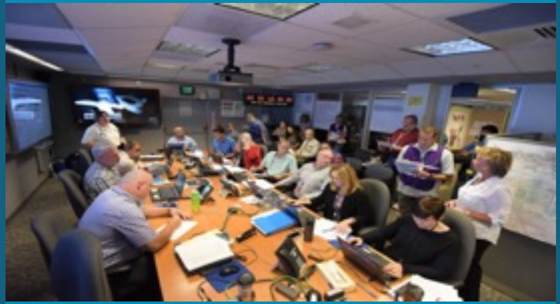
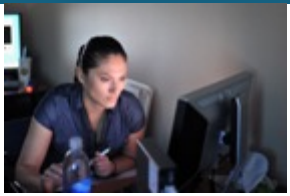
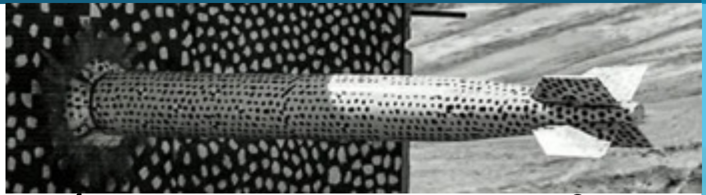
Development of SNAP Potentials for Fusion Reactor Materials







Mary Alice Cusentino[1], Mitch Wood[2], and Aidan Thompson[2]

[1]Material, Physical, and Chemical Sciences Center

[2]Center for Computing Research

2021 LAMMPS Workshop

August 12 2021

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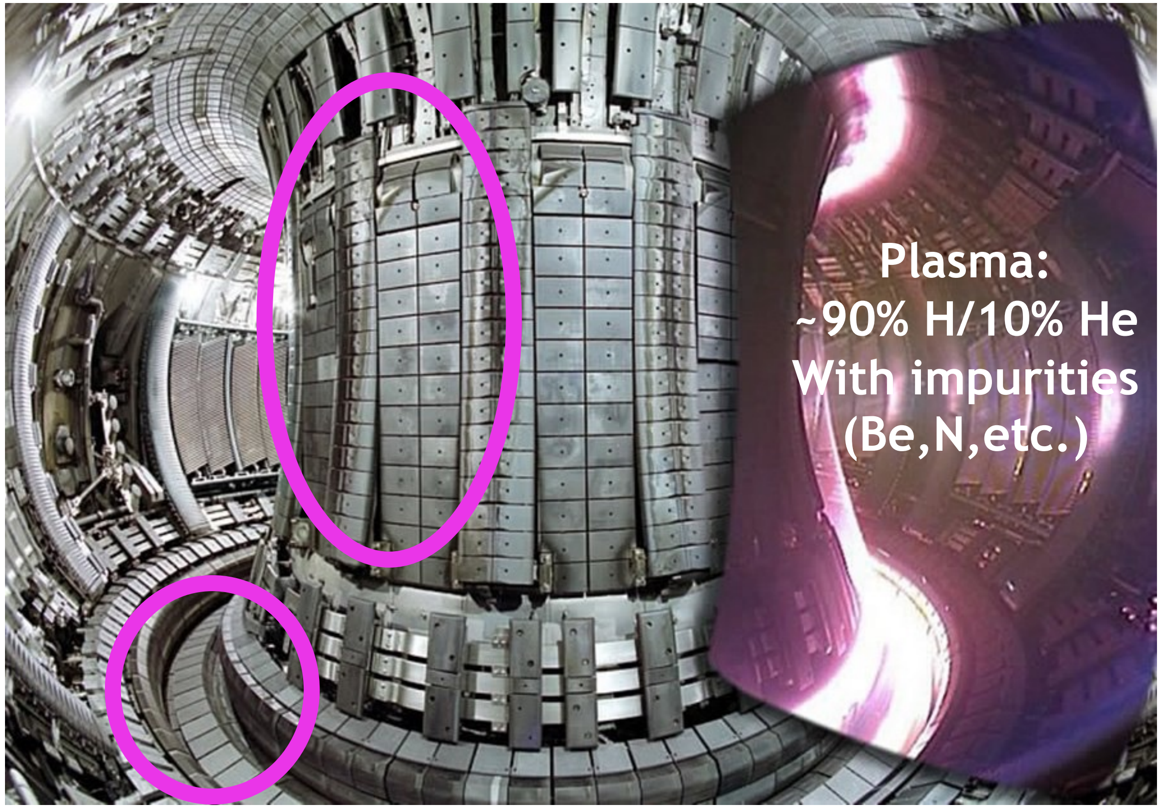
Materials for Fusion Energy

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

Beryllium First Wall



Tungsten Divertor

iter.org

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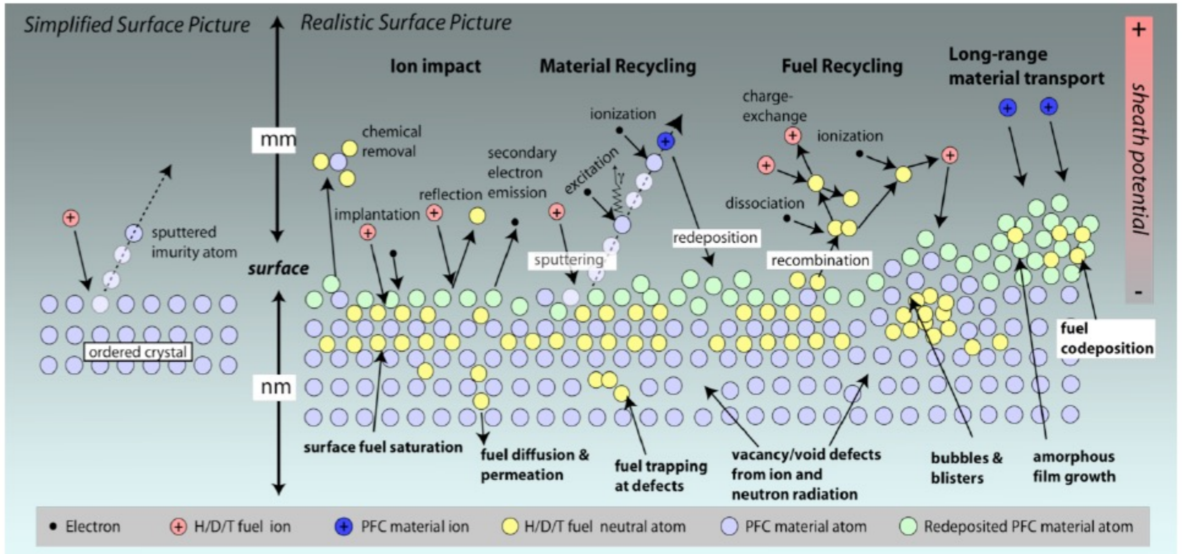

Wirth, et al. MRS Bulletin 36 (2011) 216-222

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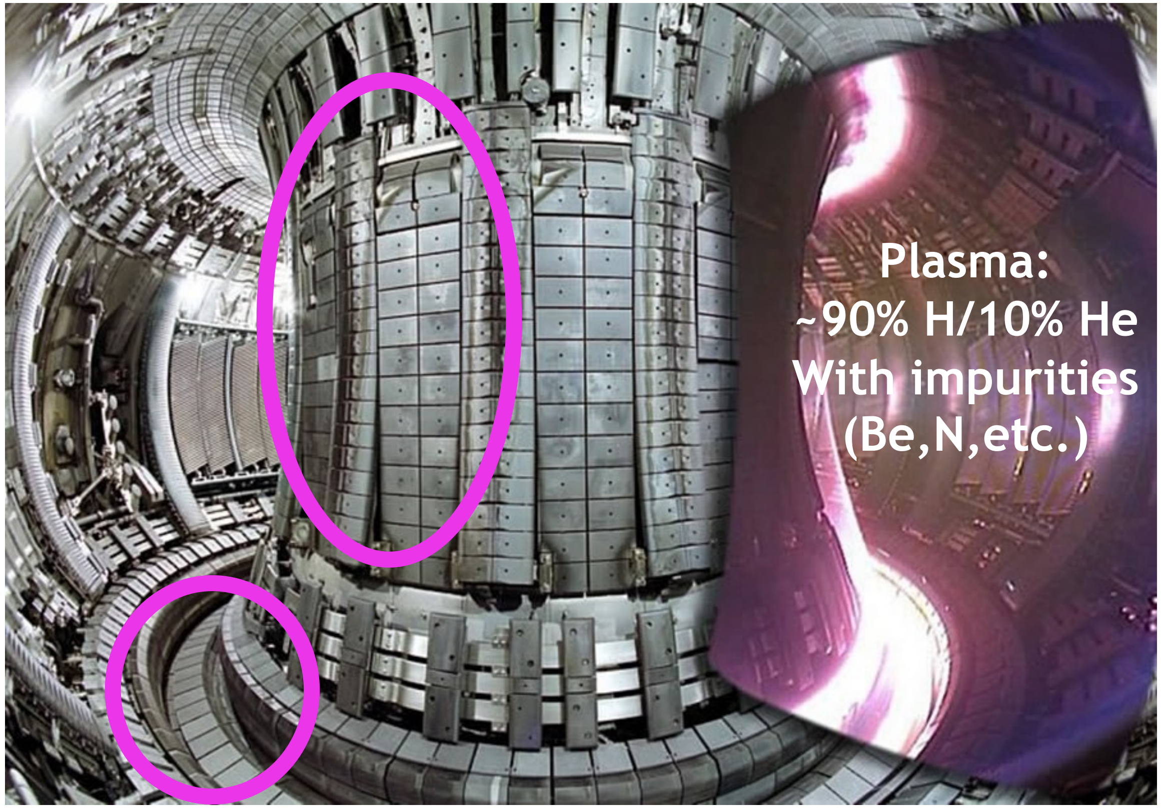

