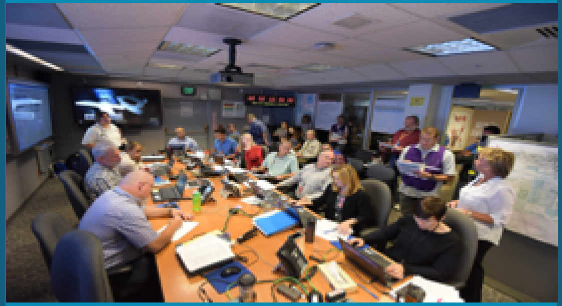
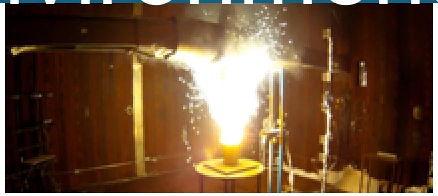
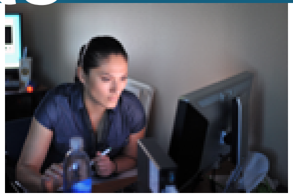
SAND2021-14821C

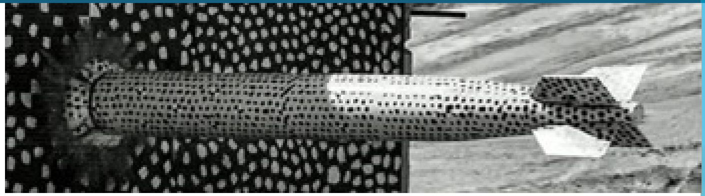
Sandia National Laboratories

Development of SNAP Machine Learned Interatomic Potentials for Materials in Extreme Environments









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2021 MRS Fall Meeting
December 6 2021

U.S. DEPARTMENT OF ENERGY NNSA National Nuclear Security Administration

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MD Approximations Change Over Time

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

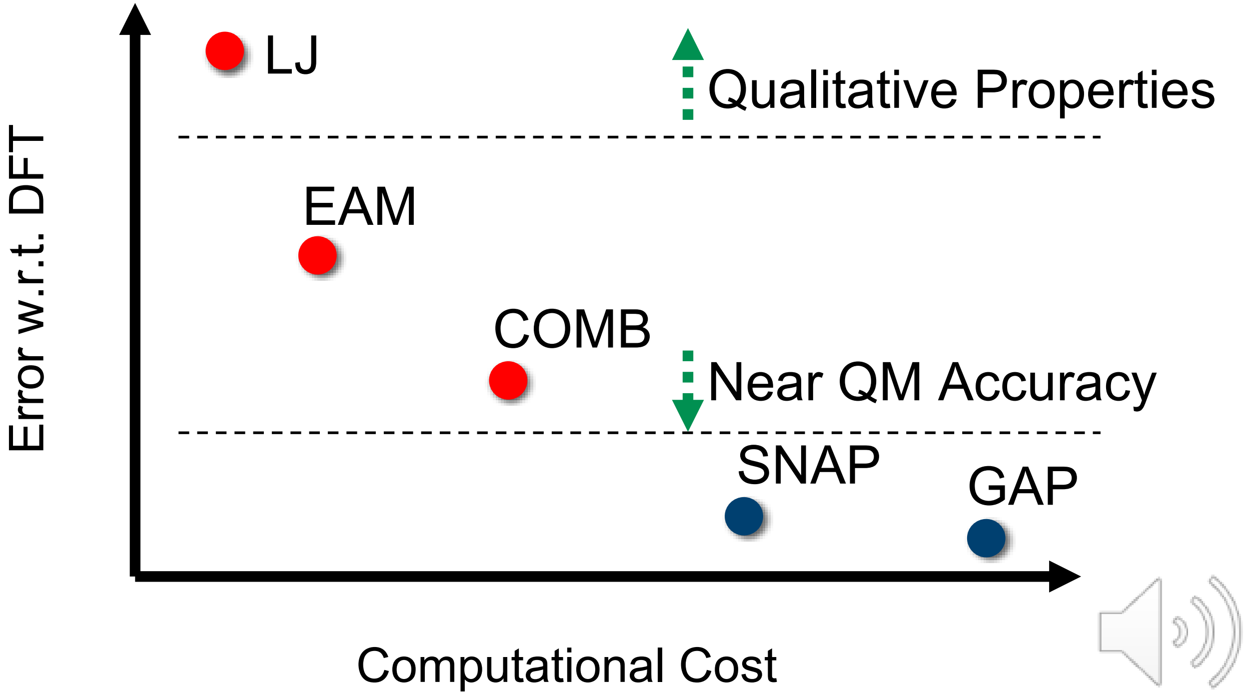
Manybody (1980s)
Stillinger-Weber, Tersoff, Embedded Atom Method

