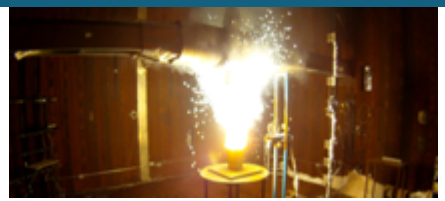
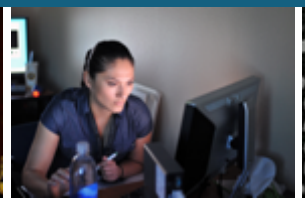
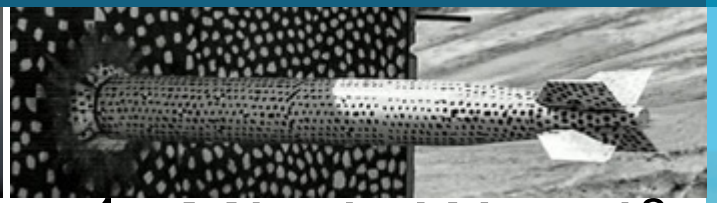
SAND2021-2055C

Sandia National Laboratories

Development of Machine Learned SNAP Potentials for Studying Radiation Damage in Materials







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2021 TMS

March 15 2021

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MD Approximations Change Over Time

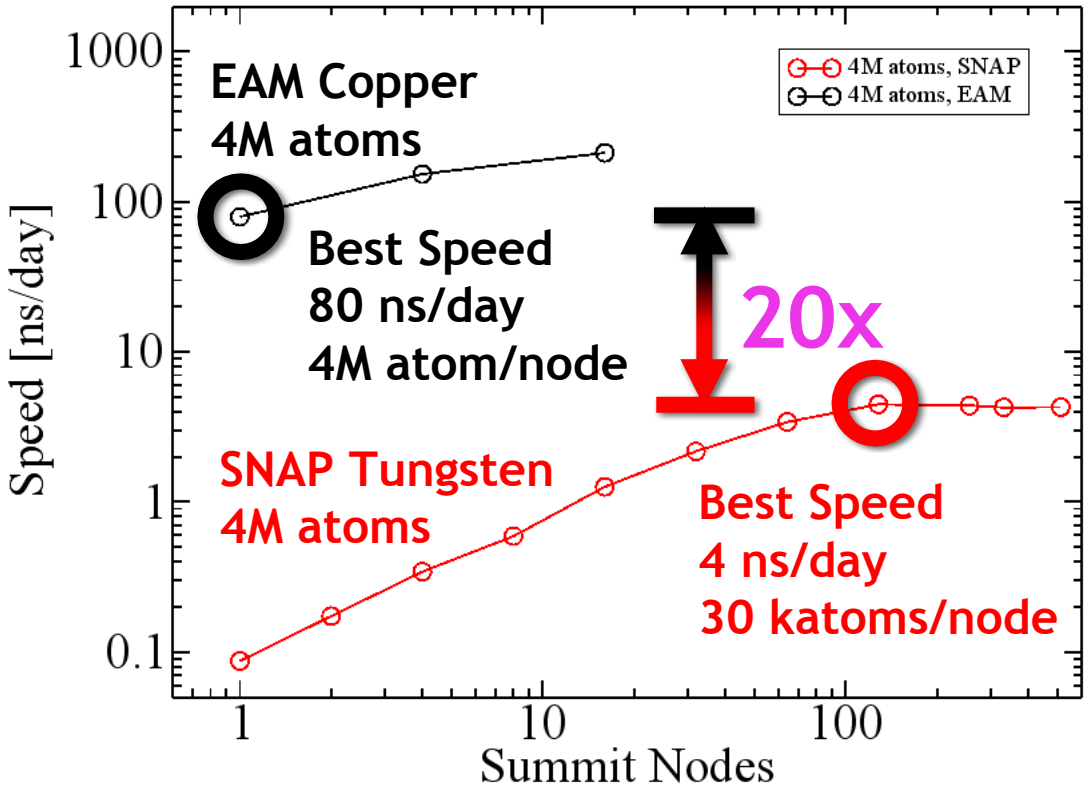
Twobody (B.C.)
Lennard-Jones, Hard Sphere, Coulomb, Bonded

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

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

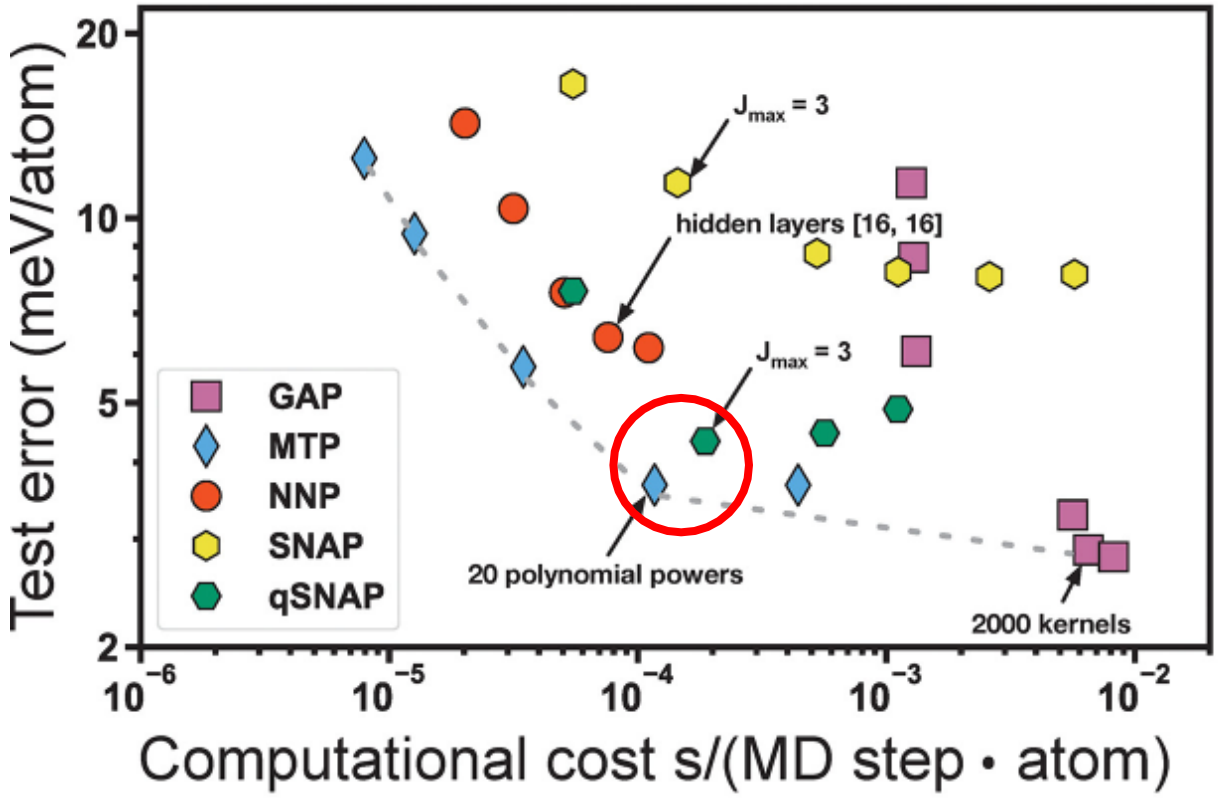
Big Data / Deep / Machine Learning (2010s)
GAP, SNAP, NN,…

GPU Timings



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

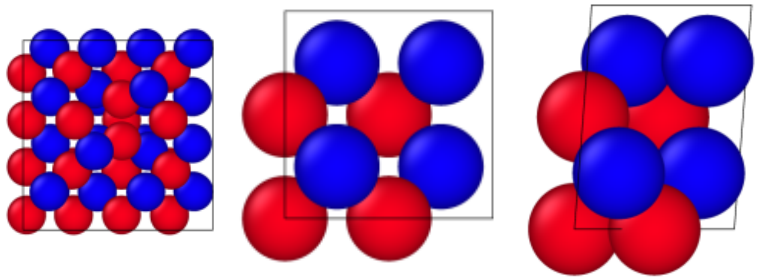
Resources are limited, which is your best choice?