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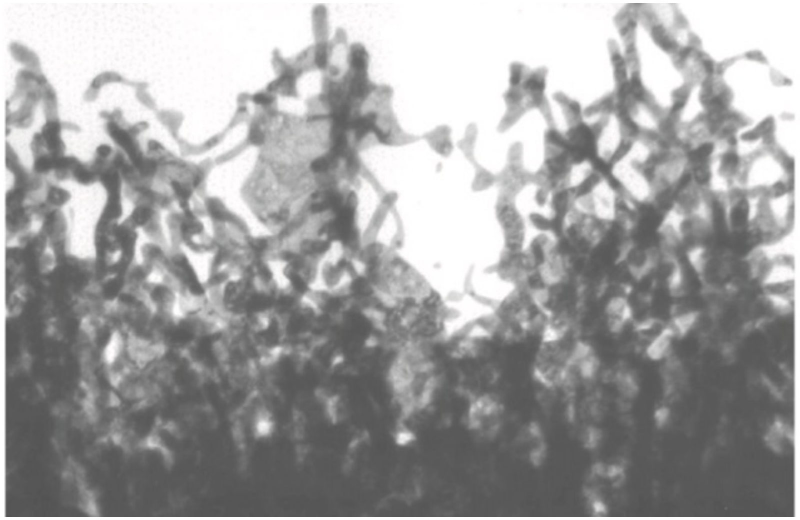
- Many complex processes that occur at the plasma/material interface that can lead to material degradation

Plasma Material Interactions in Tungsten

Material Degradation

Helium Fuzz Growth



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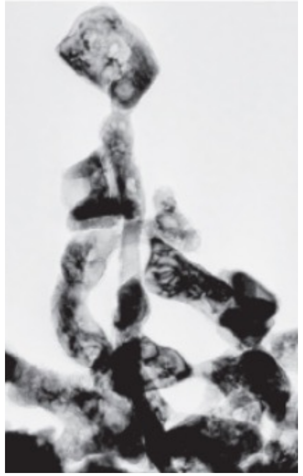

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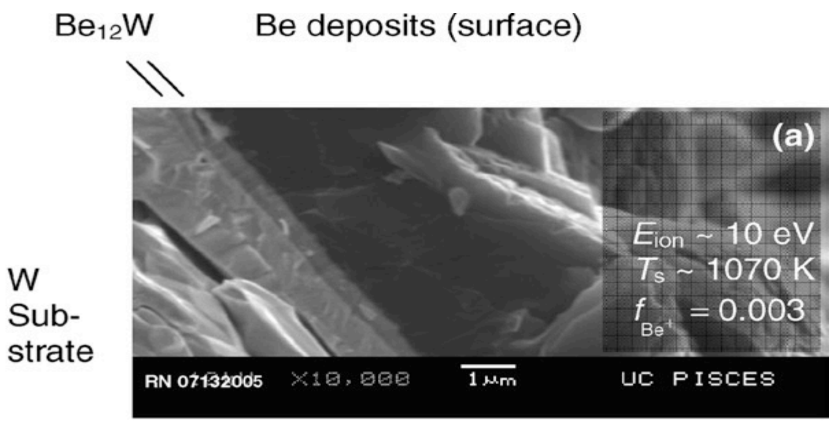
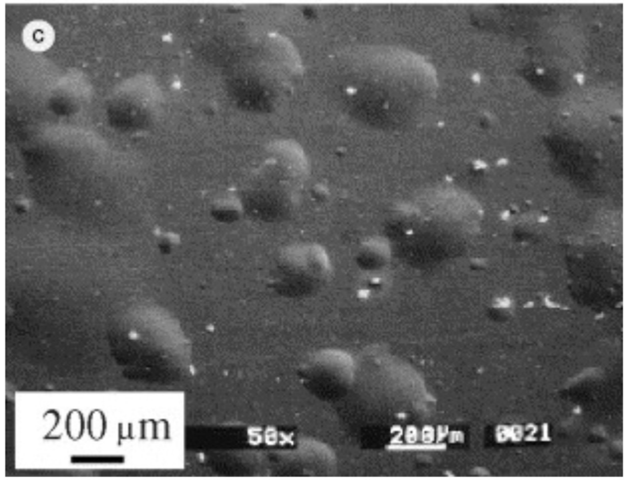
W-Be Intermetallics



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

Hydrogen Blisters



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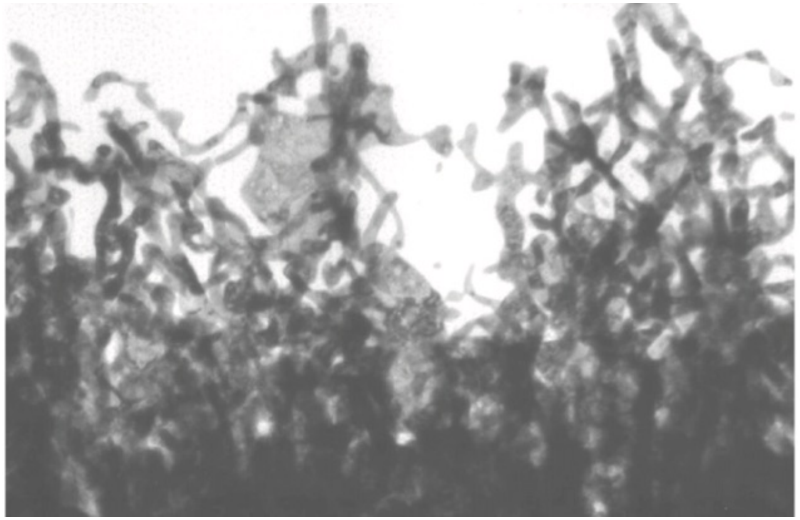

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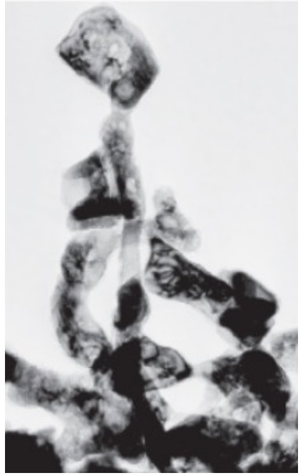

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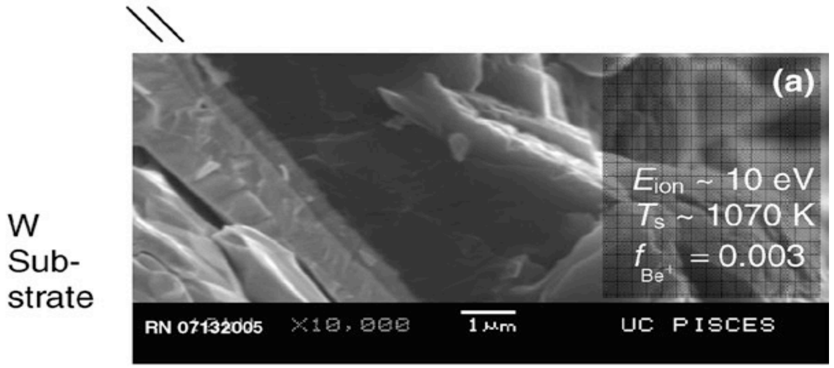

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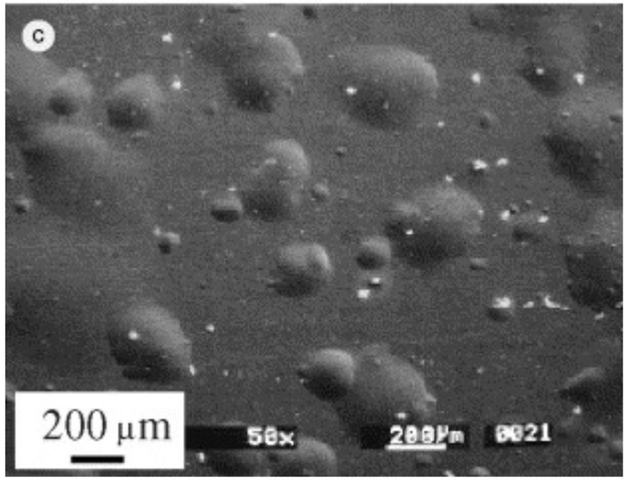

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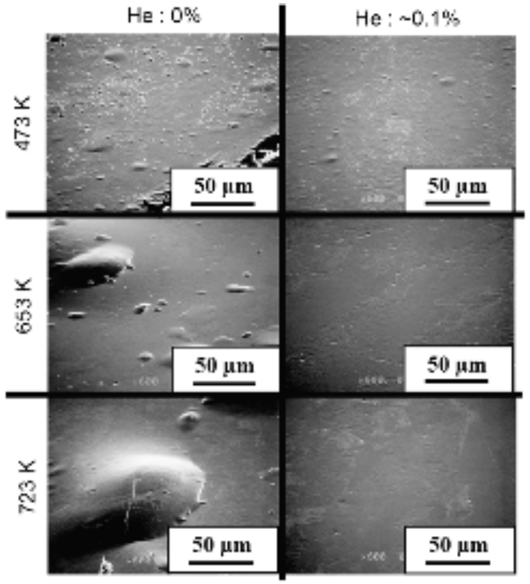
Tritium Retention

Effect of He on H Blistering



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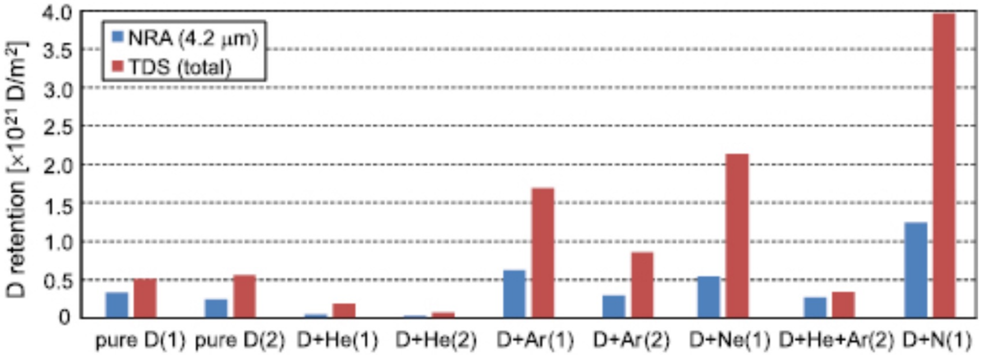

