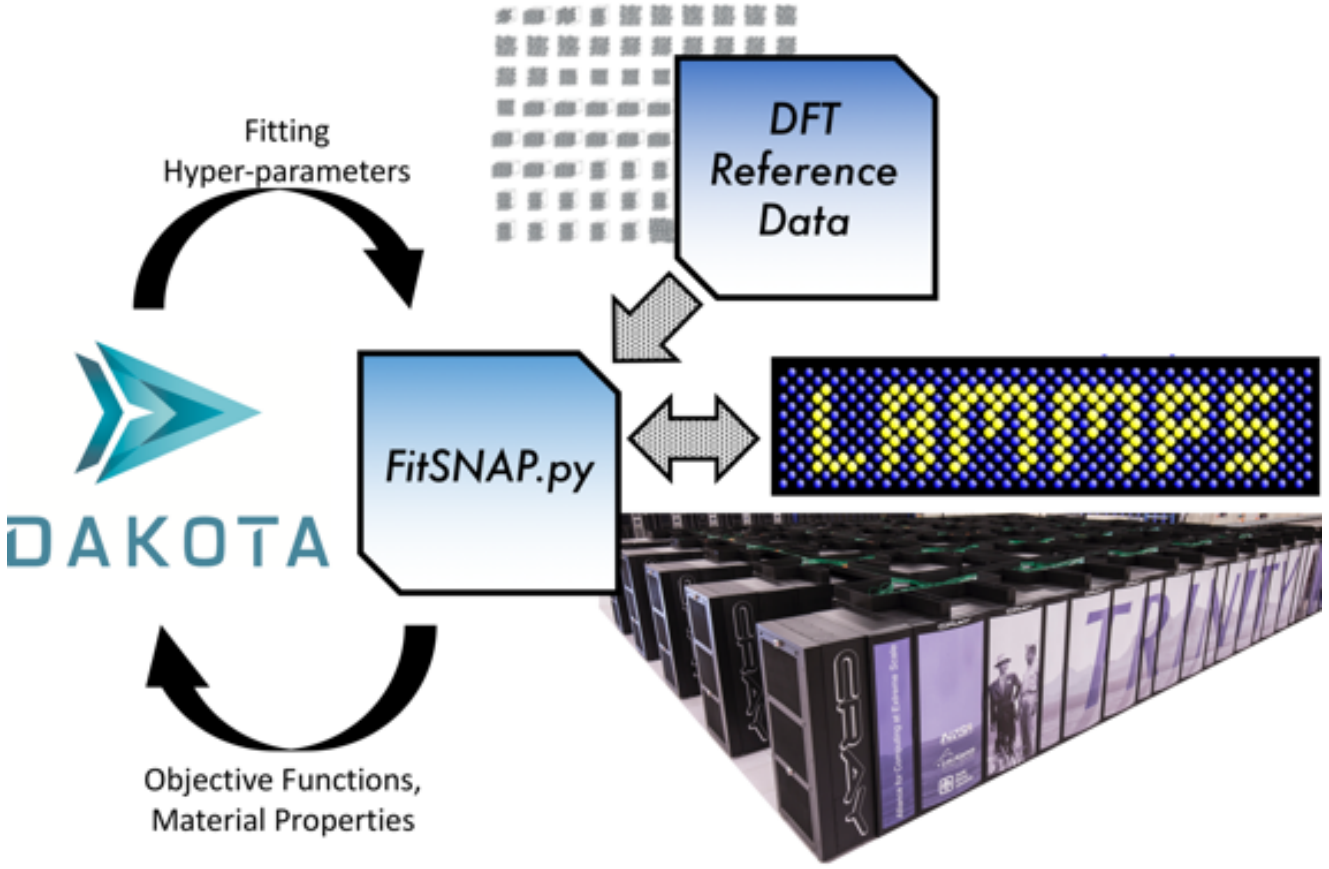
$$E_{SNAP}^i = \beta_0 + \sum_{k=1}^{K} \beta_k (B_k^i - B_{k0}^i)$$

Regression Method

- β vector fully describes a SNAP potential
- Decouples MD speed from training set size

$$\min(||\mathbf{w} \cdot D\boldsymbol{\beta} - T||^2 - \gamma_n \, ||\boldsymbol{\beta}||^n)$$

Weights Set of Descriptors DFT Training



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 Models for Simulating Plasma Material Interactions