What Makes a Machine Learned Interatomic Potential?

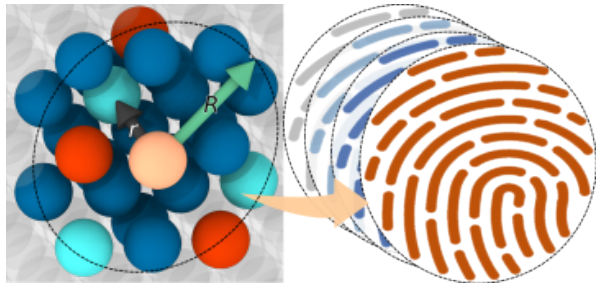
Training Data

- Generated using quantum methods
- Can include:
  - Energies
  - Forces
  - Stresses
- Variety of atomic configurations
  - Bulk structures, liquids, surfaces, defects, etc.



Descriptor

- Describes the local atomic environment
- Requirements
  - Rotation/Translation/. Permutation invariant
  - Equivariant forces
  - Smooth differentiable
  - Extensible
- Some Examples
  - Bispectrum, SOAP, ACE, Moment Tensors, etc.



Regression Method

- Linear regression
- Kernel ridge regression
- Gaussian process
- Non-linear optimization
- Neural Networks

SNAP

- Energies, forces, and stresses from DFT
- Bispectrum component descriptors
- Linear regression

SNAP Definition and Work Flow

Model Form

No Image

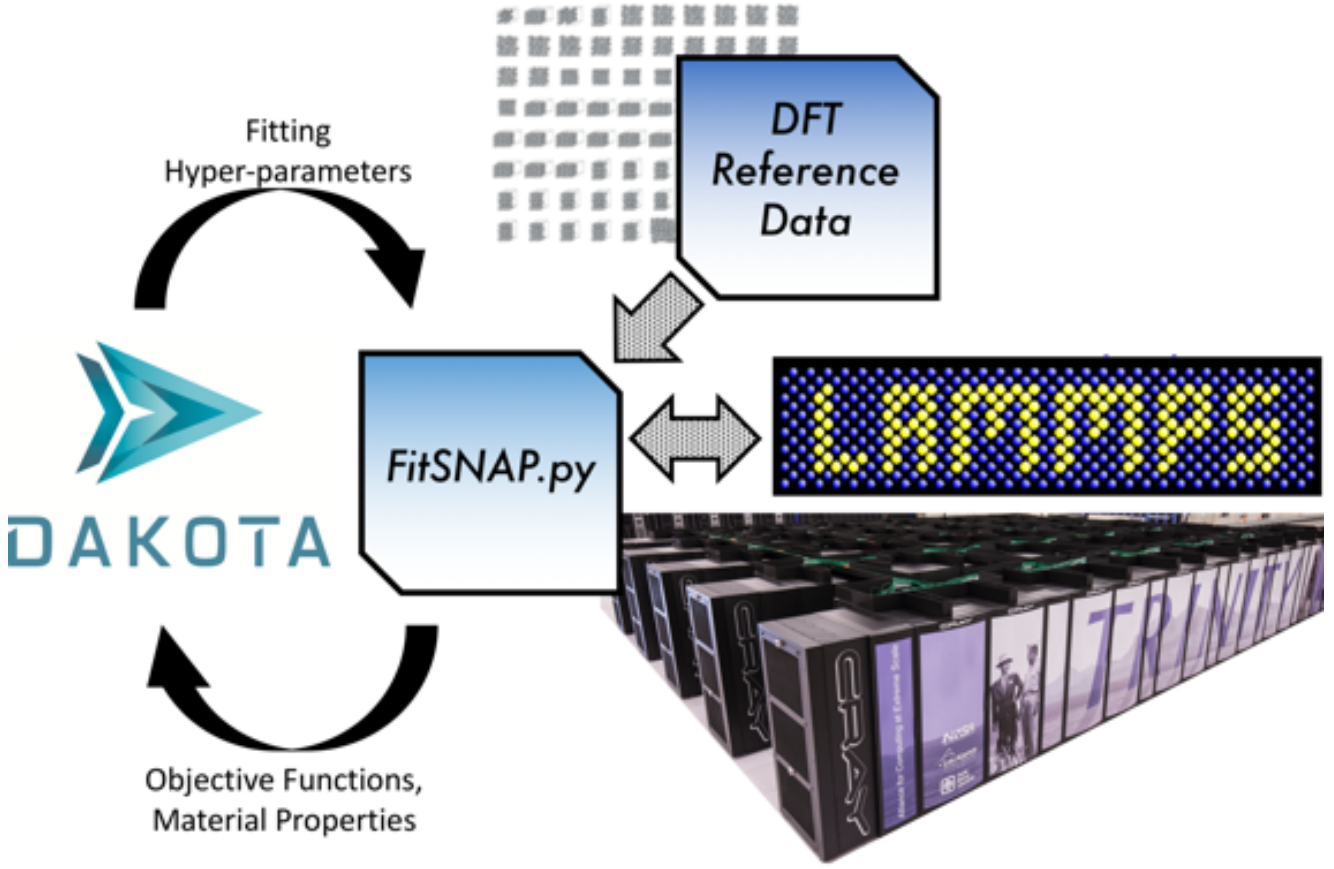
$$E^i_{SNAP} = \beta_0 + \sum_{k=1}^{K} \beta_k (B^i_k - B^i_{k0})$$