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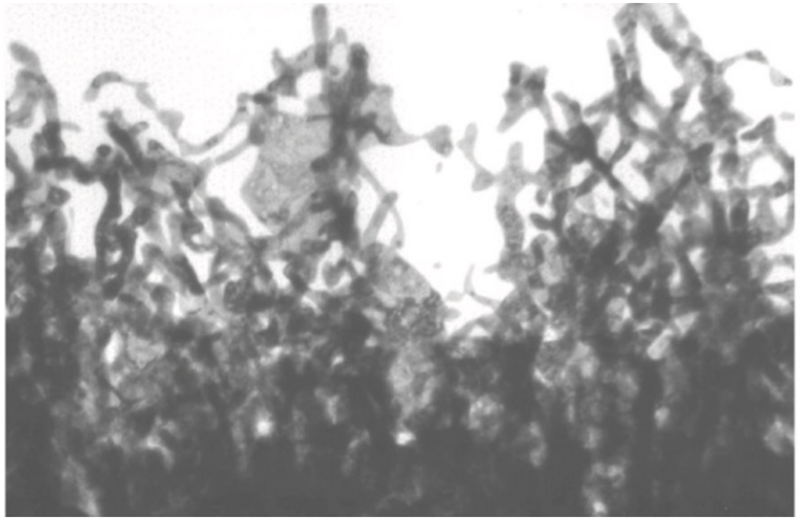

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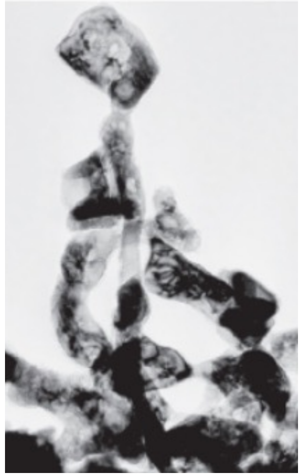

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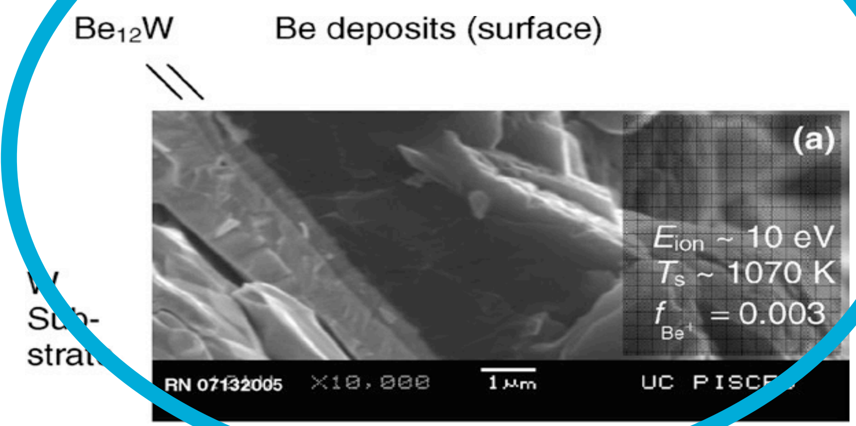

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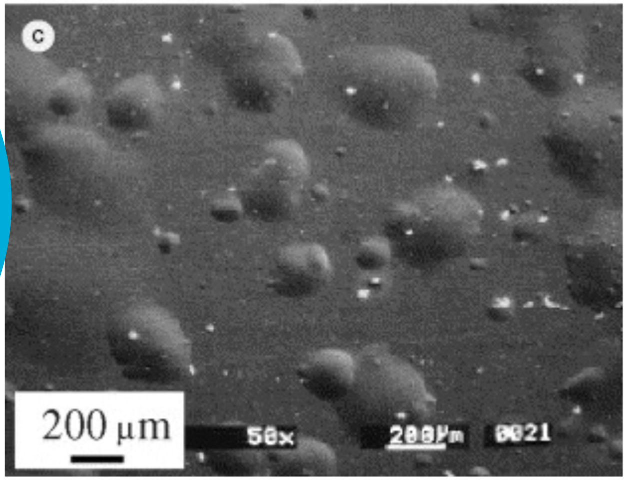

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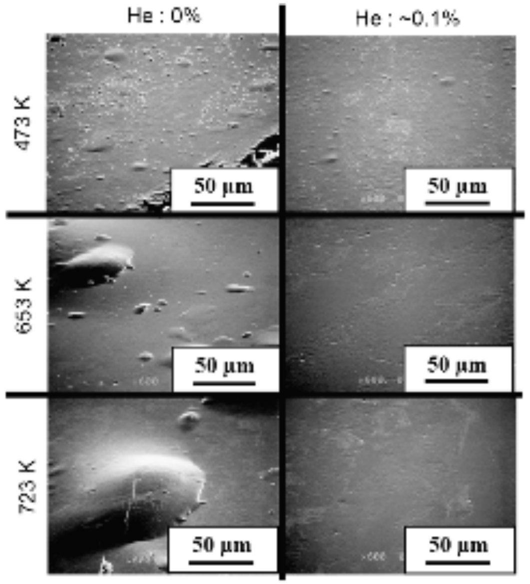

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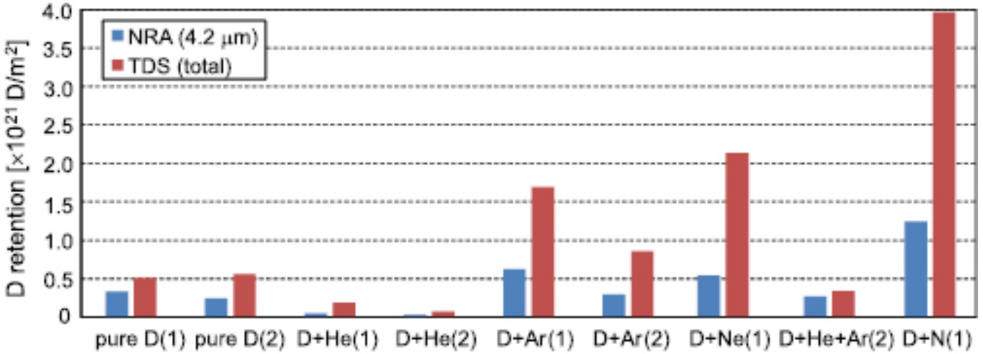

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SNAP Definition and Work Flow

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

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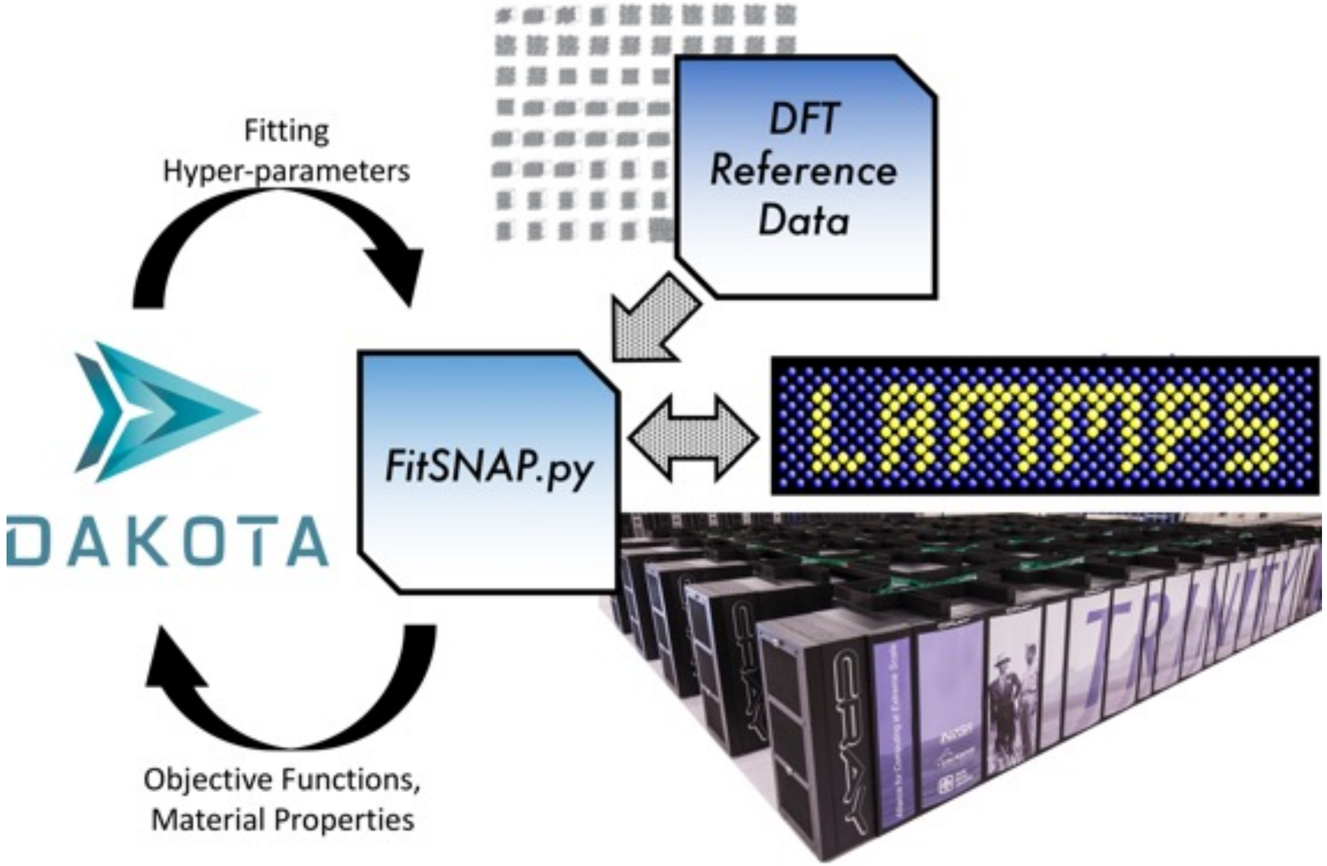