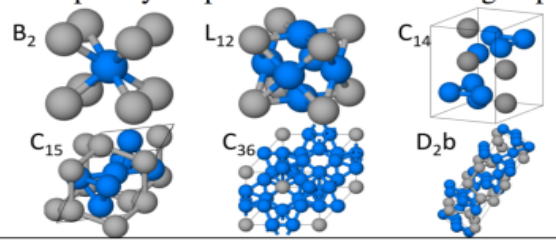
Blue: He
Purple: Be
Gray: W

W-Be SNAP Development

Training Data

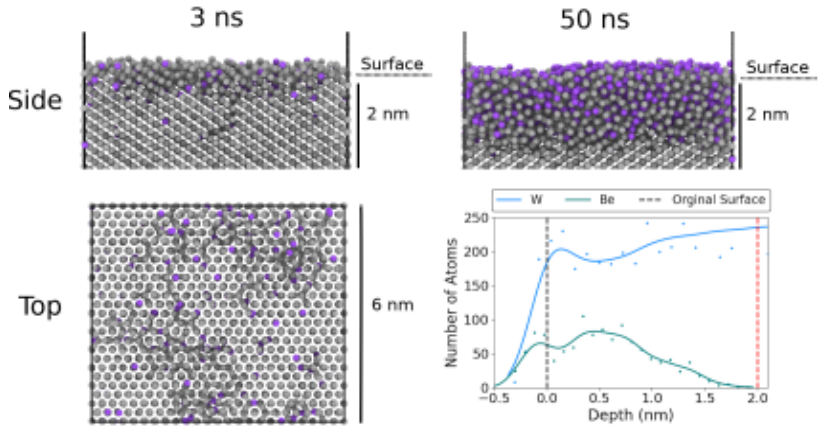
Description	N_E	N_F	σ_E	σ_F
W-Be:				
Elastic Deform†	3946	68040	$\mathbf{3 \cdot 10^5}$	$2 \cdot 10^3$
Equation of State†	1113	39627	$2 \cdot 10^5$	$4 \cdot 10^4$
DFT-MD†	3360	497124	$7 \cdot 10^4$	$6 \cdot 10^2$
Surface Adhesion	381	112527	$2 \cdot 10^4$	$\mathbf{9 \cdot 10^4}$

† Multiple crystal phases included in this group:



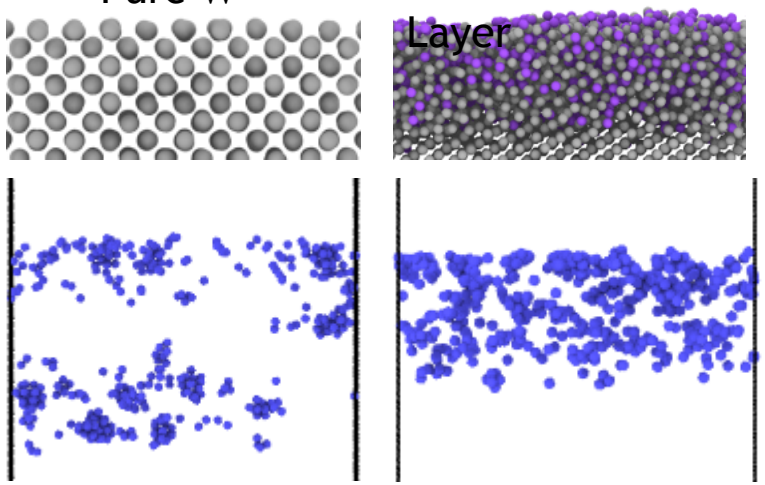
SNAP Results for W-Be

75 eV Be Implantation



SNAP Results for W-Be-He

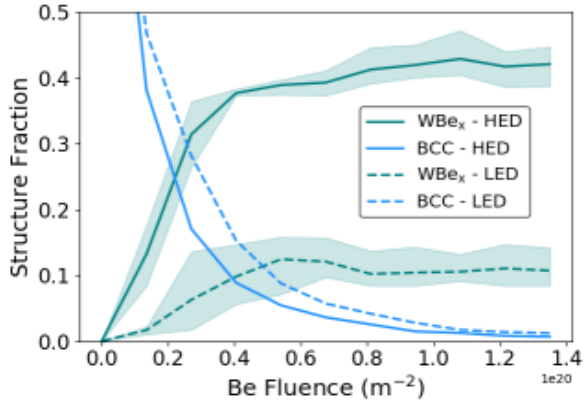
100 eV He Implantation

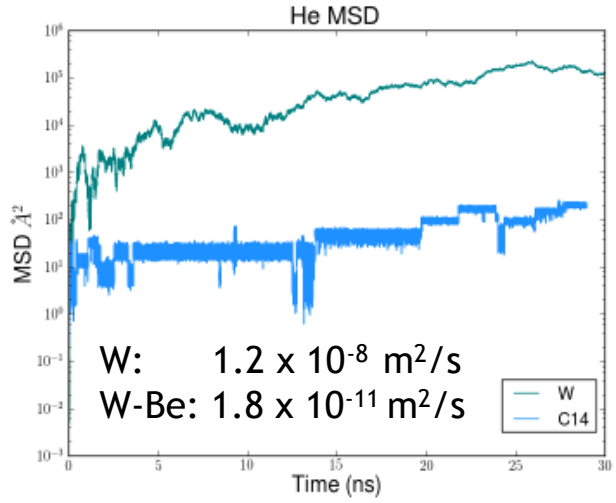


W-Be Intermetallic Formation Energies (eV)

Phase	Composition	DFT[1]	SNAP[1]	BOP[2]
B_2	WBe	0.67	0.30	-2.20
C_{14}	WBe_2	-0.87	-1.27	-4.20
C_{15}	WBe_2	-0.92	-1.15	-4.19
C_{16}	WBe_2	-0.90	-1.22	-4.20
D_2B	WBe_{12}	-0.96	-0.34	-6.69