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

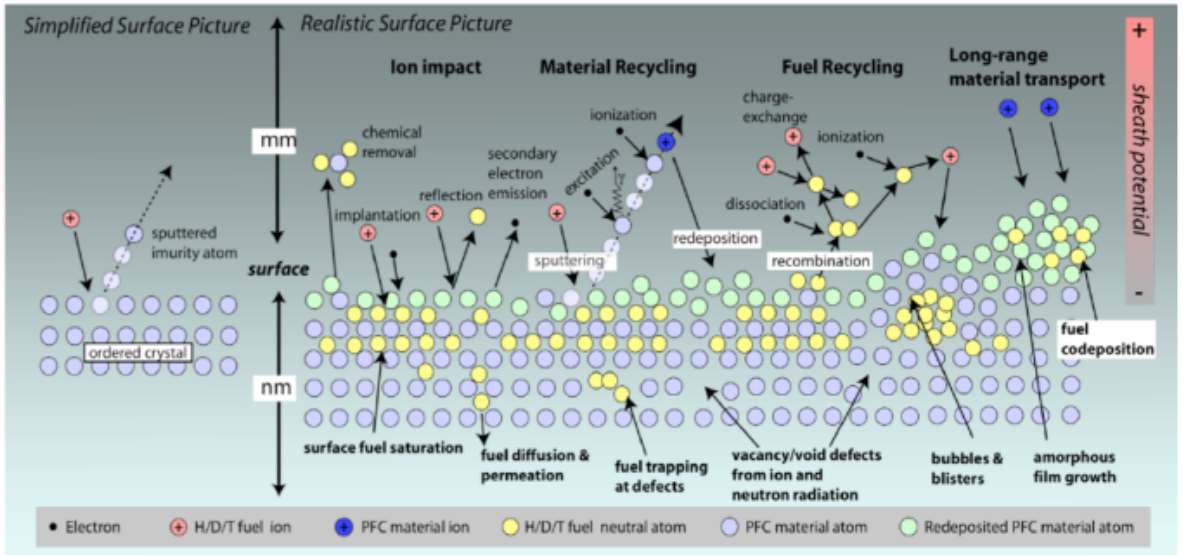


Code available: https://github.com/FitSNAP/FitSNAP

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

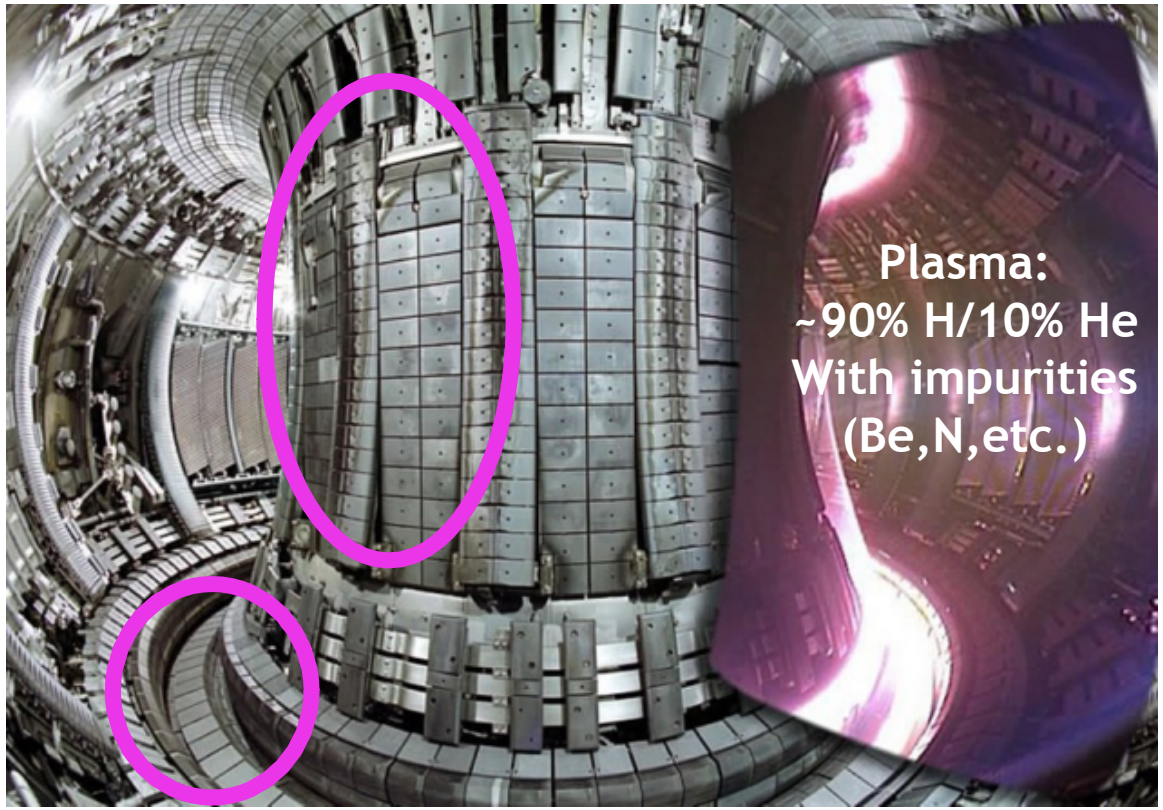
Materials for Fusion Energy

- Difficult to develop materials to handle extreme conditions within tokamak
- Large heat loads of 10-20 MW/m^3
- High particles fluxes of ~10^{24} m^{-2}s^{-1} of mixed ion species (H/He/Be/N etc.)



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

Beryllium First Wall



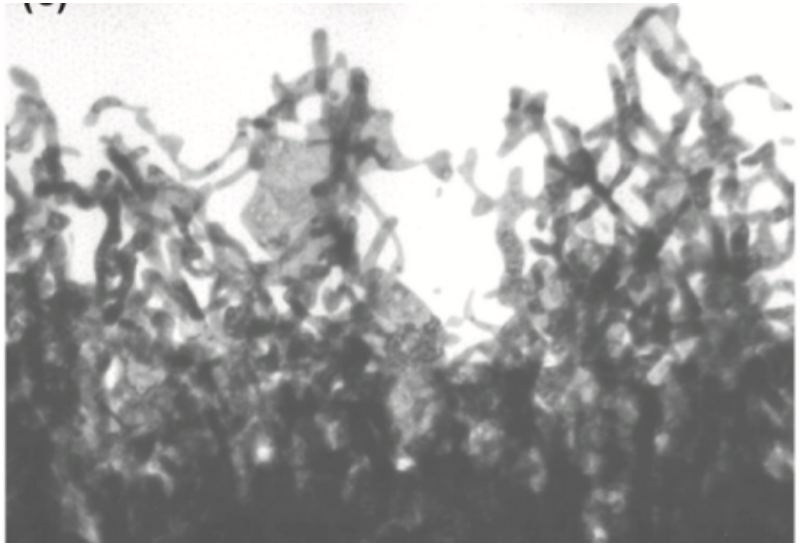
Tungsten Divertor

iter.org

- Many complex processes that occur at the plasma/material interface that can lead to material degradation

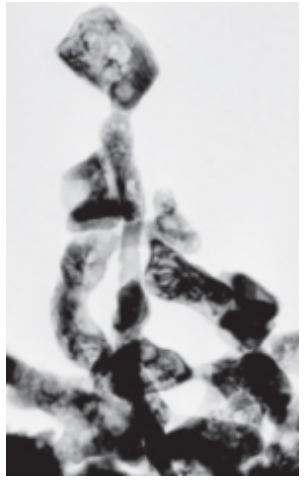
Plasma Material Interactions in Tungsten

Helium Fuzz Growth



Kajita, et al. J. Nucl. Mater, 418, (2011) 152-158

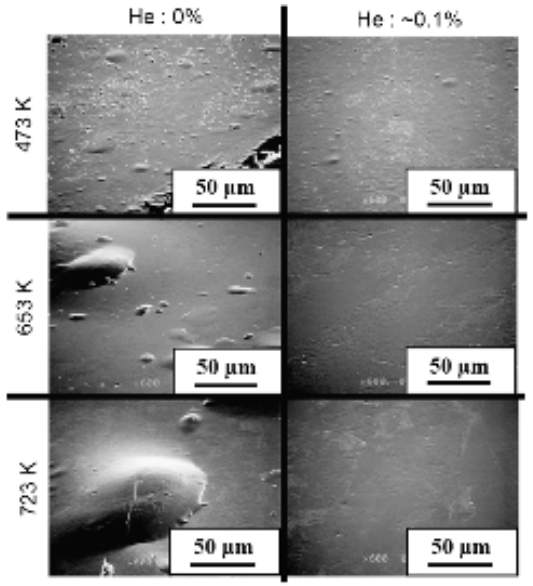
Material Degredation



Kajita, et al. Nucl. Fus. 471, 886-890 (2007)