Code available: https://github.com/FitSNAP/FitSNAP

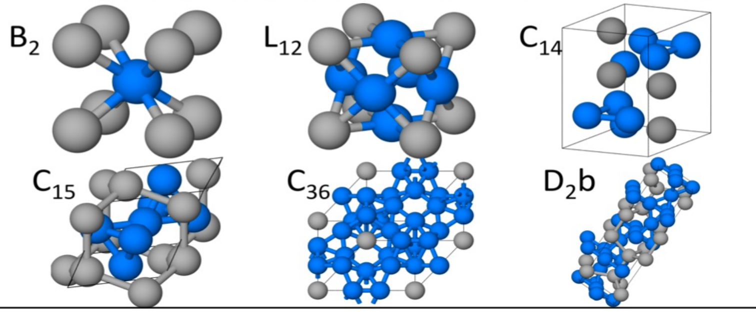
M. A. Wood, M.A. Cusentino, B.D. Wirth and A.P. Thompson, Phys. Rev. B 99, 184305

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:



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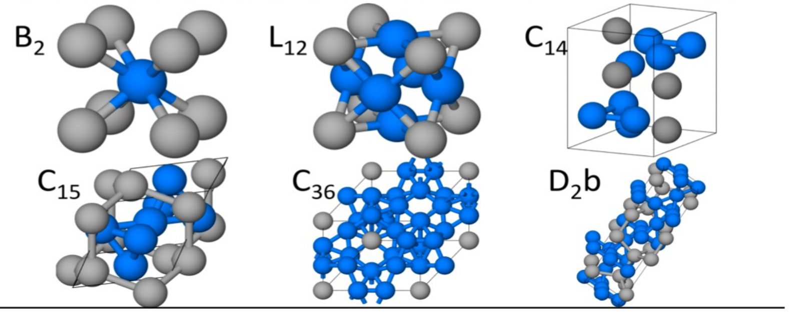

W-Be Intermetallic Formation Energies (eV)

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

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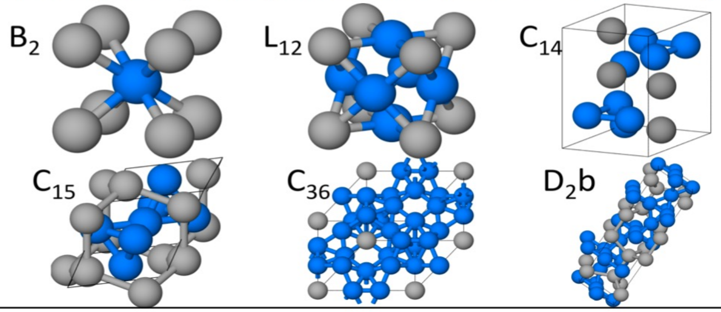

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Be Defect Formation Energies in W (eV)

	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

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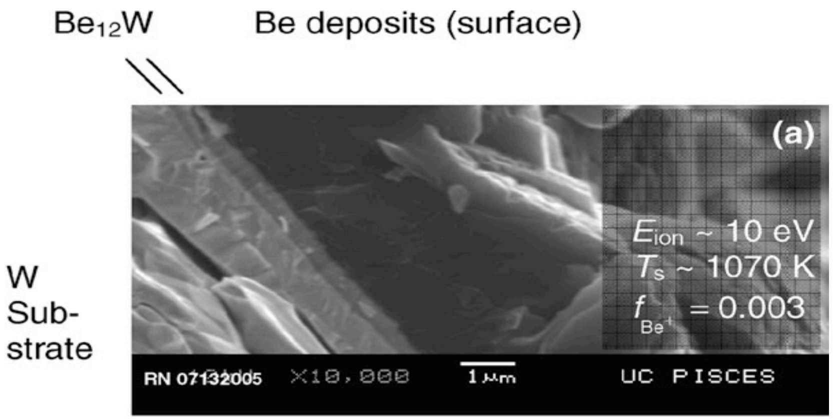
Beryllium Deposition Results in Near Surface Mixed Layer

- High energy (75 eV) and low energy (0 eV) beryllium deposition on tungsten surfaces

Experimentally Observed W-Be Intermetallics



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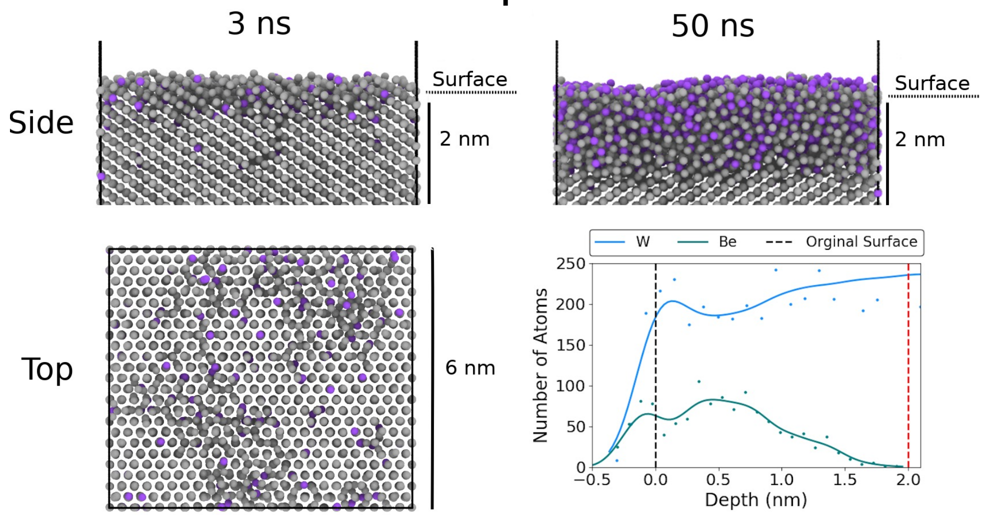
Beryllium Deposition Results in Near Surface Mixed Layer

75 eV Implantation



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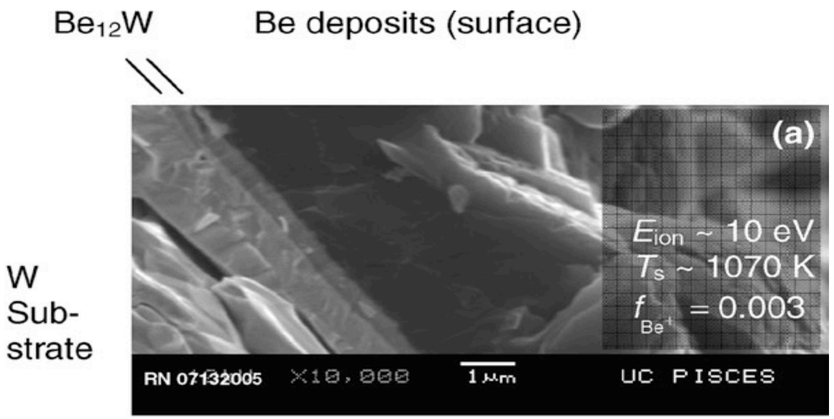

Fluence: 1.4×10^{20} m^{-2}

Cusentino, et al. Nucl. Fusion, accepted

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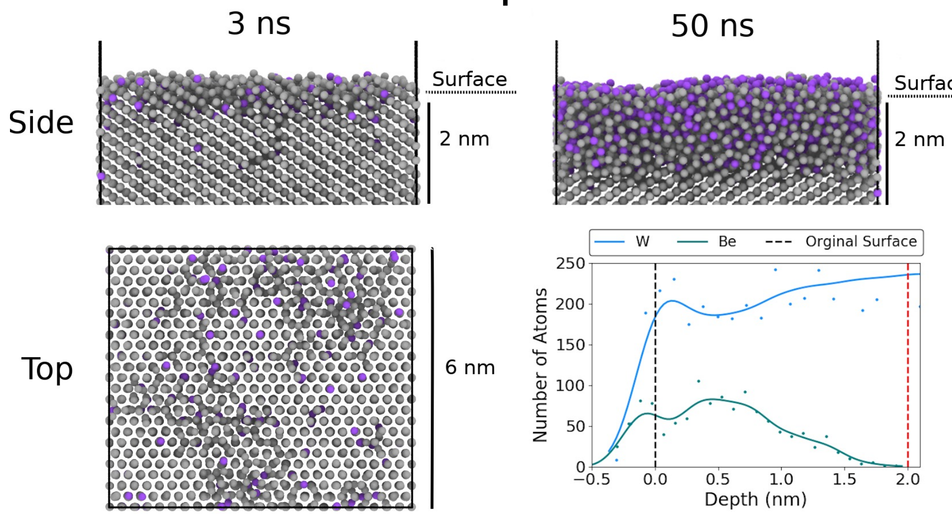