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

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)

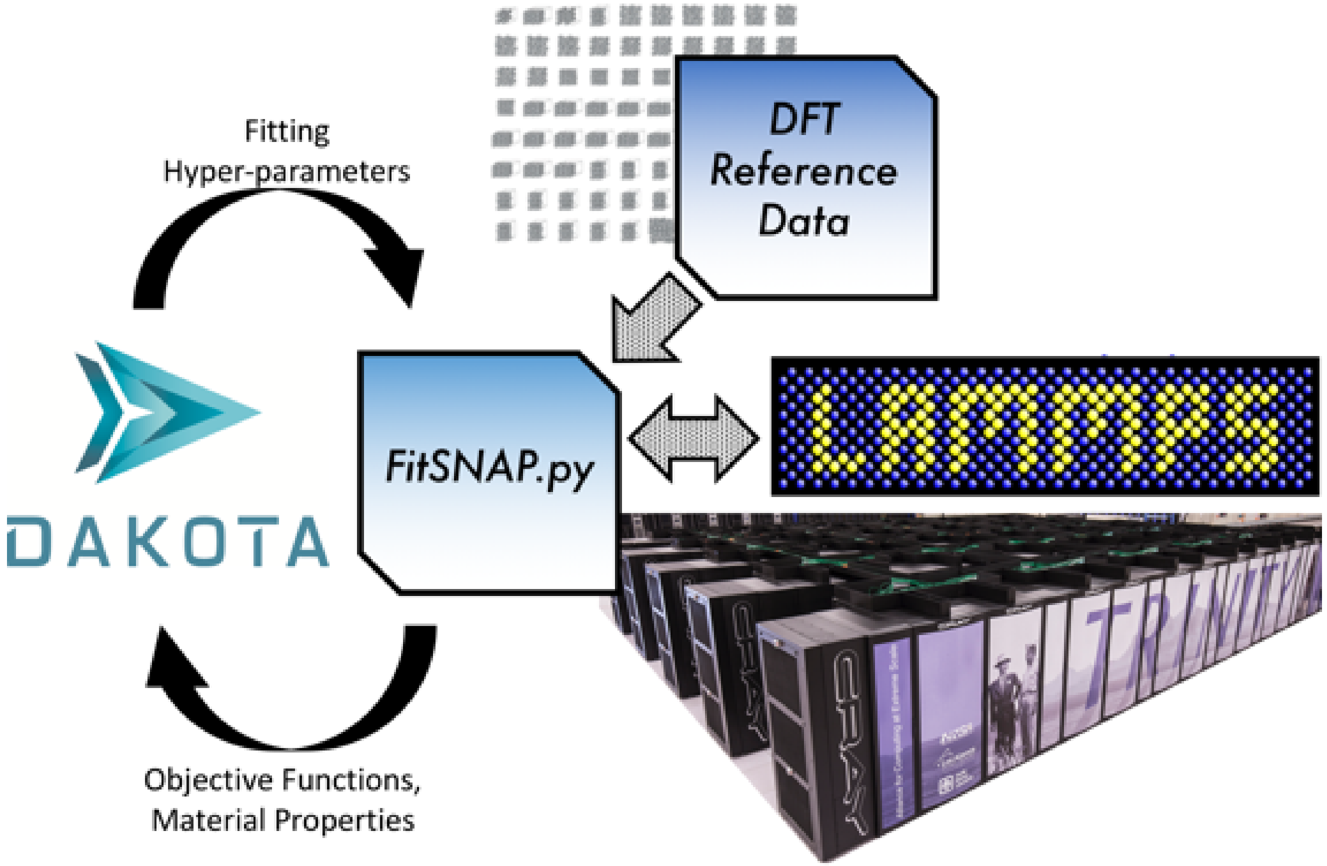
$$E^i_{SNAP} = \beta_0 + \sum_{k=1}^{K} \beta_k (B_k^i - B_{k0}^i)$$

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



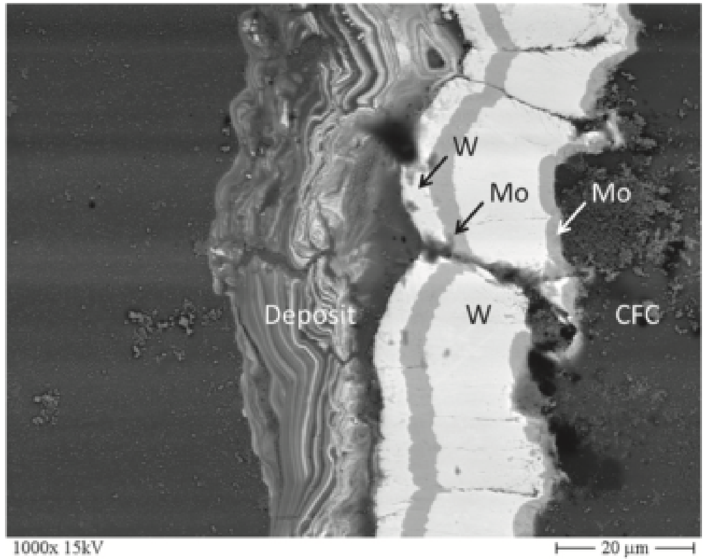
Code available: https://github.com/FitSNAP/FitSNAP