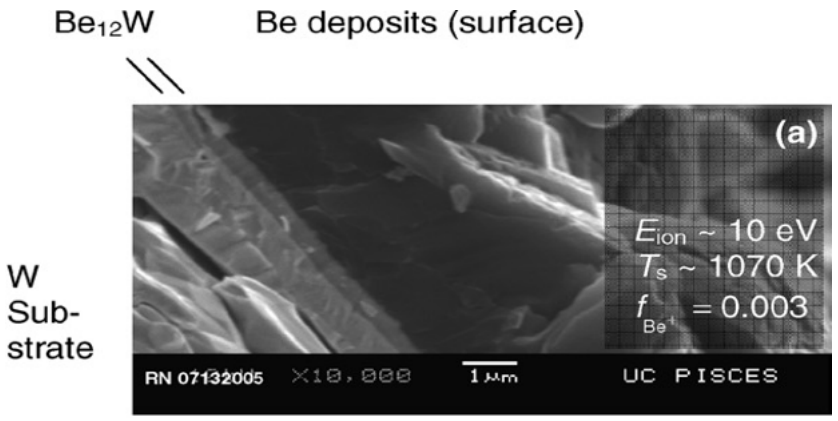
Tritium Retention

Effect of He on H Blistering



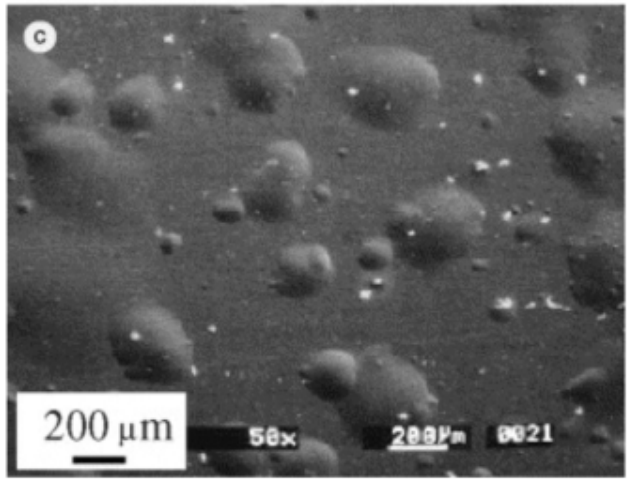
Ueda, et. al. J. Nucl. Mater. 386-388 (2009) 725-728

W-Be Intermetallics



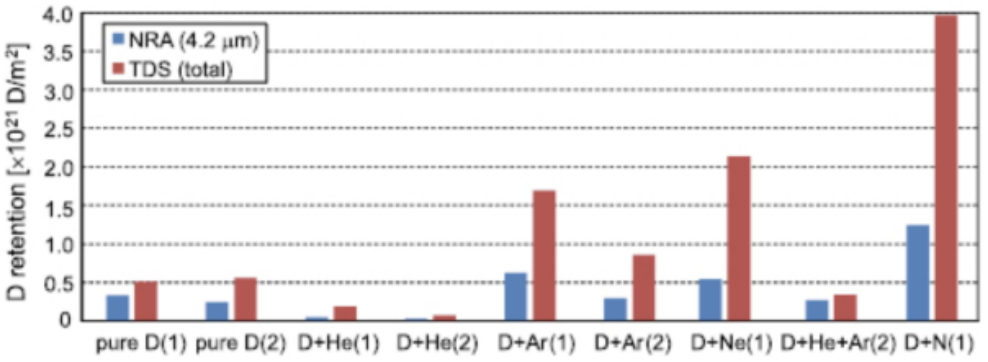
Baldwin, et. al. J. Nucl. Mater. 363-365 (2007) 1179-1183

Hydrogen Blisters



Ye, et al. J. Nucl. Mater. 313-316, 72-76 (2003)

Effect of Plasma Impurities on Hydrogen Retention



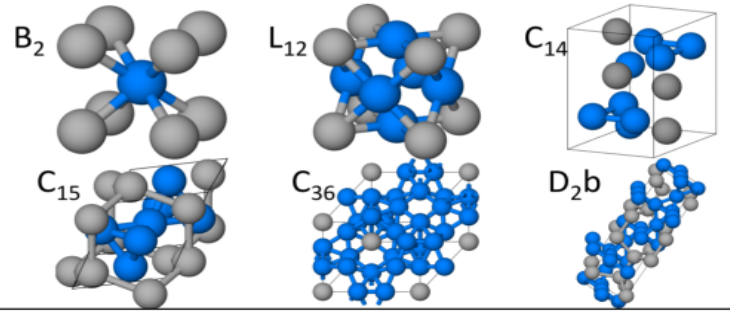
Kreter, et al. Nucl. Fus.. 59, 086029 (2019)

Tungsten-Beryllium SNAP Fitting

- Initially fit SNAP potential for pure elements
- Making a multi-element SNAP potential does sacrifice some accuracy from either pure component fit.
- Training set includes W-Be intermetallic structures

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
L_{12}	WBe_3	-0.51	-0.15	-4.58
D_2B	WBe_{12}	-0.96	-0.34	-6.69

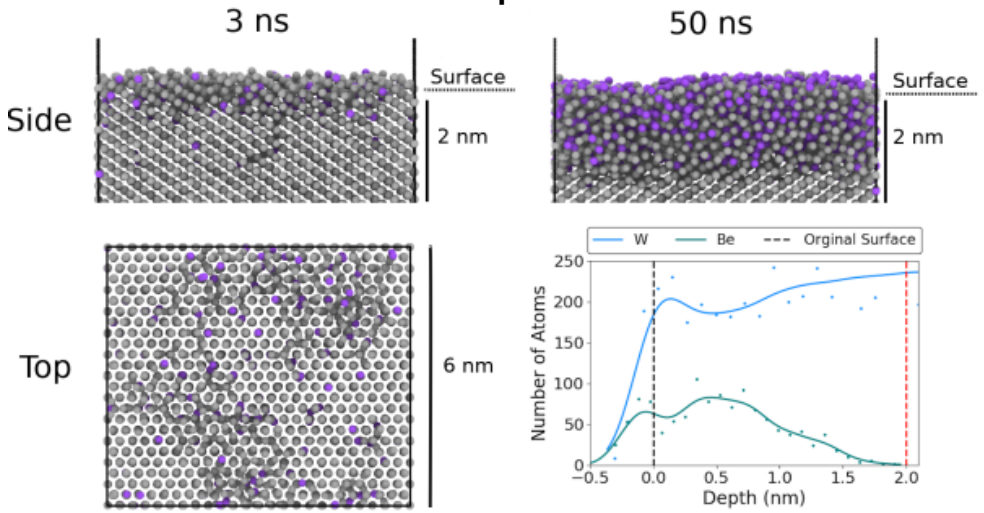
Be Defect Formation Energies in W (eV)

	DFT[1]	SNAP[1]	BOP[2]
[111] Dumbbell	4.30	3.66	0.67
Substitution	3.11	3.29	-2.00
Surface Hollow Site	-1.05	-1.39	-3.52
Tetrahedral	4.13	4.20	-0.28
[110] Dumbbell	4.86	4.29	-0.03
Octahedral	3.0	5.11	0.34
Surface Bridge Site	1.01	0.44	-1.30