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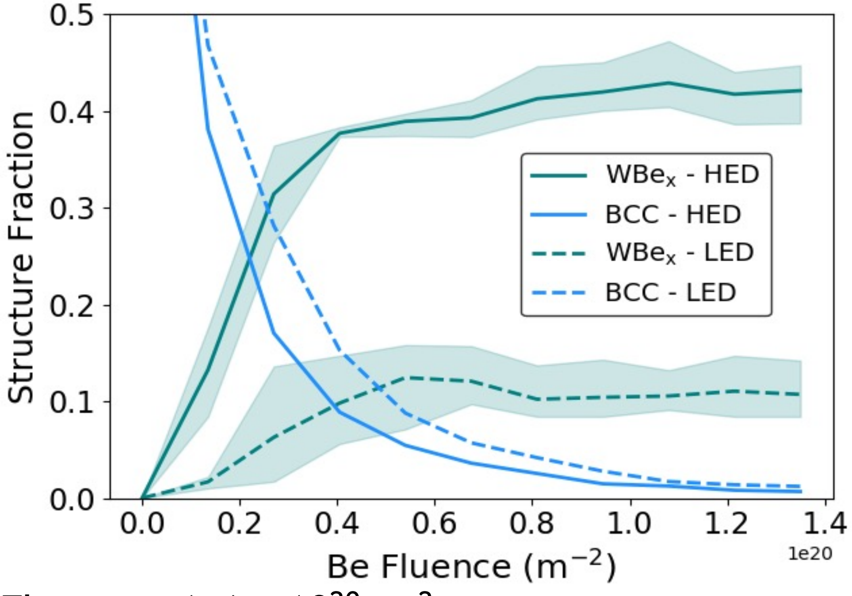
- Some intermetallic growth observed within mixed materials layer
- However, mixed materials layer appears to be kinetically trapped at MD time scales

Intermetallic Growth



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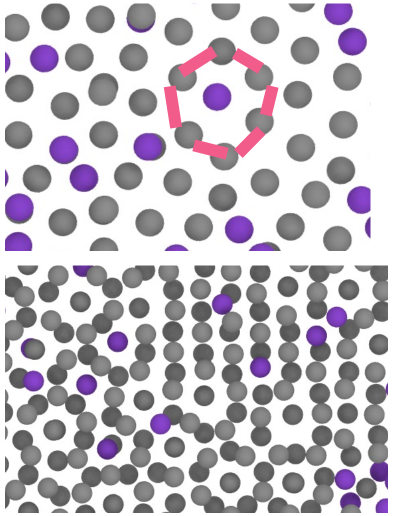

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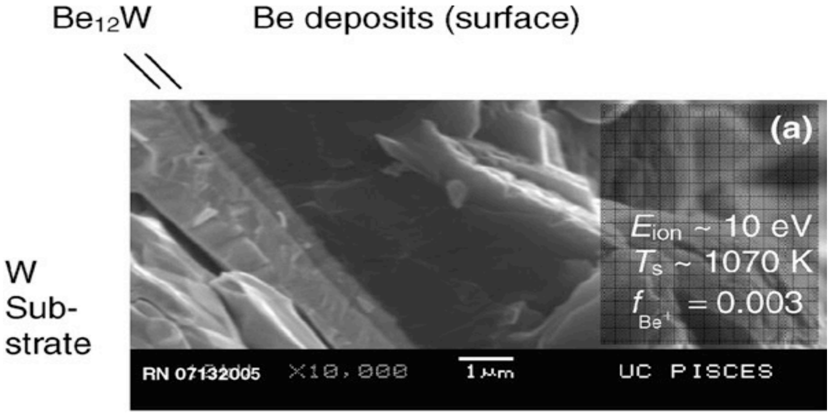
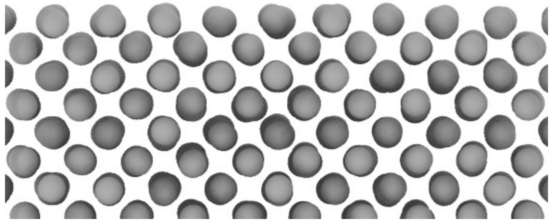


Baldwin, et. al. J. Nucl. Mater. 363-365 (2007) 1179-1183

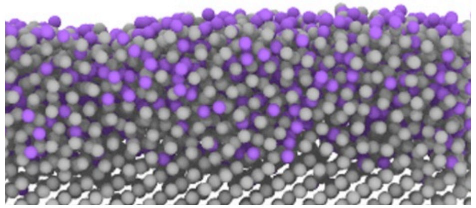
Cumulative He Implantation in W and W-Be at 2.5 x 10^{19} m^{-2}

Increasing TIme

Crystalline W

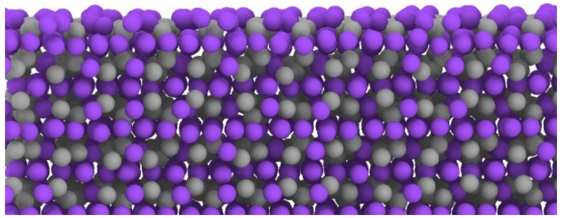


Amorphous W-Be



Blue: He
Purple: Be
Gray: W

WBe_2 C14 Structure



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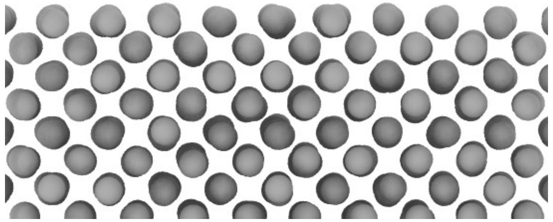

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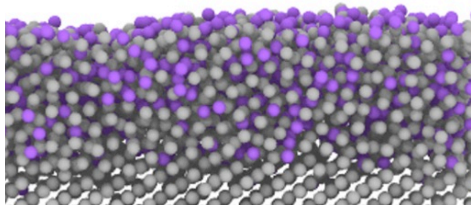

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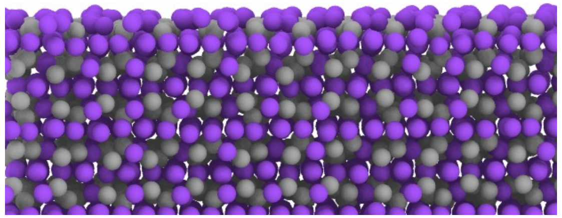

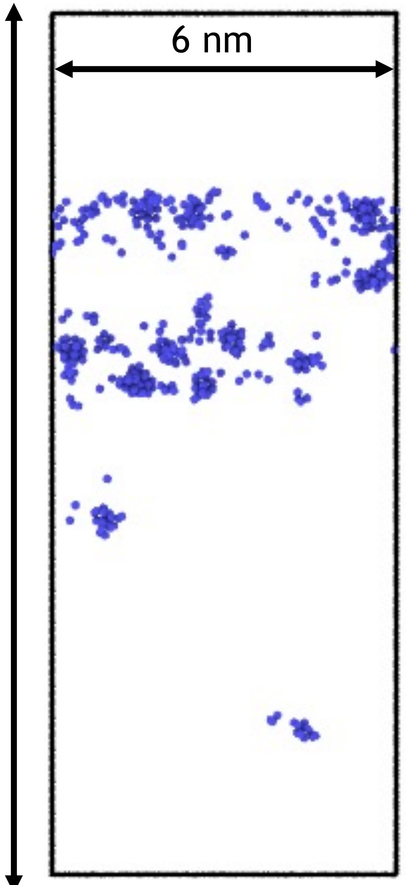

12 nm

Tungsten:

Larger He clusters distributed throughout simulation cell

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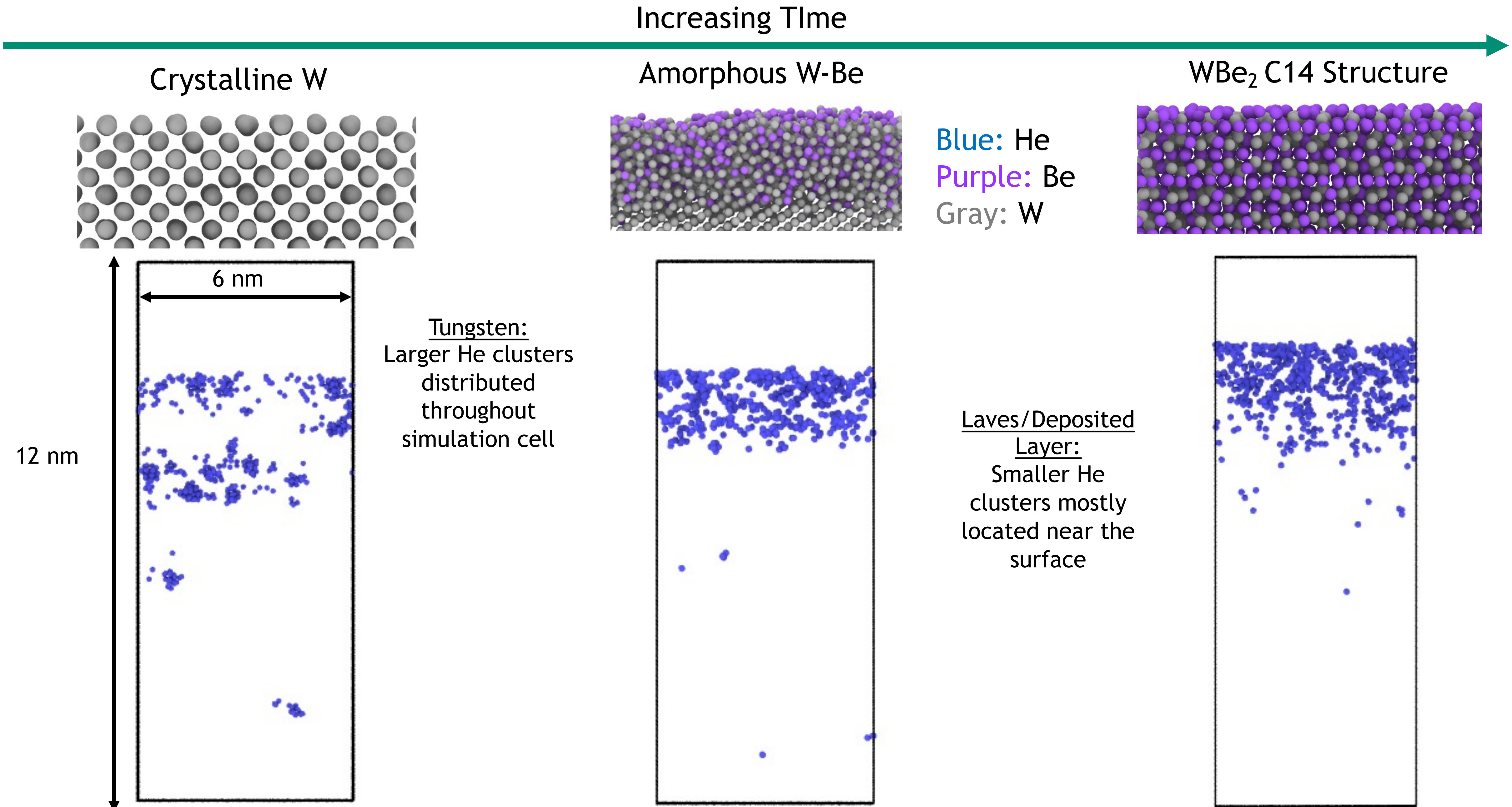