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

Plasma Material Interactions

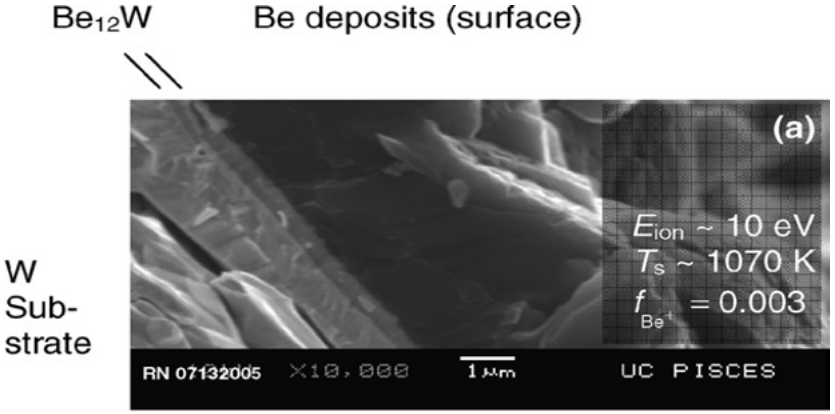
- Important to understand mixed materials effects at divertor surface
  - Material degradation, synergistic effects, implications on hydrogen retention, etc.
- Atomistic modeling will play a critical role but there is a lack of accurate interatomic potentials (IAPs) for modeling these materials especially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



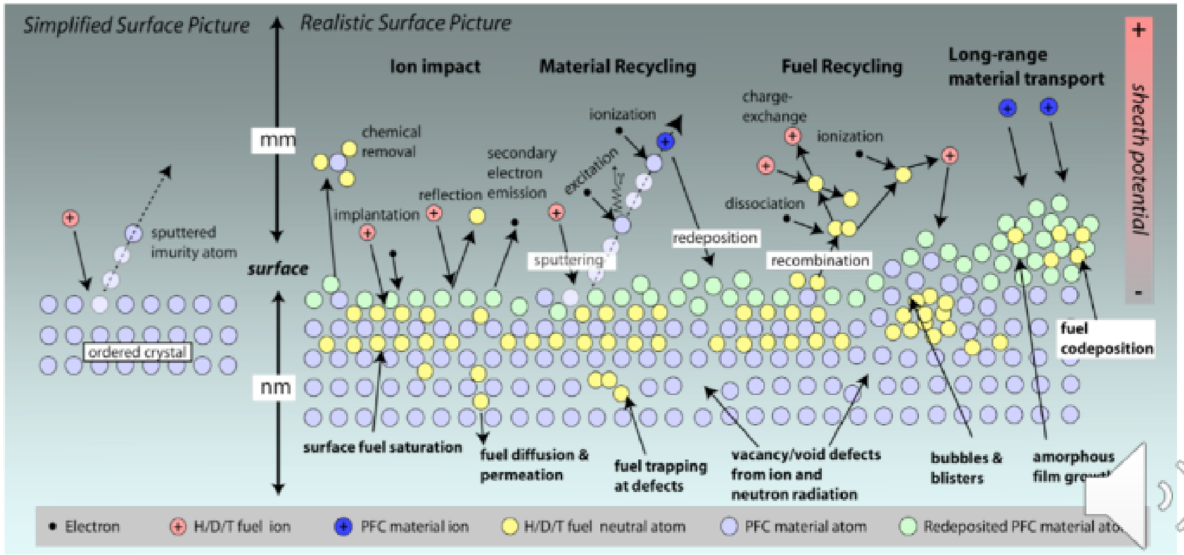
M Mayer *et al* 2016 *Phys. Scr.* **2016** 014051

Experimentally Observed W-Be Intermetallics



Baldwin, et. al. J. Nucl. Mater. 363-365 (2007) 1179-1183

Complex Physics at Plasma-Material Interface



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

SNAP Models for Simulating Plasma Material Interactions

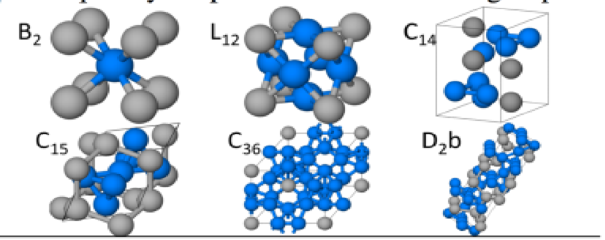
Blue: He
Purple: Be
Gray: W

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:

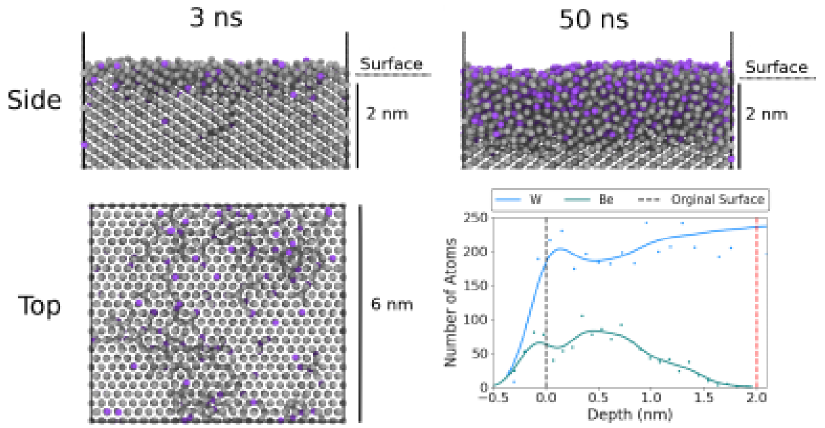


W-Be Intermetallic Formation Energies (eV)

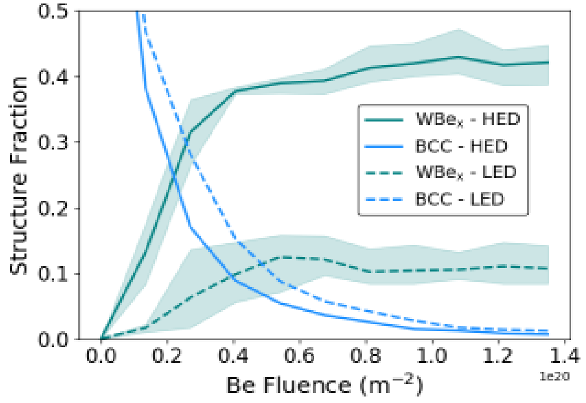
Phase	Composition	DFT[1]	SNAP[1]	BOP[2]
B_2	WBe	0.67	0.30	-2.20
C_{14}	WBe_2	-0.87	-1.27	-4.20
C_{15}	WBe_2	-0.92	-1.15	-4.19
C_{16}	WBe_2	-0.90	-1.22	-4.20
D_2B	WBe_{12}	-0.96	-0.34	-6.69