Intermetallic Growth





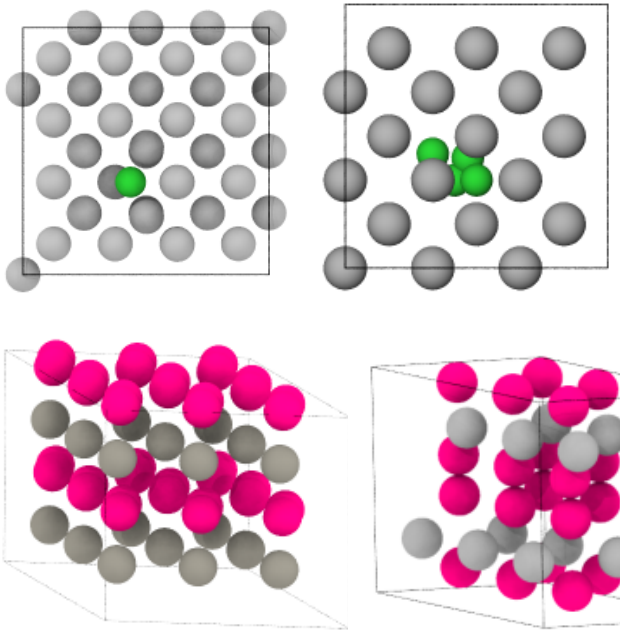
[1] M. A. Wood, et al. 2019 Phys. Rev. B 99, 184305
[2]] C. Björkas et al 2010 J. Phys.: Condens. Matter 22 352206
[3] M.A. Cusentino, et al. 2021 Nucl. Fusion 61 046049
[4] M.A. Cusentino, et al. 2020 Nucl. Fusion 60 126018

Building SNAP Models for Hydrogen and Nitrogen

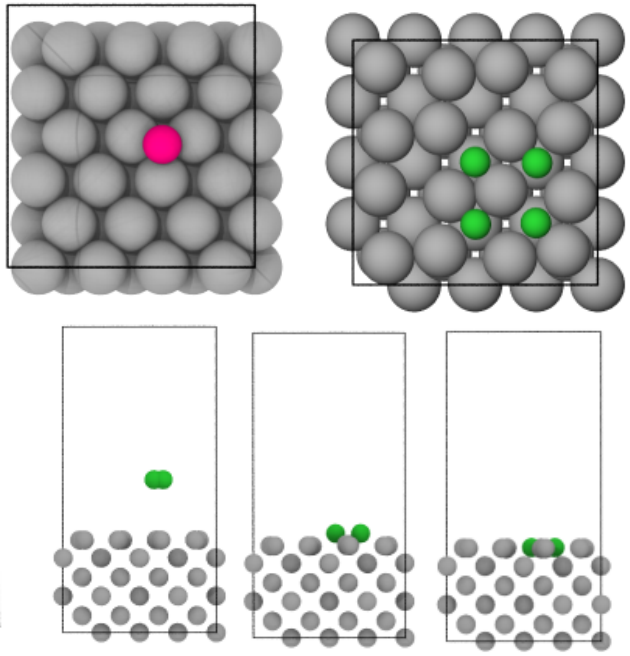
W: Grey
H: Green
N: Pink

- 90% of plasma impinging on divertor is hydrogen
  - Concern of hydrogen trapping in divertor
- Nitrogen also present as impurity species
  - Experiments indicate formation of tungsten nitride layer that results in increased hydrogen retention
- Additional training data required:

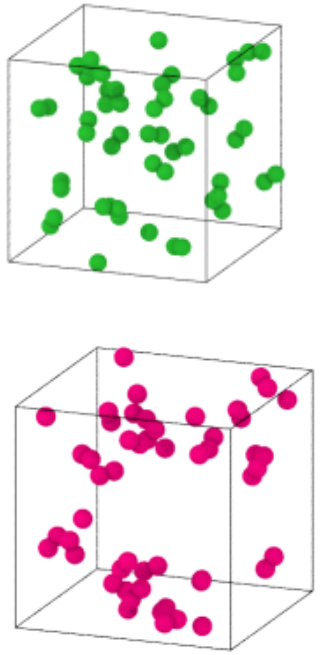
Bulk Configurations



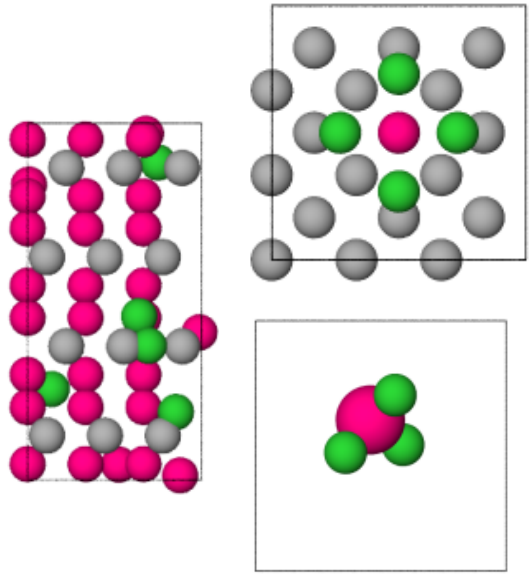
Surface Configurations



Gaseous Configurations



Moving to W-N-H



Fitted Properties

Defect Formation Energies

H Defects	DFT (eV)	SNAP (eV)
E_f^{Tet}(eV)	0.88	2.50
E_f^{Oct}(eV)	1.26	3.24
E_f^{Sub}(eV)	4.08	5.38
E_f^{H2}(eV)	-4.74	-4.75

N Defects	DFT (eV)	SNAP (eV)
E_f^{Tet}(eV)	1.85	1.89
E_f^{Oct}(eV)	1.11	1.09
E_f^{Sub}(eV)	4.72	2.90
E_f^{N2}(eV)	-9.79	-9.47