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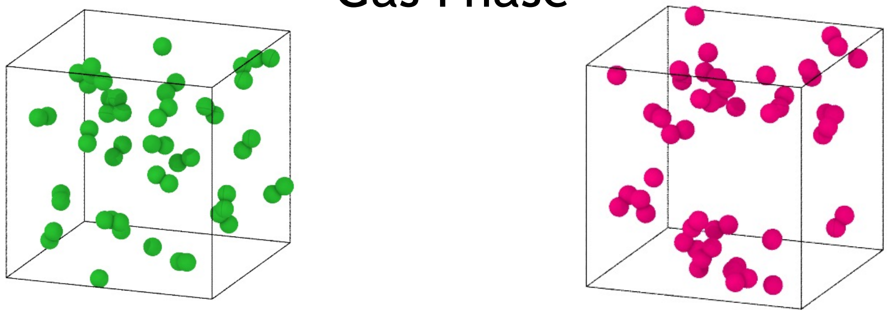
Laves/Deposited Layer:
Smaller He clusters mostly located near the surface

Extending SNAP for W-H and W-N

- Additional training data needed
- Pure H/N data:
  - Dimers, trimers, DT-MD of gas dimers

Gas Phase



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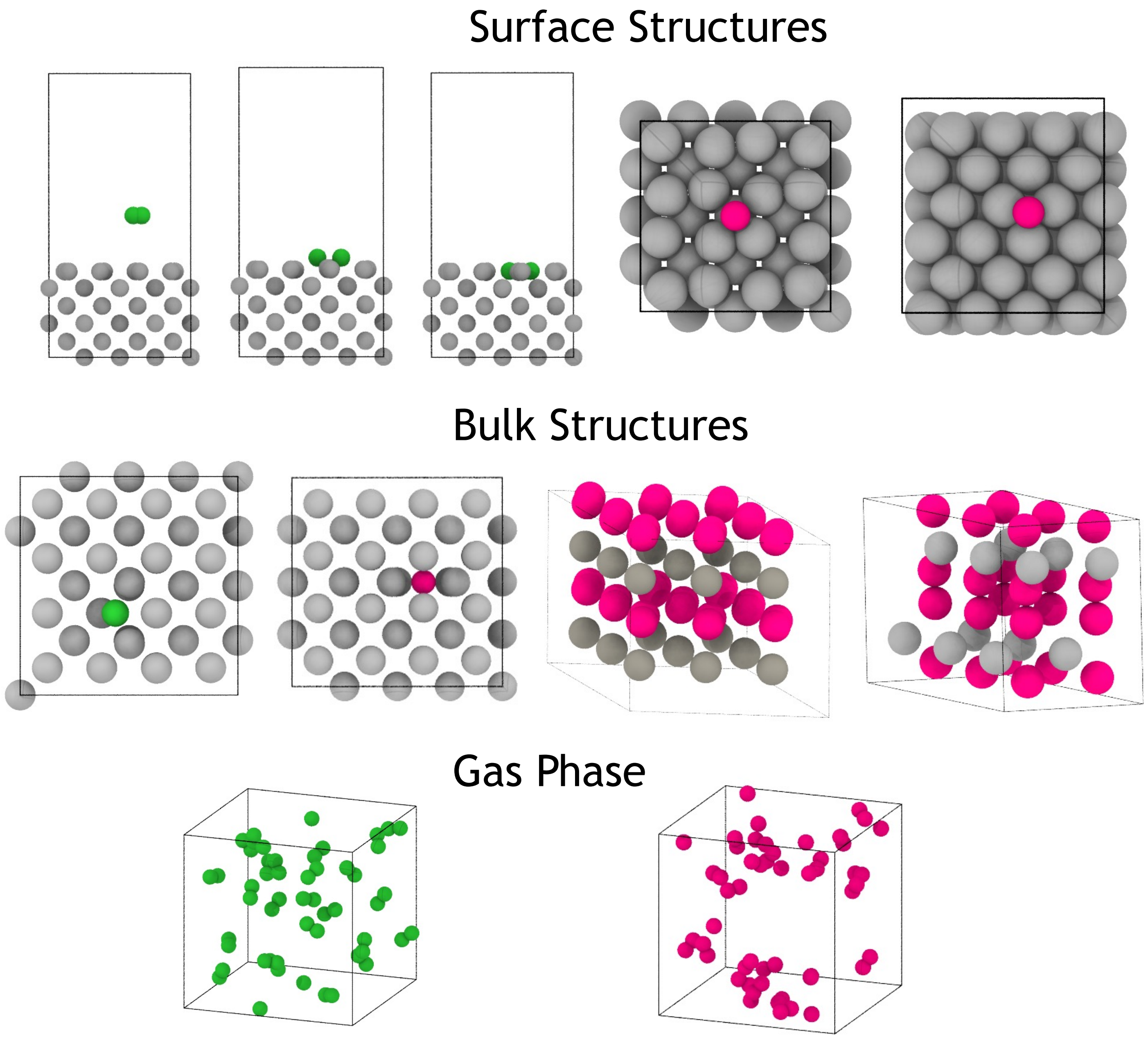

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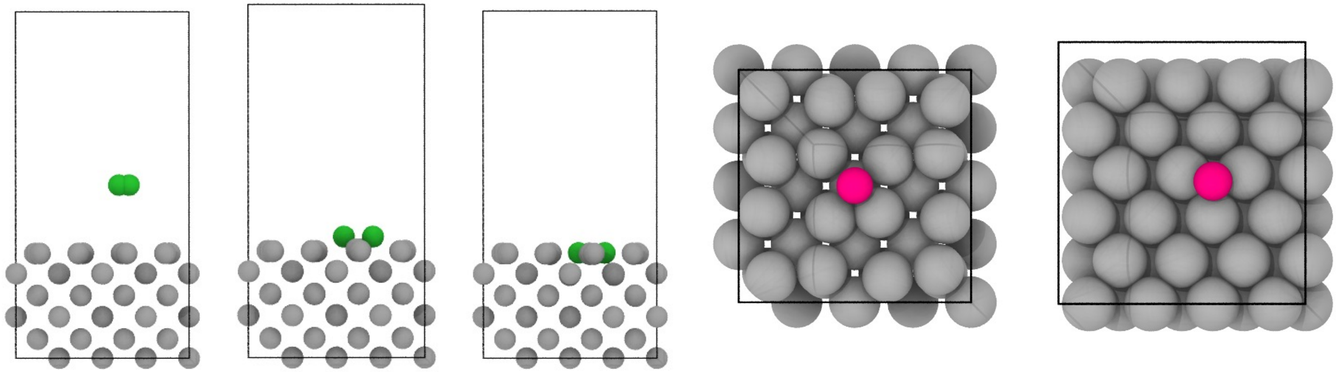
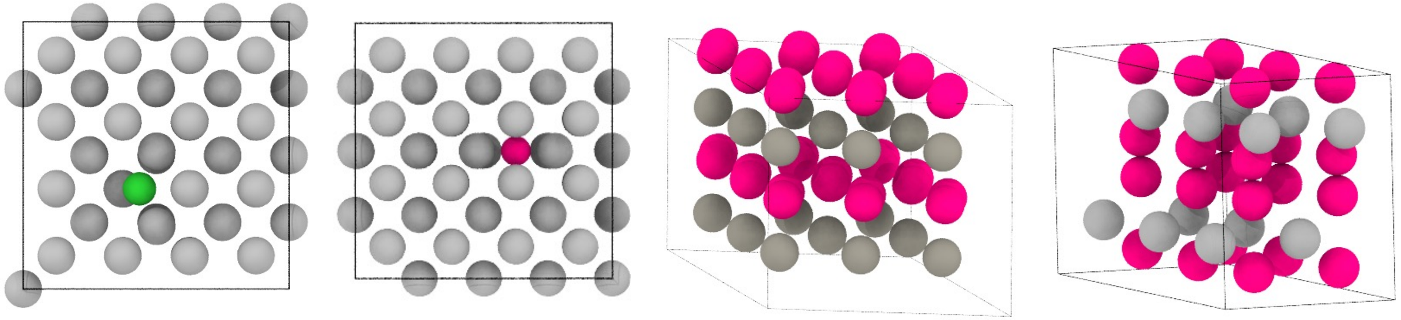
  - W_xN_y bulk configurations
- Additional objective functions added:
  - W-H/N bulk defect formation energies
  - H/N surface adsorption energies
  - W_xN_y cohesive energies

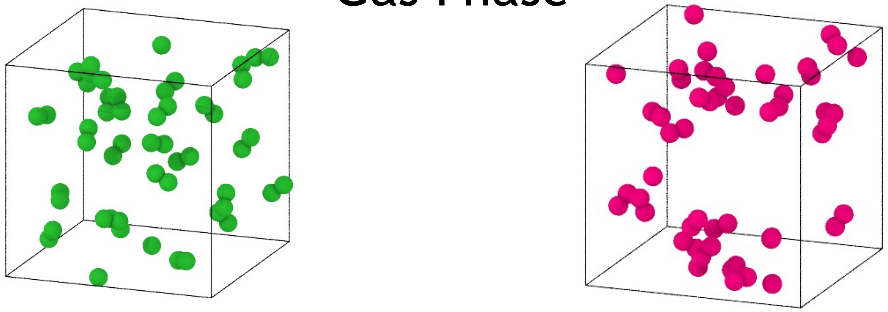
Surface Structures



Bulk Structures



Gas Phase



W: Grey H: Green N: Pink

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

- Have never used SNAP for gaseous species before
- Hydrogen and nitrogen training 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