SNAP Results for W-Be

75 eV Be Implantation



Intermetallic Growth

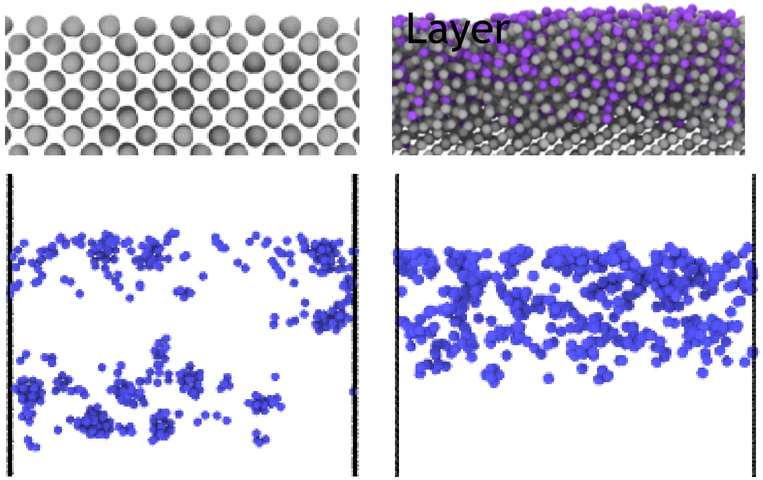


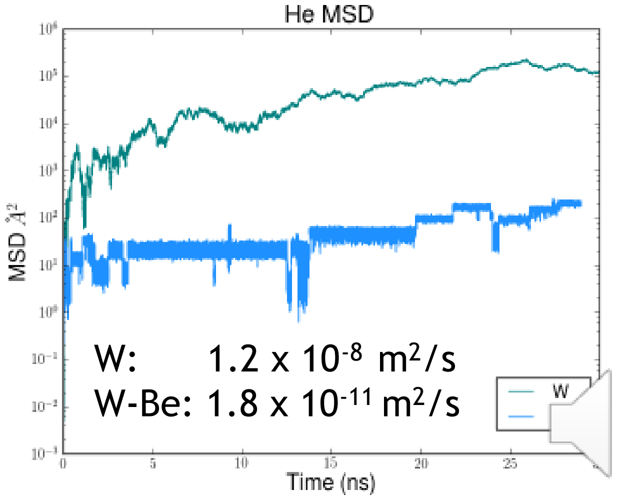
SNAP Results for W-Be-He

100 eV He Implantation

Pure W

W-Be Mixed Layer

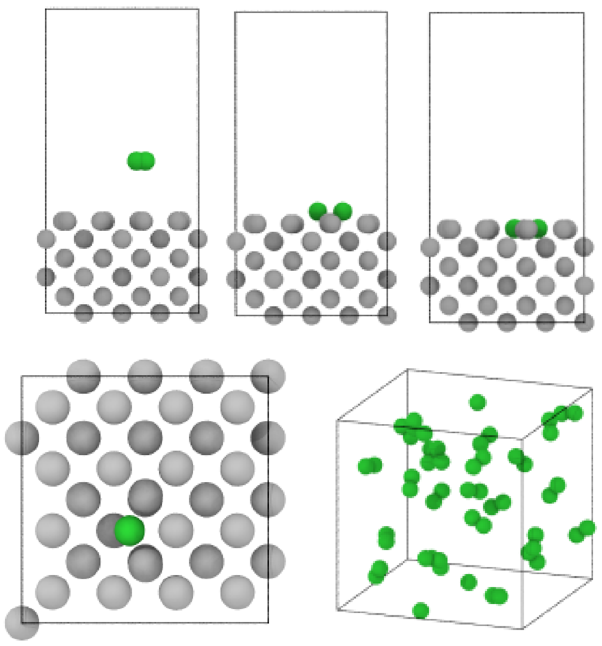




[1] M. A. Wood, et al. 2019 Phys. Rev. B 99, 184305
[2]] C. Björkas et al 2010 J. Phys.: Condens. Matter 22 352206
[3] M.A. Cusentino, et al. 2021 Nucl. Fusion 61 046049
[4] M.A. Cusentino, et al. 2020 Nucl. Fusion 60 126018

SNAP Results for W-H

Training Data



Fitted Properties

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

Initial Results

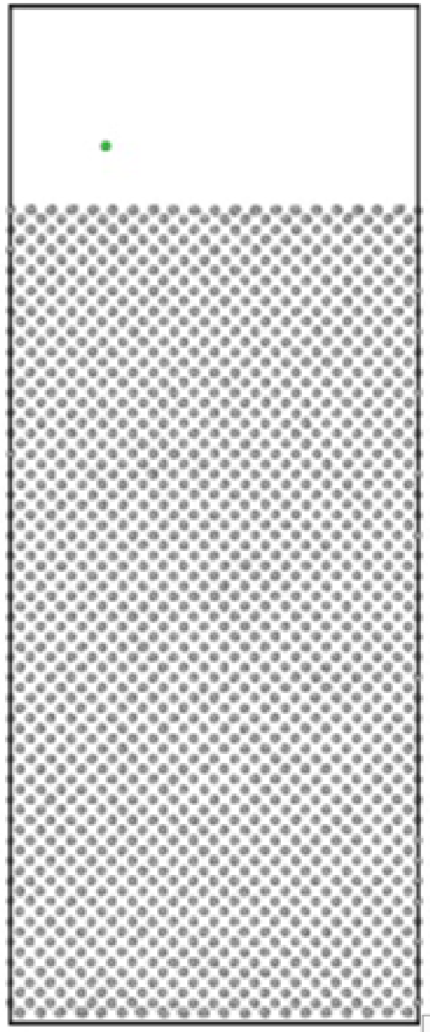
Defect Formation Energies

Bulk 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

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	-0.81
(111) Ads. Site	A	A
(111) Ads. Energy	-0.59	-0.93