[1] M. A. Wood, M.A. Cusentino, B.D. Wirth and A.P. Thompson, Phys. Rev. B 99, 184305
[2] C. Björkas et al 2010 J. Phys.: Condens. Matter 22 352206

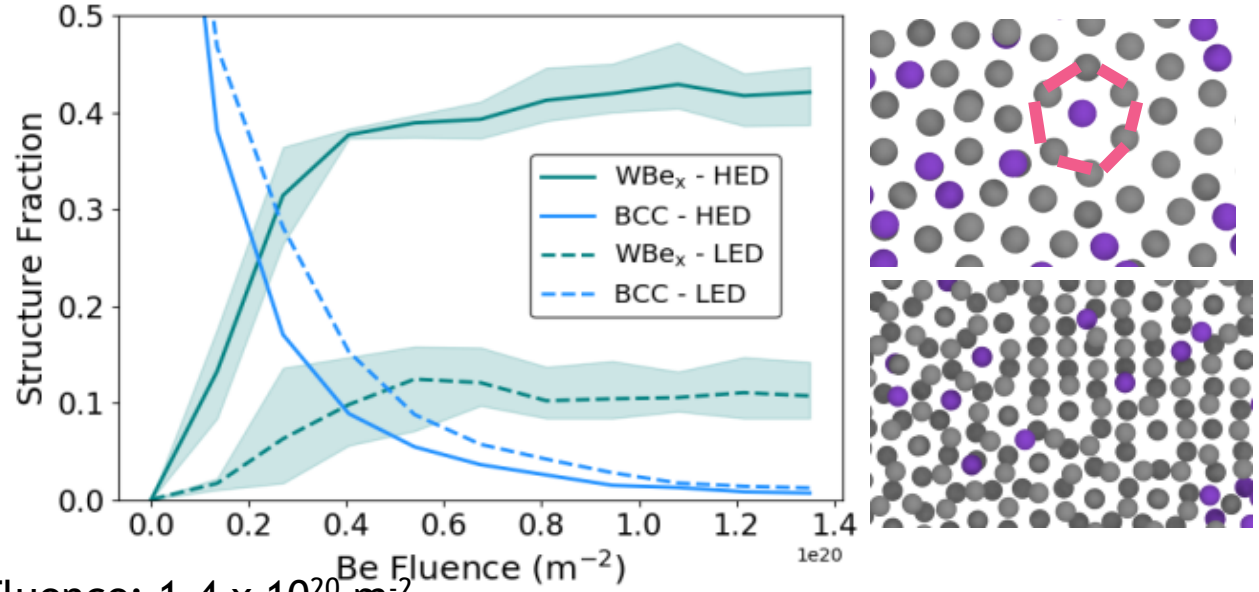
Beryllium Deposition Results in Near Surface Mixed Layer

75 eV Implantation



- High energy (75 eV) and low energy (0 eV) beryllium deposition on tungsten surfaces
- Formation of disordered mixed materials layer in first 2 nm of surface
- Some intermetallic growth observed within mixed materials layer
- However, mixed materials layer appears to be kinetically trapped at MD time scales

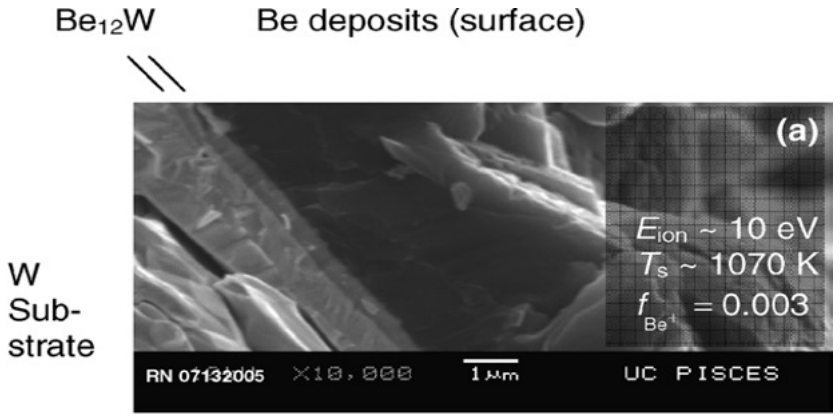
Intermetallic Growth



Fluence: 1.4 x 10^{20} m^{-2}

Cusentino, et al. Nucl. Fusion, in review

Experimentally Observed W-Be Intermetallics

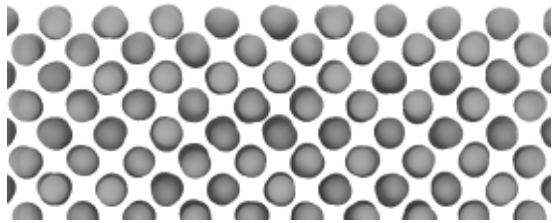


Baldwin, et. al. J. Nucl. Mater. 363-365 (2007) 1179-1183

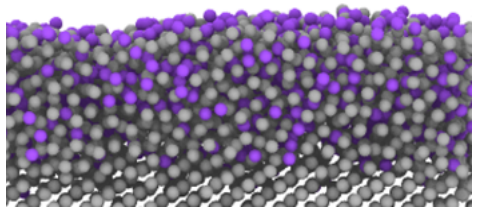
Be Disrupts Helium Diffusion and Bubble Growth in W