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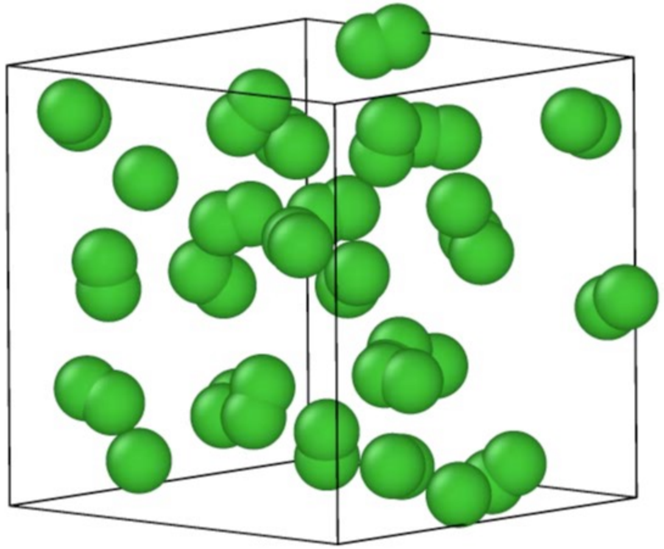
Poor Clustering Behavior



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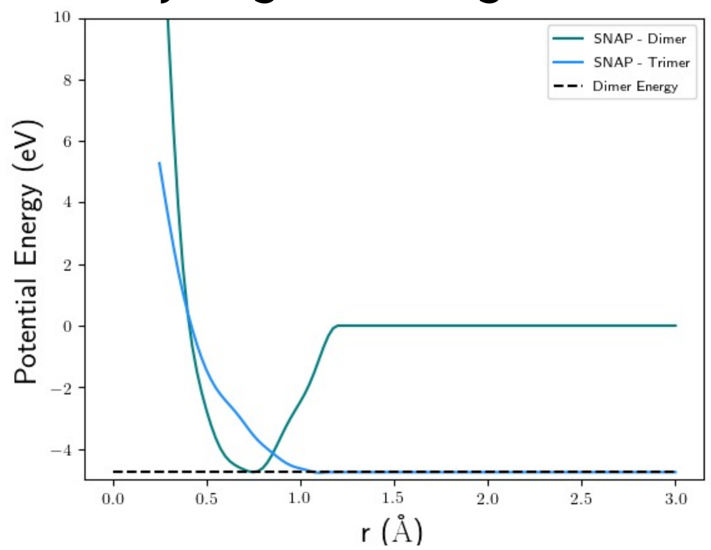
Hydrogen Binding Curves



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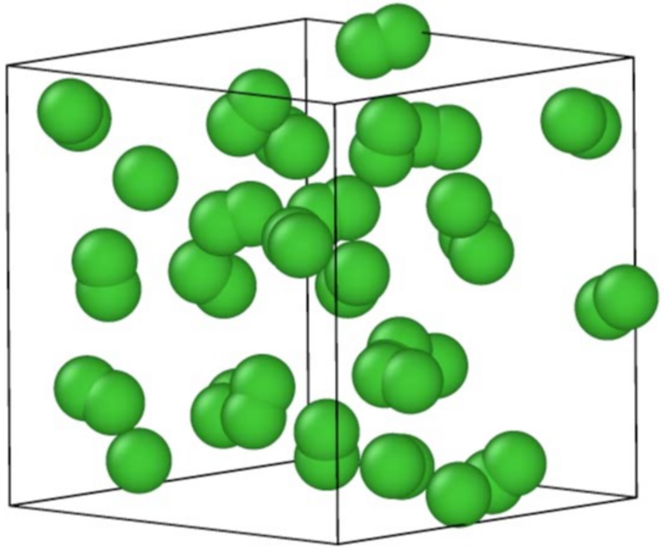
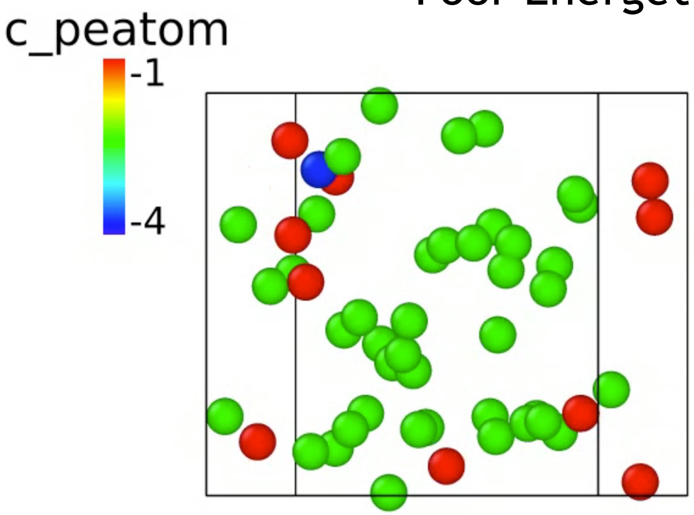


Poor Energetics

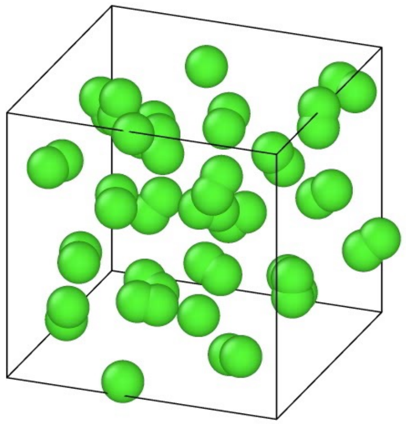


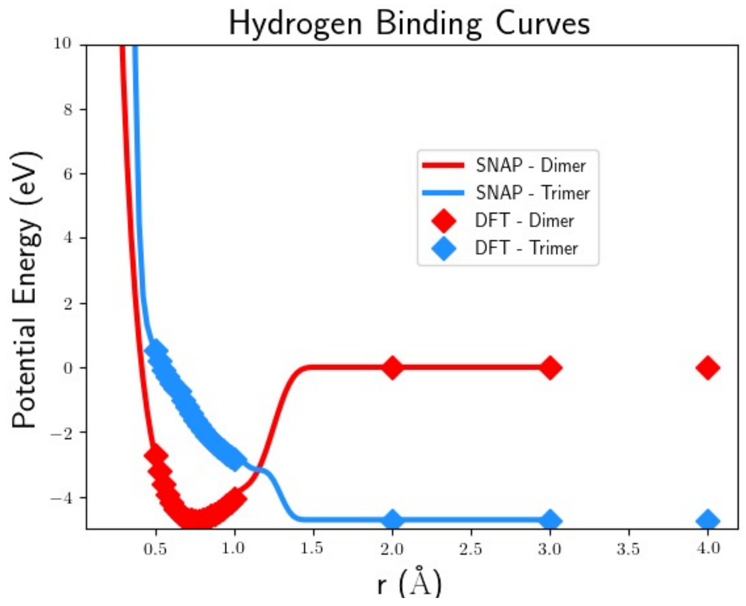
Atoms colored by potential energy

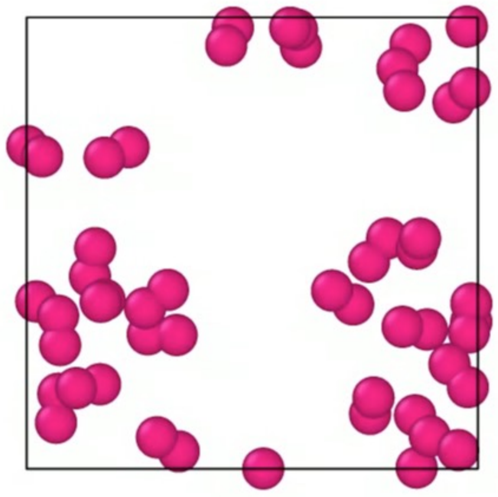
- Green is nominal H2 energy
- Reproduces correct binding curves

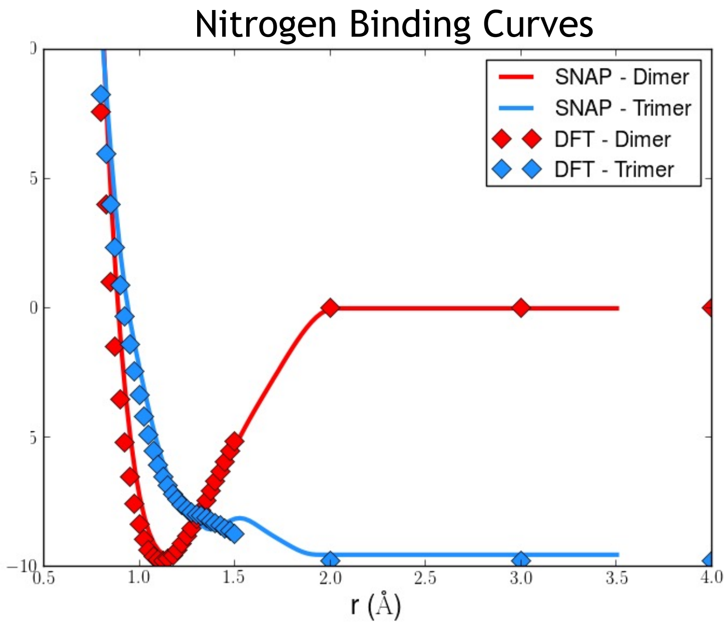
Changes to Fitting Results in Better Hydrogen and Nitrogen Potentials