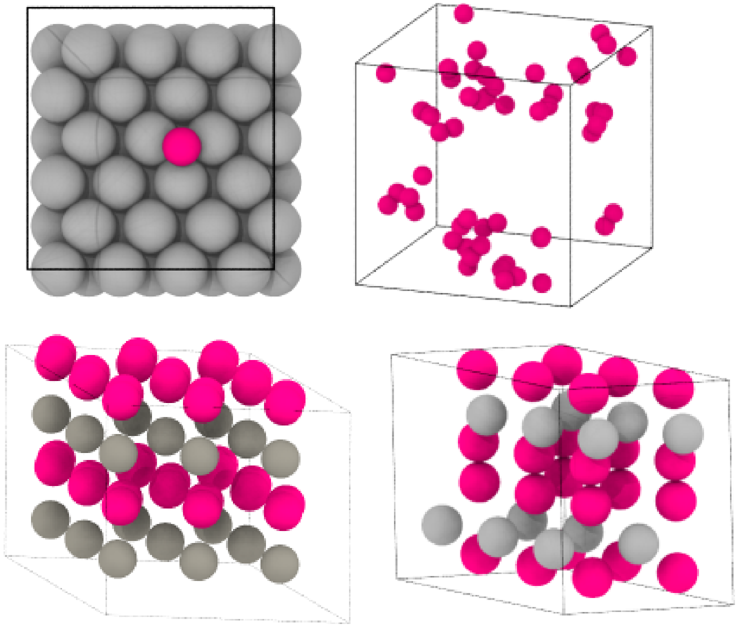
75 eV H Implantation



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	1.89
E_f^{Oct}(eV)	1.11	1.09
E_f^{Sub}(eV)	4.72	2.90
E_f^{N2}(eV)	-9.79	-9.47

Surface Adsorption Energies

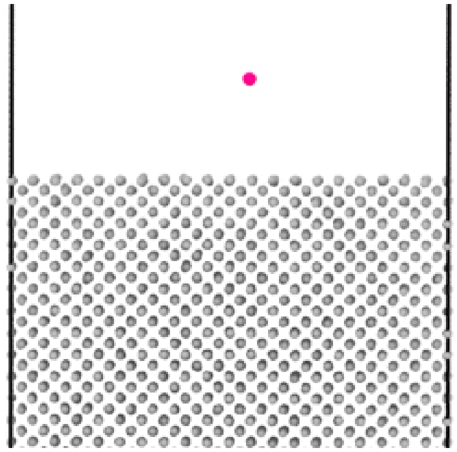
	DFT (eV)	SNAP (eV)
(100) Ads. Site	Hollow	Hollow
(100) Ads. Energy	-3.52	-4.33
(110) Ads. Site	Hollow	Hollow
(110) Ads. Energy	-3.59	-2.97

W_xN_y Formation Energies

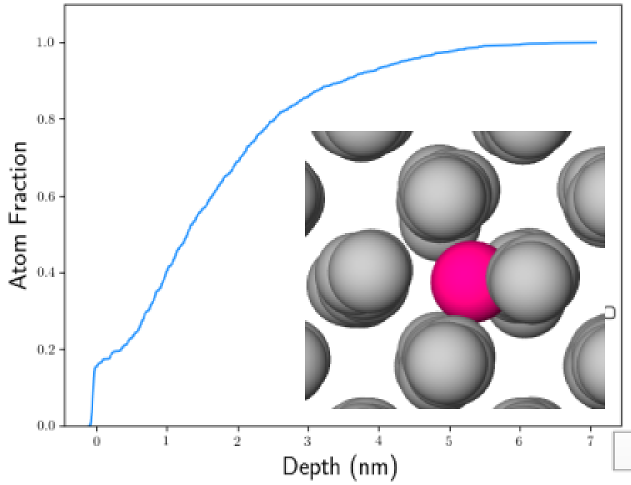
	DFT (eV)	SNAP (eV)
WN_2- P62mmc	-1.82	-1.82
WN_2- P6m2	-0.91	-1.75
WN - NiAs	-0.84	-0.74
WN - WC	-0.23	-1.51
W_2N	-0.03	3.29

Initial Results

75 eV Single N Implantation



75 eV N Depth Profile

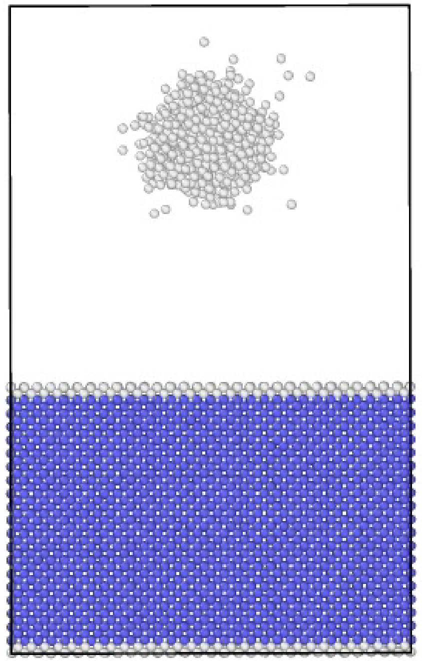


W: Grey H: Green N: Pink

SNAP for Modeling Thermal Spray Process

- Develop SNAP potential for modeling thermal spray deposition process for tantalum
- Training data focused on liquid, solid and liquid -solid interfaces of tantalum
- SNAP well reproduces fitted properties and has been used to simulation thermal spray deposition process