W_xN_y Formation Energies

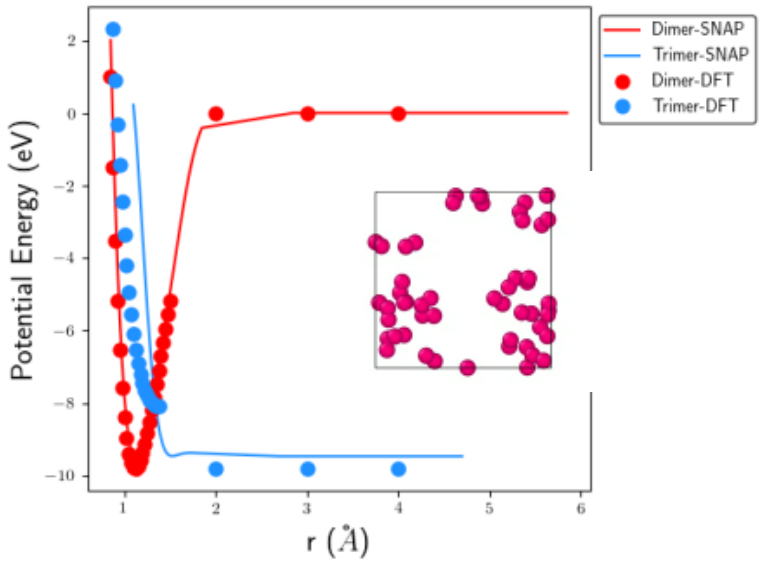
N Defects	DFT (eV)	SNAP (eV)
WN_2- P62mmc	-1.82	-1.82
WN_2- P6m2	-0.91	-1.75
WN - NiAs	-0.84	-1.74
WN - WC	-0.23	-1.51
W_2N	-0.03	3.29

Adsorption Energies

H Ads.	DFT (eV)	SNAP (eV)
(100) Ads. Site	Bridge	Bridge
(100) Ads. Energy	-0.96	-1.57
(100) H_2 Ads. Energy	-0.80	-0.76
(110) Ads. Site	Hollow	Hollow
(110) Ads. Energy	-0.75	-0.69
(111) Ads. Site	Bridge	Bridge
(111) Ads. Energy	-0.59	-1.42

N Ads.	DFT (eV)	SNAP (eV)
(100) Ads. Site	Hollow	Hollow
(100) Ads. Energy	-3.52	-4.33
(100) N_2 Ads. Energy	-2.94	-8.63
(110) Ads. Site	Hollow	Bridge
(110) Ads. Energy	-3.59	-2.58
(111) Ads. Site	Bridge	Hollow
(111) Ads. Energy	-3.08	-3.44