Increasing TIme

Crystalline W

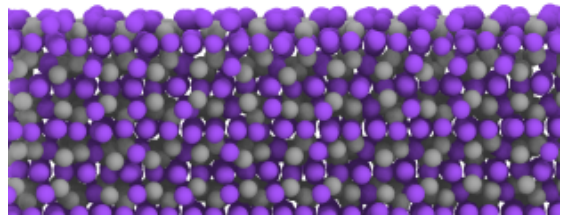


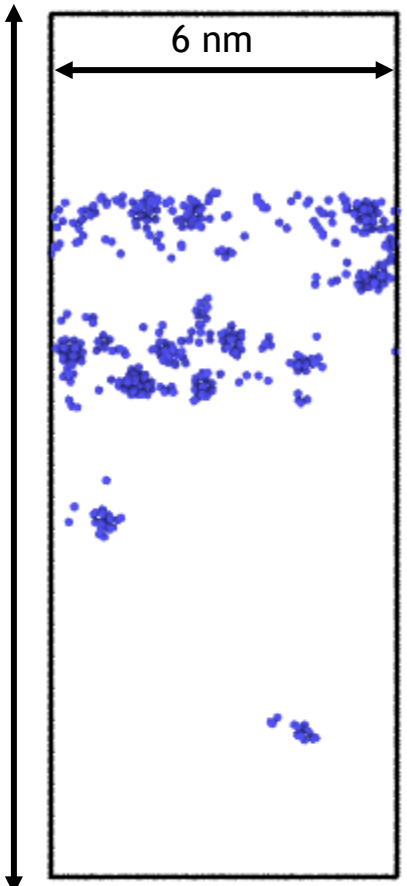
Amorphous W-Be

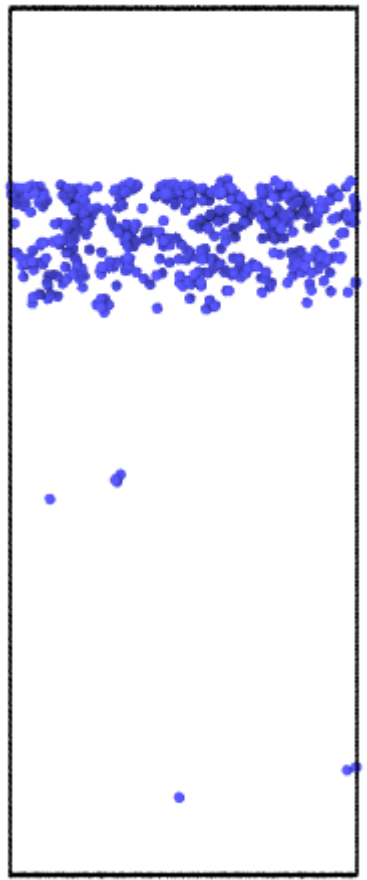


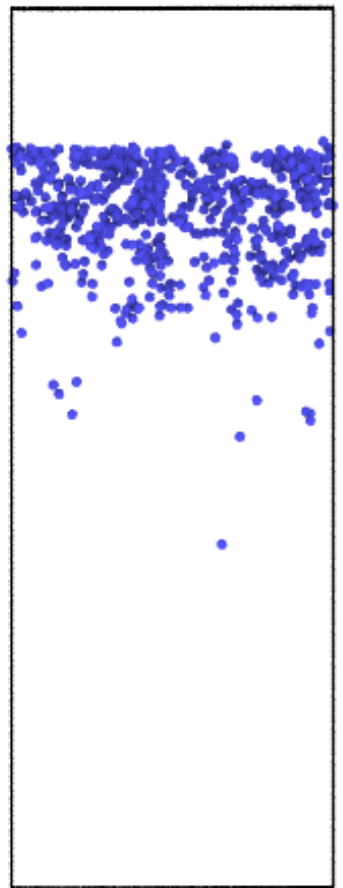
Blue: He
Purple: Be
Gray: W

WBe_2 C14 Structure









Tungsten:
Larger He clusters distributed throughout simulation cell

Laves/Deposited Layer:
Smaller He clusters mostly located near the surface

Fluence:
2.5×10^{19} m^{-2}

M.A. Cusentino *et al* 2020
Nucl. Fusion **60** 126018

Extending SNAP for W-H and W-N

<u>Pure H or N Data</u>

- Dimer and Trimer binding curve
- Molecular binding curves
- Random configurations of molecules at varying densities
- DFT-MD

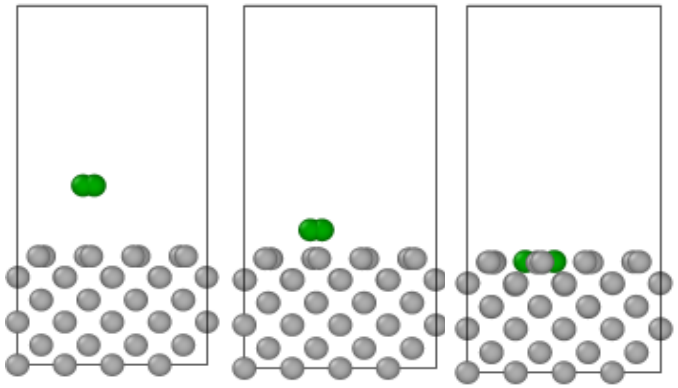
<u>W-H Data</u>

- H and H_2 adsorption on W surface
- H defects in bulk tungsten
- Sheared/Strained configurations of H defects in bulk W

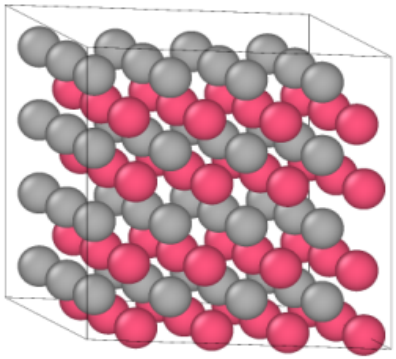
<u>W-N Data</u>

- N adsorption and surface diffusion on (100), (110), (111) surfaces
- N_2 dissociation on (100), (110), (111) surfaces
- NEB of N into bulk W for (100) and (110) surface
- N defects in bulk W
- W_xN_x bulk structures
- W_xN_x sheared/strained structures

H_2 Adsorption



WN NiAs Structure



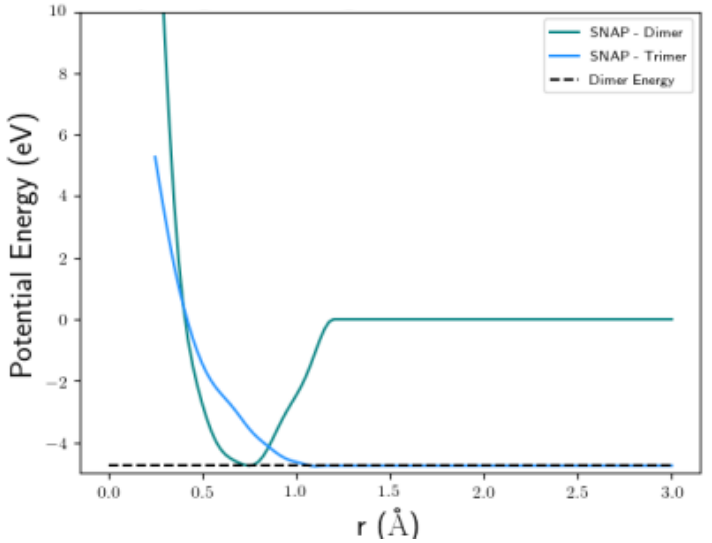
<u>Objective Functions</u>

- Energy/force errors on training data
- W or W_xN_x cohesive energies
- W and W-H or W-N defect formation energies
- H/N dimer and trimer binding energies
- H/N atom and molecular surface binding energies

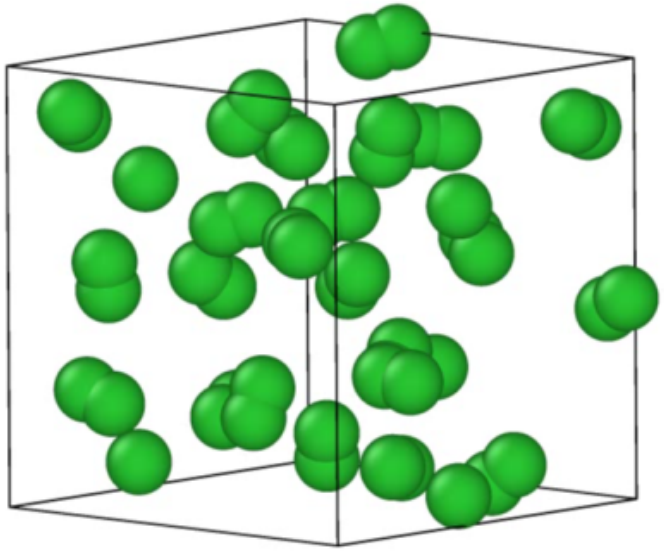
Challenges in Developing W-H and W-N SNAP Potentials

- Have never used SNAP for gaseous species before
- Hydrogen and nitrogen raining data is also more sparse compared to crystalline structures i.e. tungsten
- Difficult resides in how to get correct gas behavior (like forming dimers but not trimers) without inherent physics built -in to potential form