CNA Coloring:
White = Liquid/Surface
Blue = BCC



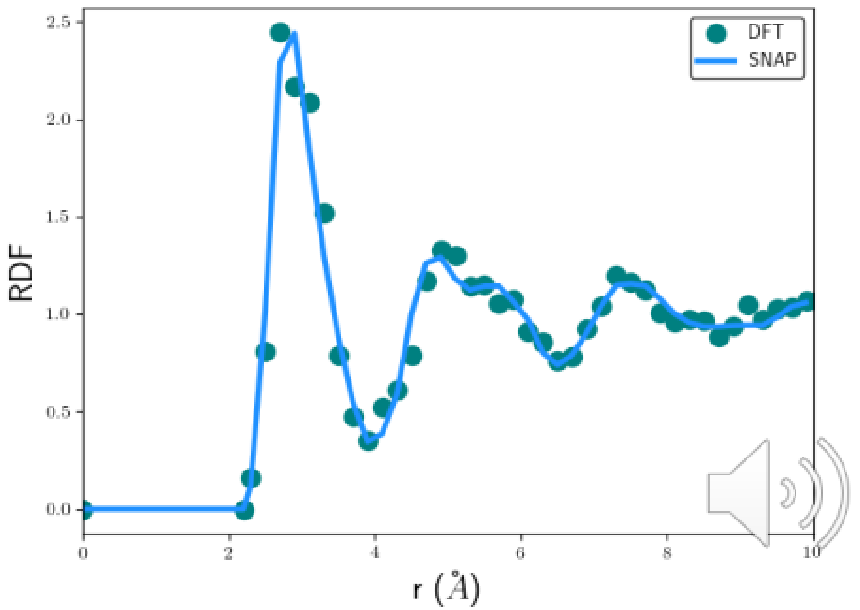
Cohesive Energies and Atomic Volumes

Structure	DFT E_{coh} (eV)	SNAP E_{coh} (eV)	DFT Vol./atom (Å/atom)	SNAP Vol/atom (Å/atom)
BCC	-8.10	-8.12	18.13	17.11
A15	-8.07	-8.09	18.61	16.81
FCC	-7.85	-7.89	18.79	20.41
HCP	-7.81	-7.85	18.0	19.95

Defect	DFT E_f (eV)	SNAP E_f (eV)
Substitutional	-8.10	-8.12
<111> Dumbbell	-8.07	-8.09
<110> Dumbbell	-7.85	-7.89

Elastic Constants	DFT (GPa)	SNAP (GPa)
C11	240.2	269.3
C12	186.3	163.0
C13	66.8	75.5

Liquid RDF



SNAP for Modeling Strength Properties in Tin

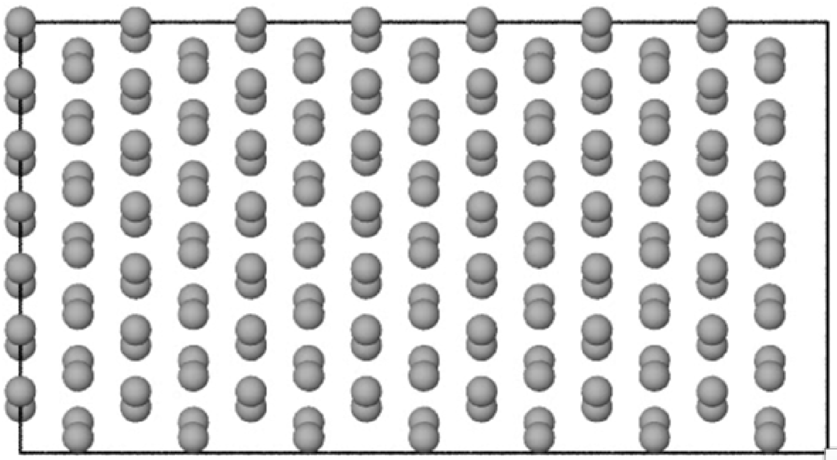
- Develop SNAP potential for modeling phase transitions of tin
- Training data focused on beta, gamma, and delta phase tin but properties depend on exchange correlation functional used
- SNAP can reproduces phase stability and transition pressures

Transition Pressures (GPa)	SNAP	Exp.
$\alpha \to \beta$	1.0	1
$\beta \to \gamma$	15.1	14
$\gamma \to \delta$	55.9	50

Cohesive Energies and Atomic Volumes

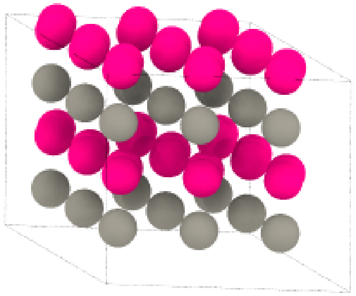
	Ecoh (eV) SNAP	Ecoh (eV) DFT	Vol (Å^3) SNAP	Vol (Å^3) DFT
Alpha	-3.95	-3.85	35.85	36.93
Beta	-3.78	-3.81	29.67	28.45
Gamma	-3.75	-3.79	28.39	27.83
Delta	-3.74	-3.77	24.98	24.98