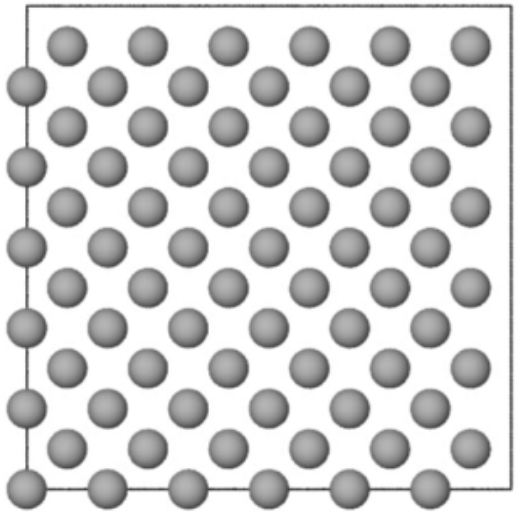
Nitrogen Binding Curves

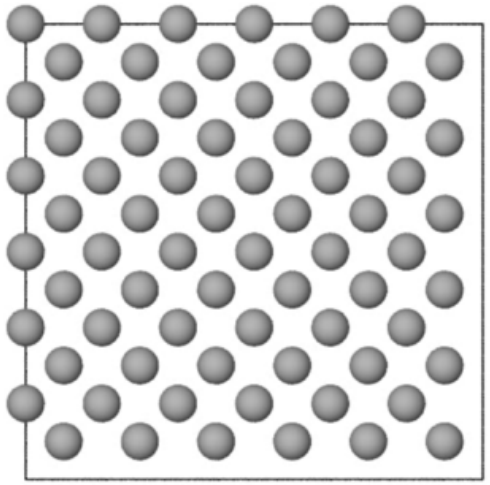


Post-Fitting Testing

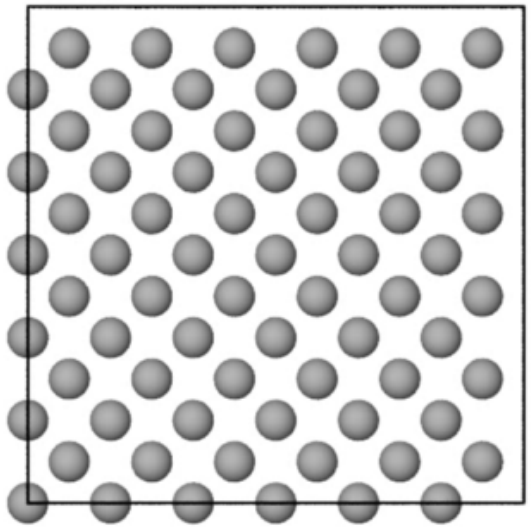
W: Grey
H: Green
N: Pink

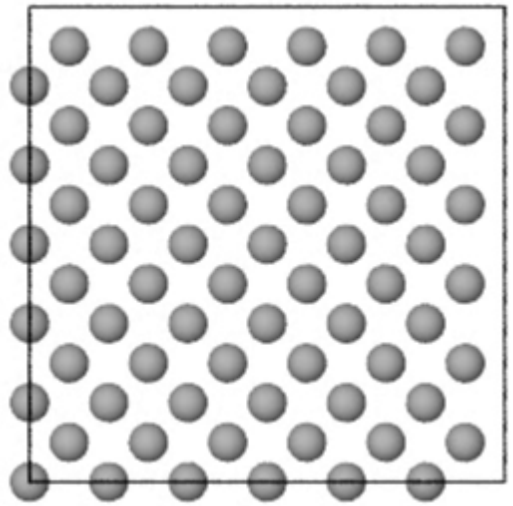
Bulk Dynamics



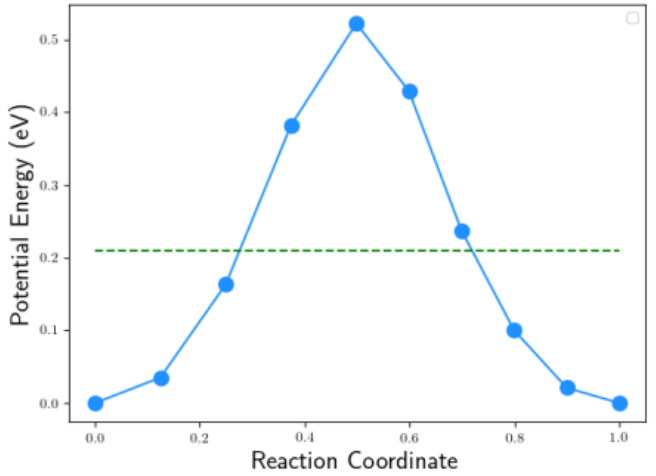


Surface Dynamics

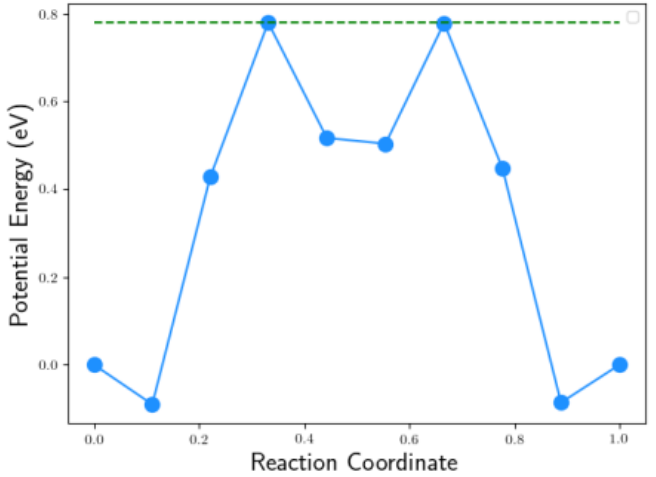




NEB Barriers (Bulk)