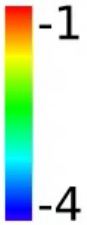
Hydrogen Binding Curves



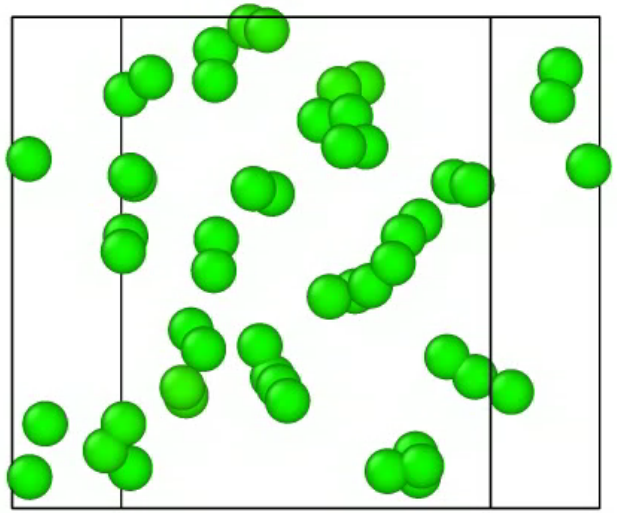
Poor Clustering Behavior



c_peatom



Poor Energetics

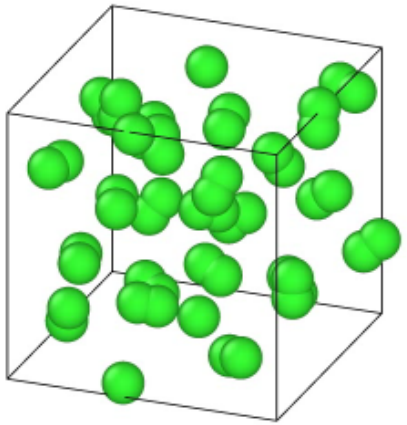


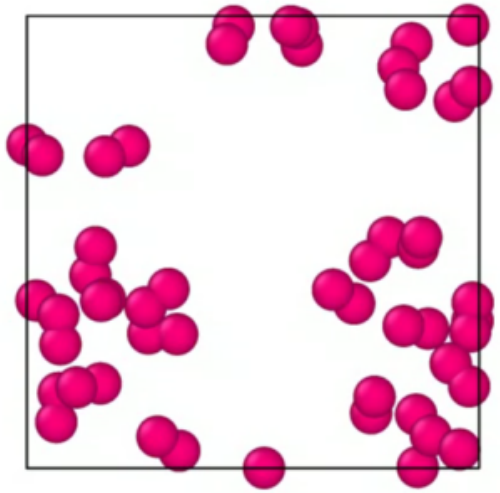
Movie colored by PE/atom

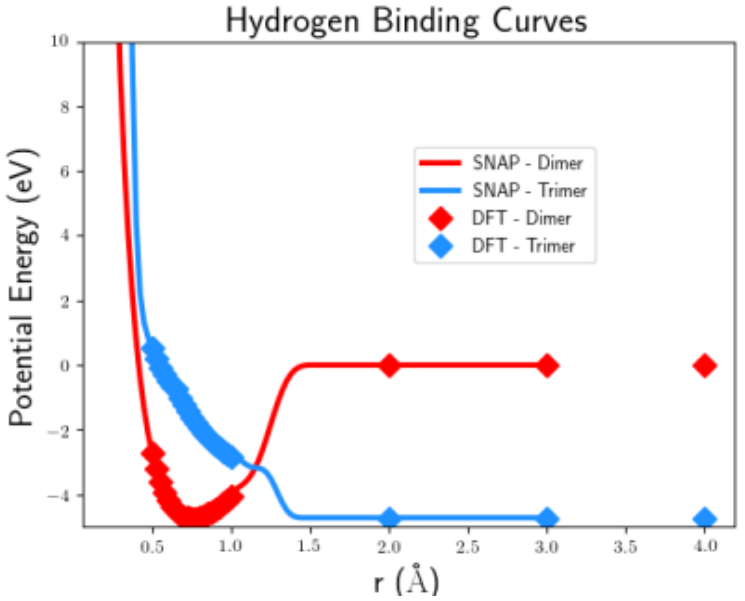
- Green is nominal H2 energy
- Reproduces correct binding curves

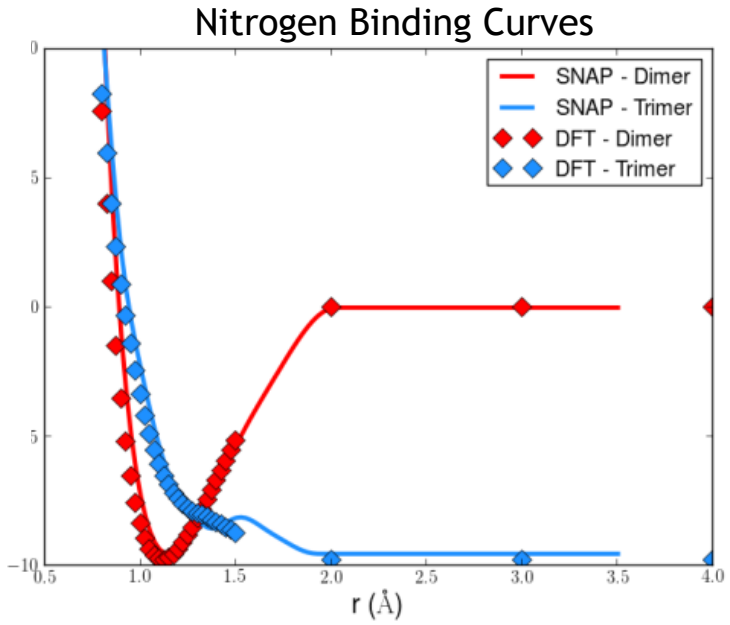
Changes to Fitting Results in Better Hydrogen and Nitrogen Potentials

- Modifications to fitting workflow yielded better results in reproducing correct gas species behavior
- Adjustments included:
  - Only including training data near potential energy well
  - Making radial cutoff much shorter (1.5 Å for H and 2.0 Å for N)
  - Adding extra objective function for dynamics behavior
  - Adjusted ZBL cutoff
  - Adjusted objective function for binding curves

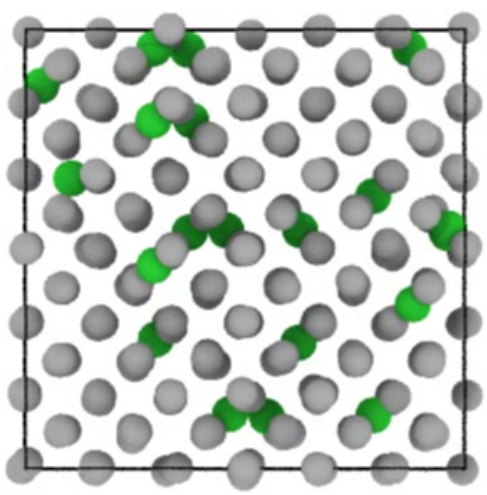


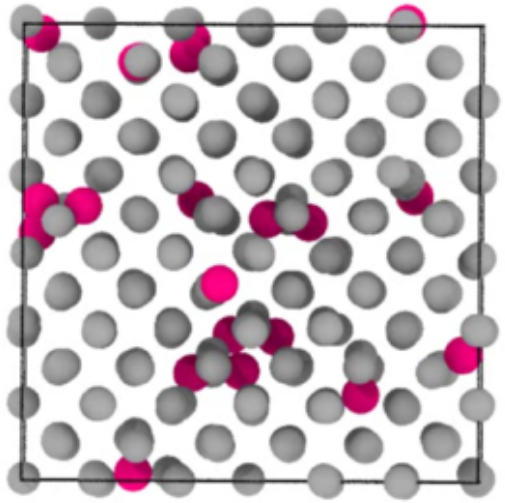






Preliminary Results for W-H and W-N SNAP Bulk Properties





W-H Bulk Properties

	DFT	SNAP
E_f^{H2} (eV)	-4.75	-4.74
E_f^{Tet} (eV)	0.88	0.85
E_f^{Oct} (eV)	1.26	1.17
E_f^{Sub} (eV)	4.08	4.25
E_f^{V} (eV)	3.27	3.30