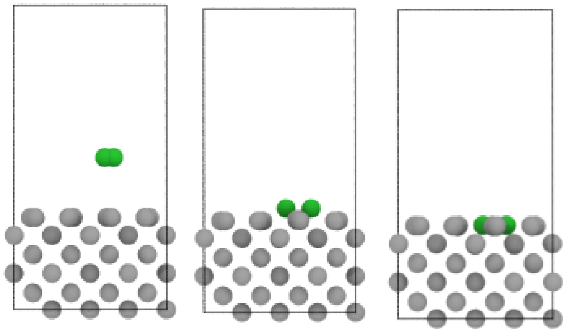
Beta Phase at 300 K

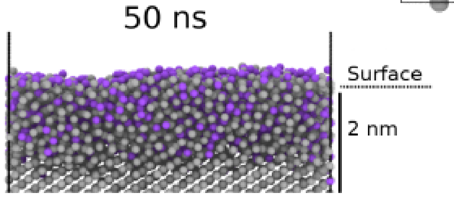


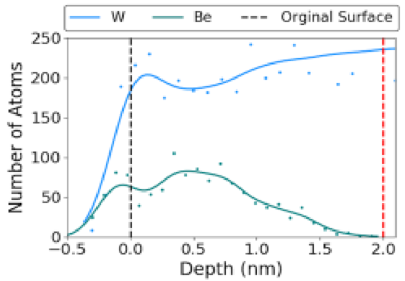
Summary

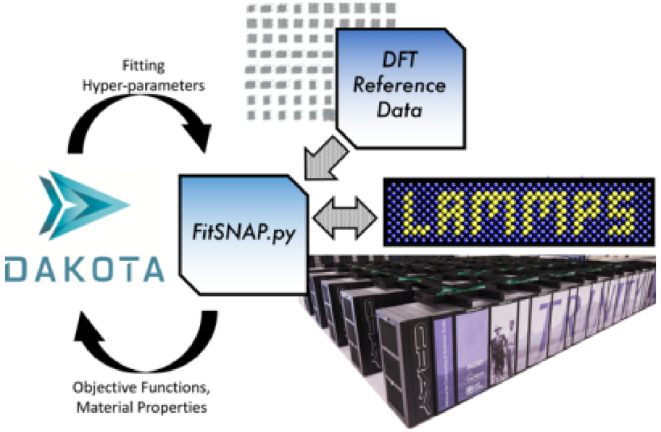
- SNAP is a robust ML-IAP that has been applied to a variety of materials for extreme conditions with high accuracy
- A W-Be-He has been successfully developed to study plasma material interactions relevant for fusion energy reactors
- The current SNAP potential is being extended for W-H and W-N and SNAP can reproduce key material properties for gas-metal interactions
- A SNAP tantalum potential has been developed that has been used to model the thermal spray process
- A SNAP tin potential is being developed and current potential [illegible] produce the phase transition pressure

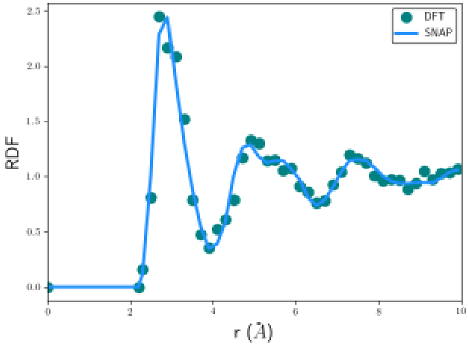


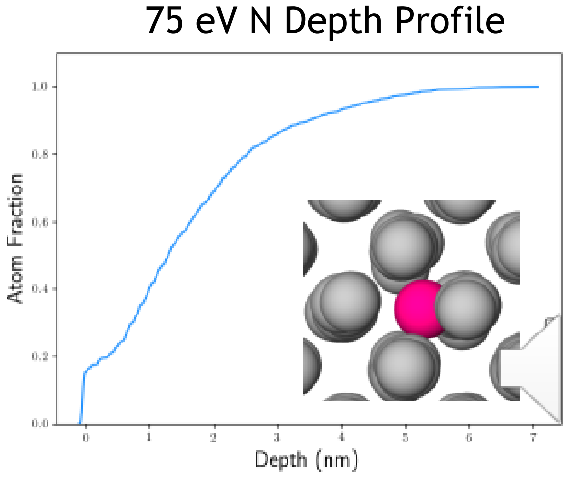












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