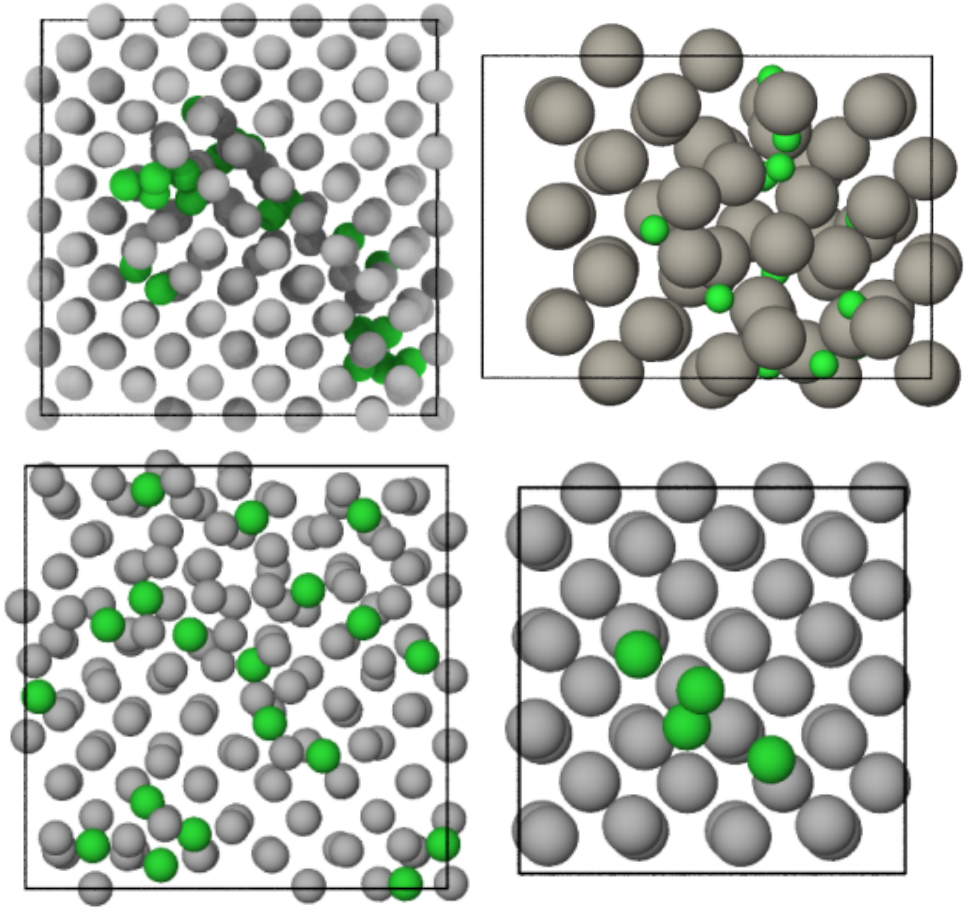


Nitrogen



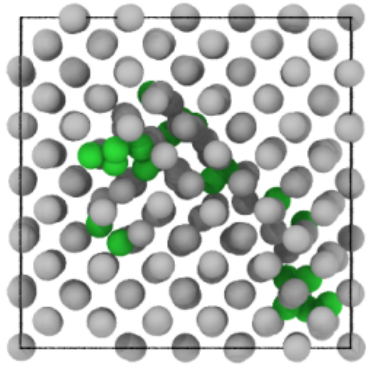
Expanding Training Data Based on Early Potentials