W_xN_x Cohesive Energies

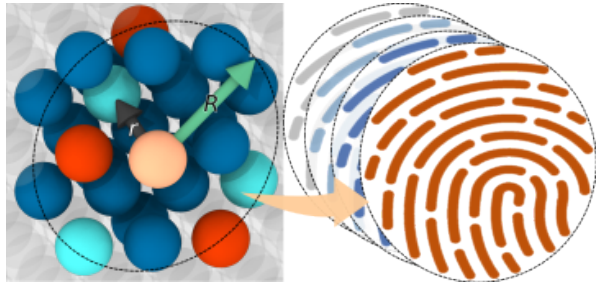
	DFT	SNAP
P62mmc (WN_2) (eV)	-1.84	-2.64
P6m2 (WN_2) (eV)	-0.92	-2.63
NiAs (WN) (eV)	-0.83	-1.35
WC (WN) (eV)	-0.24	-1.00
$MoSi_2$ (W_2N) (eV)	-0.07	-0.06

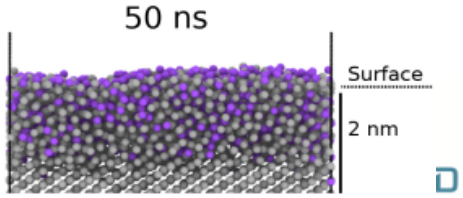
W-N Bulk Properties

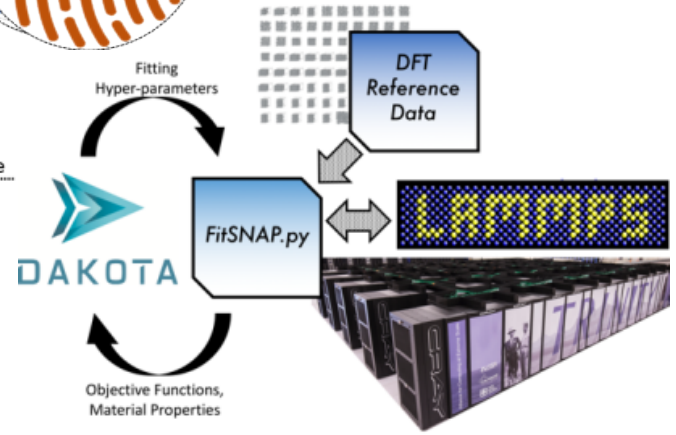
	DFT	SNAP
E_f^{H2} (eV)	-9.79	-9.71
E_f^{Tet} (eV)	1.26	1.45
E_f^{Oct} (eV)	0.53	0.56
E_f^{Sub} (eV)	4.15	1.23
E_f^{V} (eV)	3.27	2.95

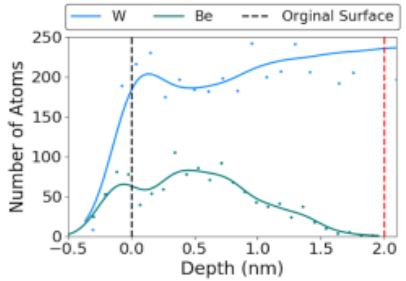
Summary

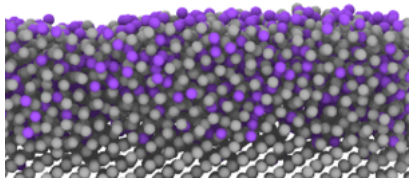
- SNAP is a versatile ML interatomic potential that has been applied to a variety of materials including materials for fusion energy
- A W-Be SNAP potential has been developed and used to study Be implantation in W and extended to simulation He implantation W-Be materials
- The current SNAP potential is being extended for W -H and W-N and SNAP can reproduce gas species behavior both in vacuum and in metals
- Future work entails the development of one W-Be-H -He-N potential for studying fusion energy materials

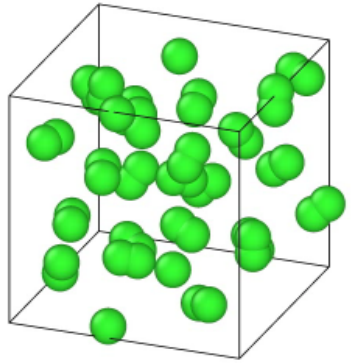


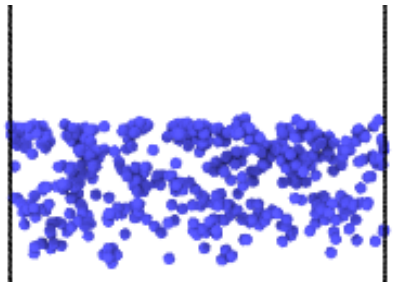












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EXASCALE COMPUTING PROJECT

Office of Science

Variations of SNAP

Quadratic SNAP

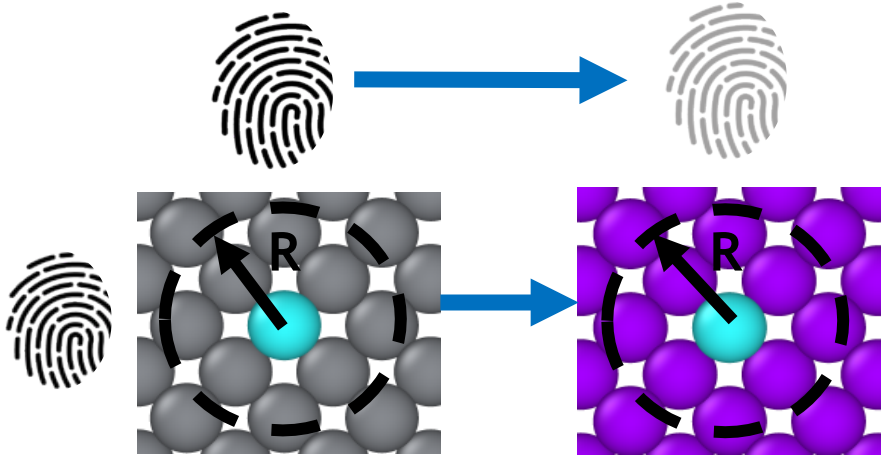
$$E^i_{SNAP} = \boldsymbol{\beta} \cdot \mathbf{B}^i + \frac{1}{2}(\mathbf{B}^i)^T \cdot \boldsymbol{\alpha} \cdot \mathbf{B}^i$$

- Linear terms are 4-body
- Quadratic terms are 7-body
- Number of linear coefficients grows as $O(J^3)$
- Number of quadratic coefficients grows as = $O(J^6)$

Neural Network SNAP

SNAP for Multiple Elements

WD-SNAP



EME-SNAP