Initial “Poorly” Behaving Potentials

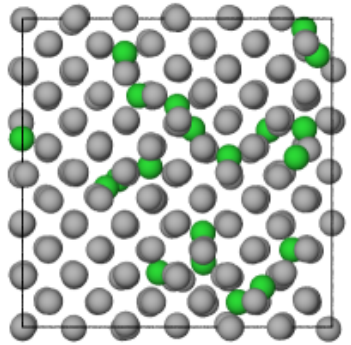


Introduce Additional Training Data
“By Hand” Active Learning

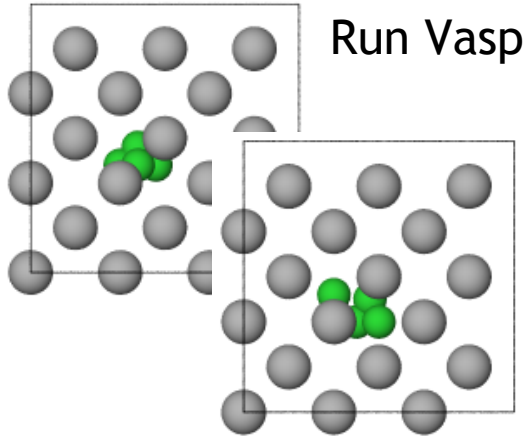
Testing:
Poor Behavior



SNAP Refit:
Better Behavior

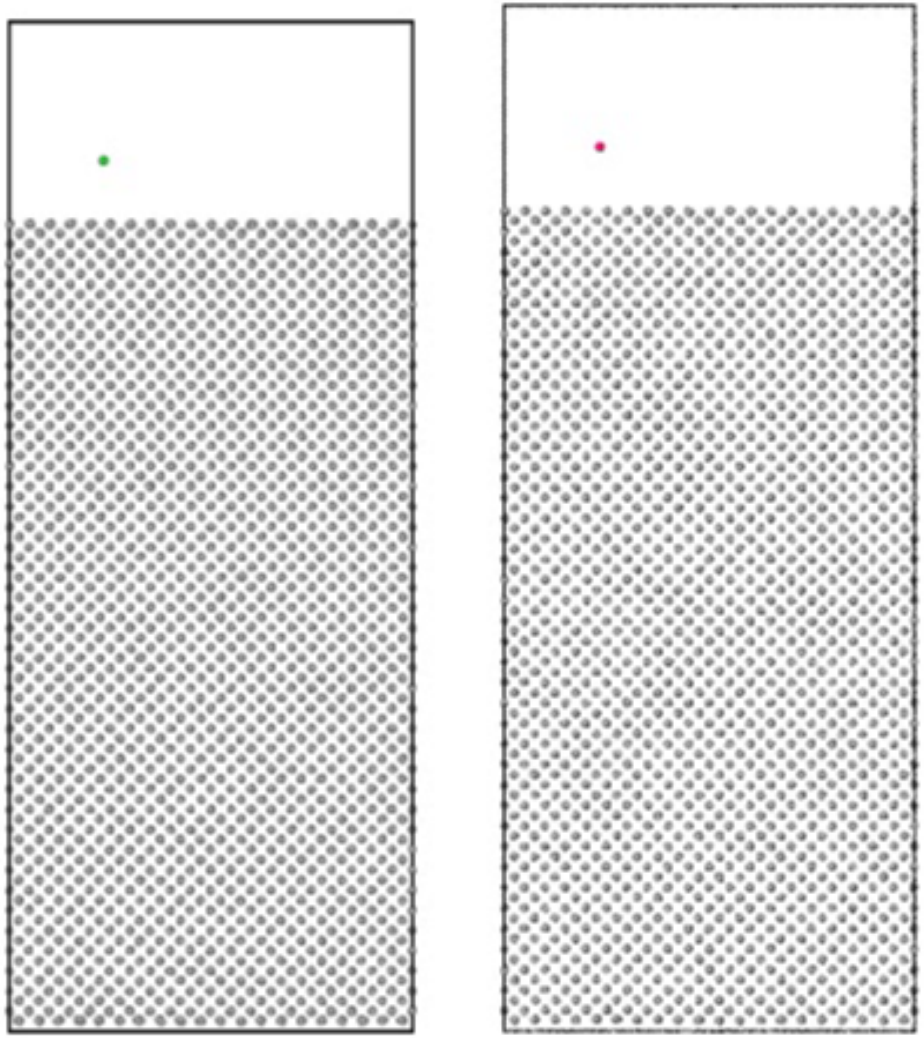


Run Vasp

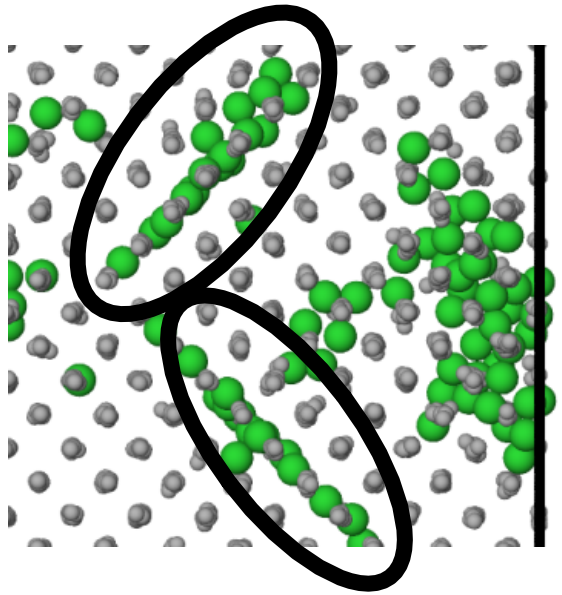


Production Implantation Simulations

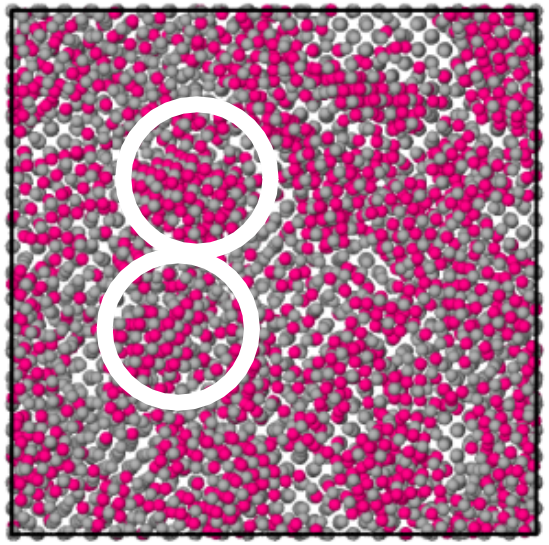
- 75 eV hydrogen (left) or nitrogen (right) into (100) tungsten at 1000 K
- Atoms implanted every 10 ps
- Hydrogen:
  - Diffuses throughout the material
  - Forms oriented platelets that were similarly observed with other potentials at high H concentrations
- Nitrogen
  - Remains very close to the surface, 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

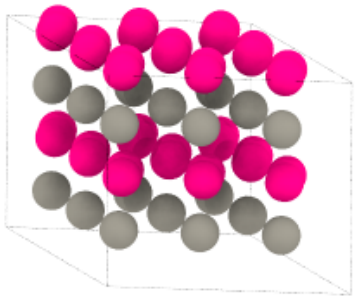


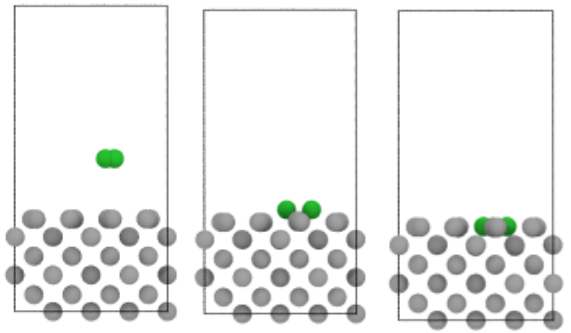
W_xN_x Formation

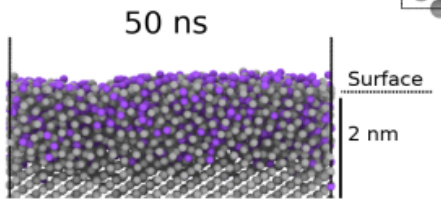


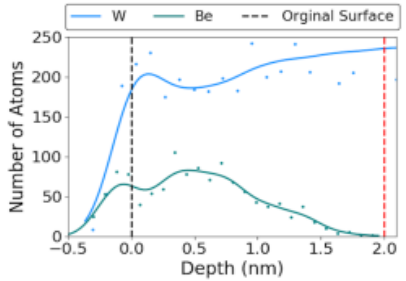
Summary

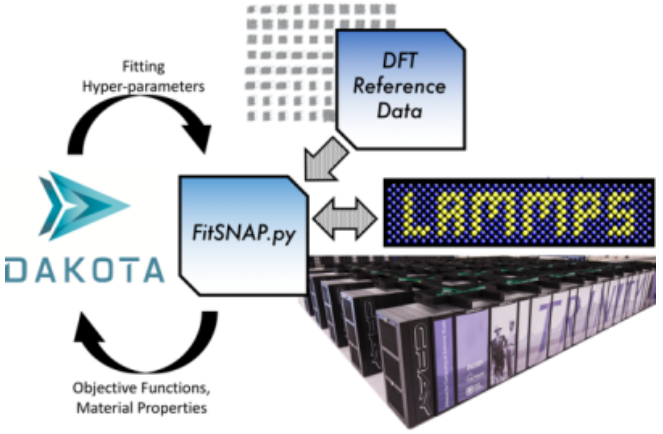
- SNAP is a robust ML-IAP that has been applied to a variety of materials for extreme conditions with high accuracy
- A W-Be-He has been successfully developed to study plasma material interactions relevant for fusion energy reactors
- The current SNAP potential is being extended for W-H and W-N and SNAP can reproduce key material properties for gas-metal interactions
- Initial post-fitting testing has assisted in finding poor behavior of early potentials so that additional training data can be generated
- 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

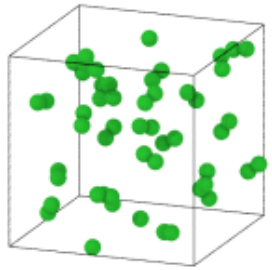


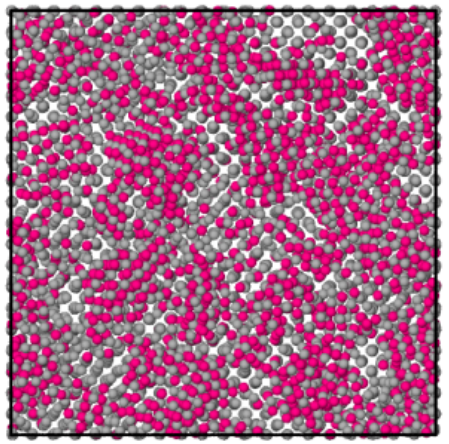












Contact:
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EXASCALE COMPUTING PROJECT

Office of Science

MD Approximations Change Over Time

Twobody (B.C.)
Lennard-Jones, Hard Sphere, Coulomb, Bonded

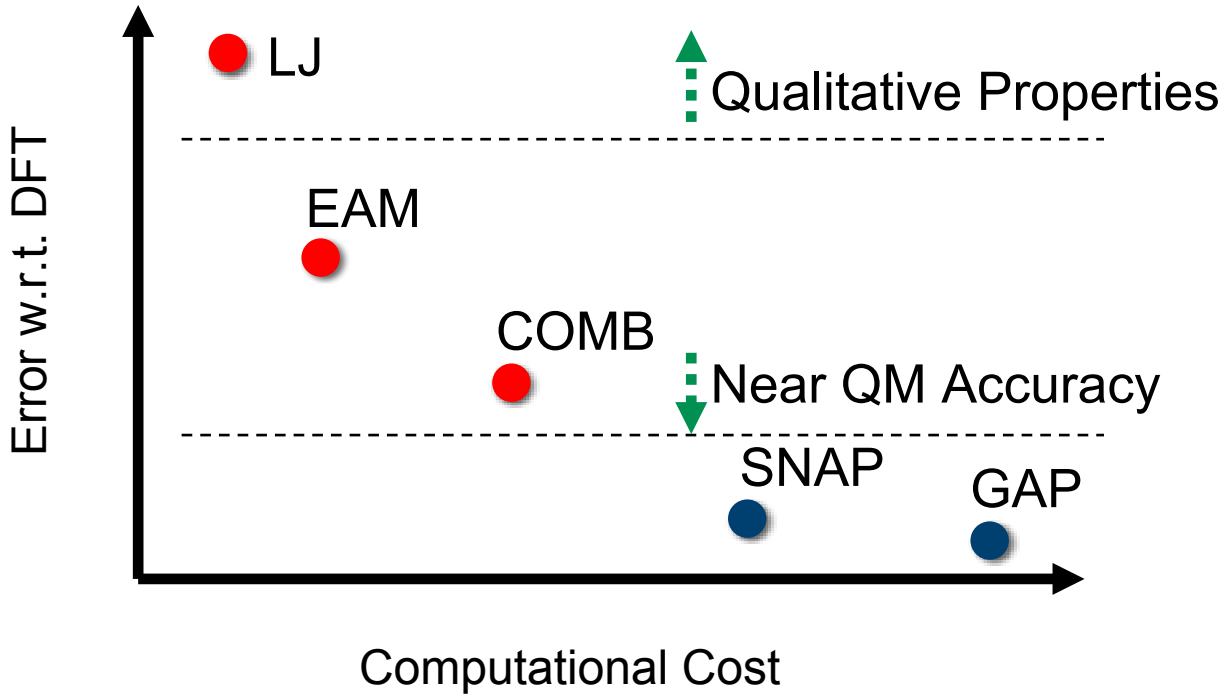
Manybody (1980s)
Stillinger-Weber, Tersoff, Embedded Atom Method

Advanced (90s-2000s)
REBO, BOP, COMB, ReaxFF

Big Data / Deep / Machine Learning (2010s)
GAP, SNAP, NN,…

Plimpton and Thompson, MRS Bulletin (2012).

Resources are limited, which is your best choice?



Gayatri, Moore *et al.* (2020) https://arxiv.org/abs/2011.12875