- 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) compared to W (4.6 Å)
  - Adding extra objective function for dynamics behavior
  - Adjusted ZBL cutoff
  - Adjusted objective function for binding curves







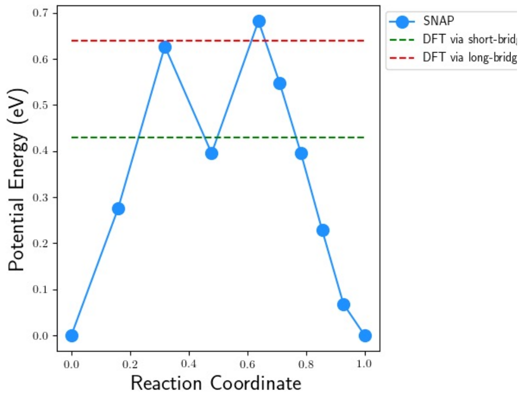


Tradeoff Between Surface and Bulk Behavior

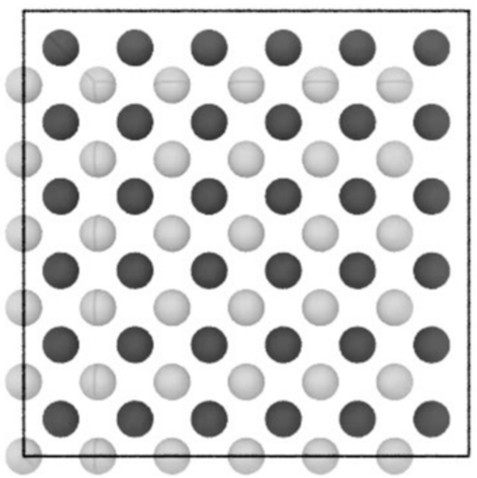
Potential for H on Surfaces

	DFT (eV)	SNAP (eV)
(100) Ads. Site	Bridge	Bridge
(110) Ads. Energy	-0.96	-0.95
(100) Ads. Site	Hollow	Hollow
(110) Ads. Energy	-0.75	-0.43

NEB Surface Hop



Top-down Surface View



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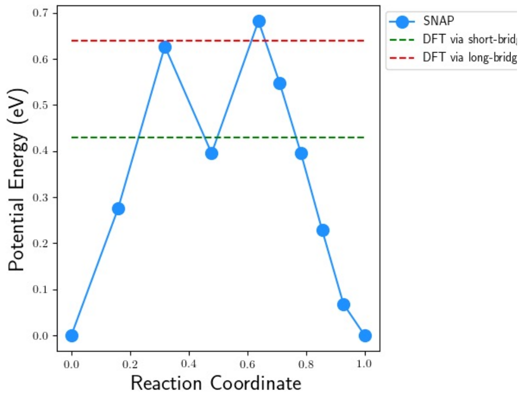
Potential for H in Bulk

	DFT	SNAP
E_f^{Tet}(eV)	0.88	0.88
E_f^{Oct}(eV)	1.26	1.26
E_f^{Sub}(eV)	4.08	4.02

NEB Surface Hop



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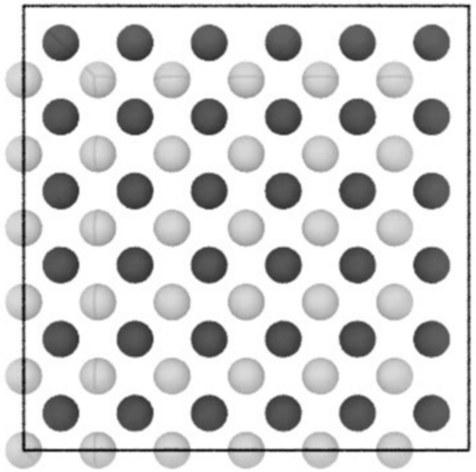
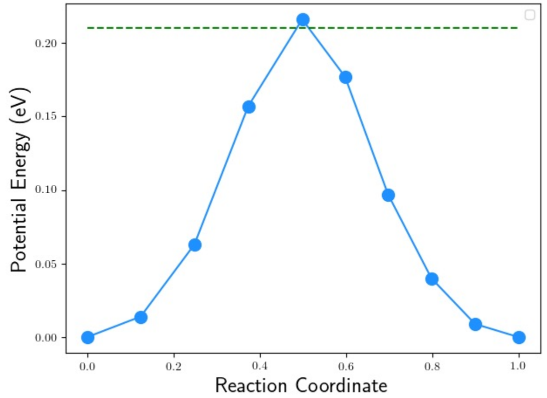
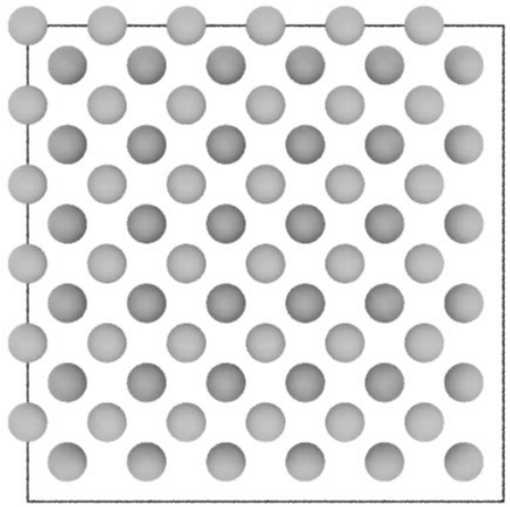


NEB Bulk Hop



Bulk Tungsten



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(100) Ads. Site	Bridge	Bridge
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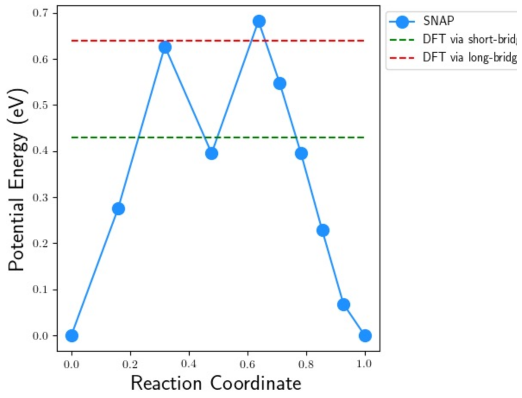

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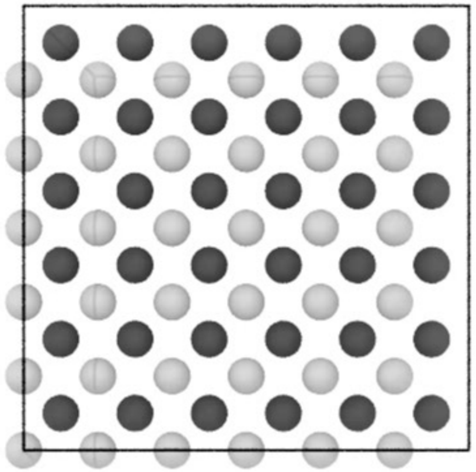
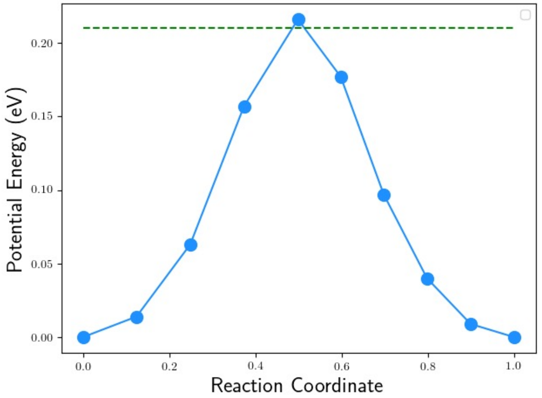
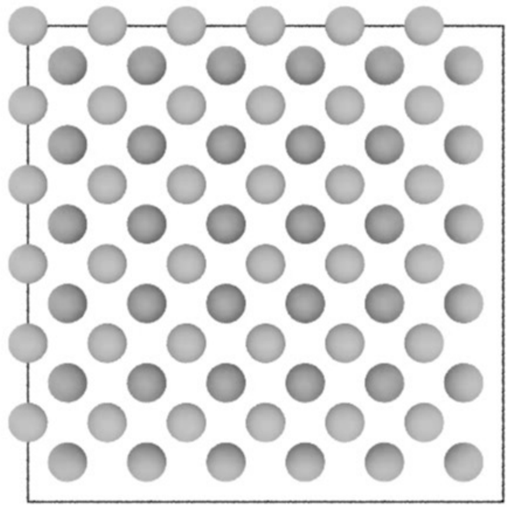


	DFT	SNAP
E_f^{Tet}(eV)	0.88	8.89
E_f^{Oct}(eV)	1.26	9.34
E_f^{Sub}(eV)	4.08	3.87

NEB Bulk Hop



Bulk Tungsten



	DFT (eV)	SNAP (eV)
(100) Ads. Site	Bridge	Hollow
(110) Ads. Energy	-0.96	-3.54
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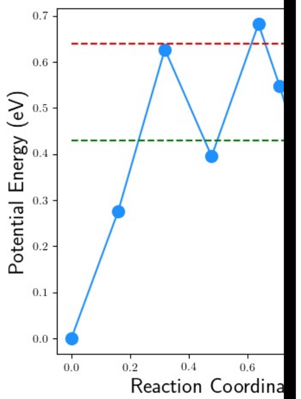
Tradeoff Between Surface and Bulk Behavior

Potential for H on Surfaces

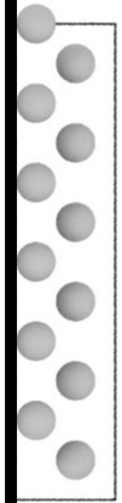
(100) A…	
(110) Ad…	
(100) A…	
(110) Ad…	

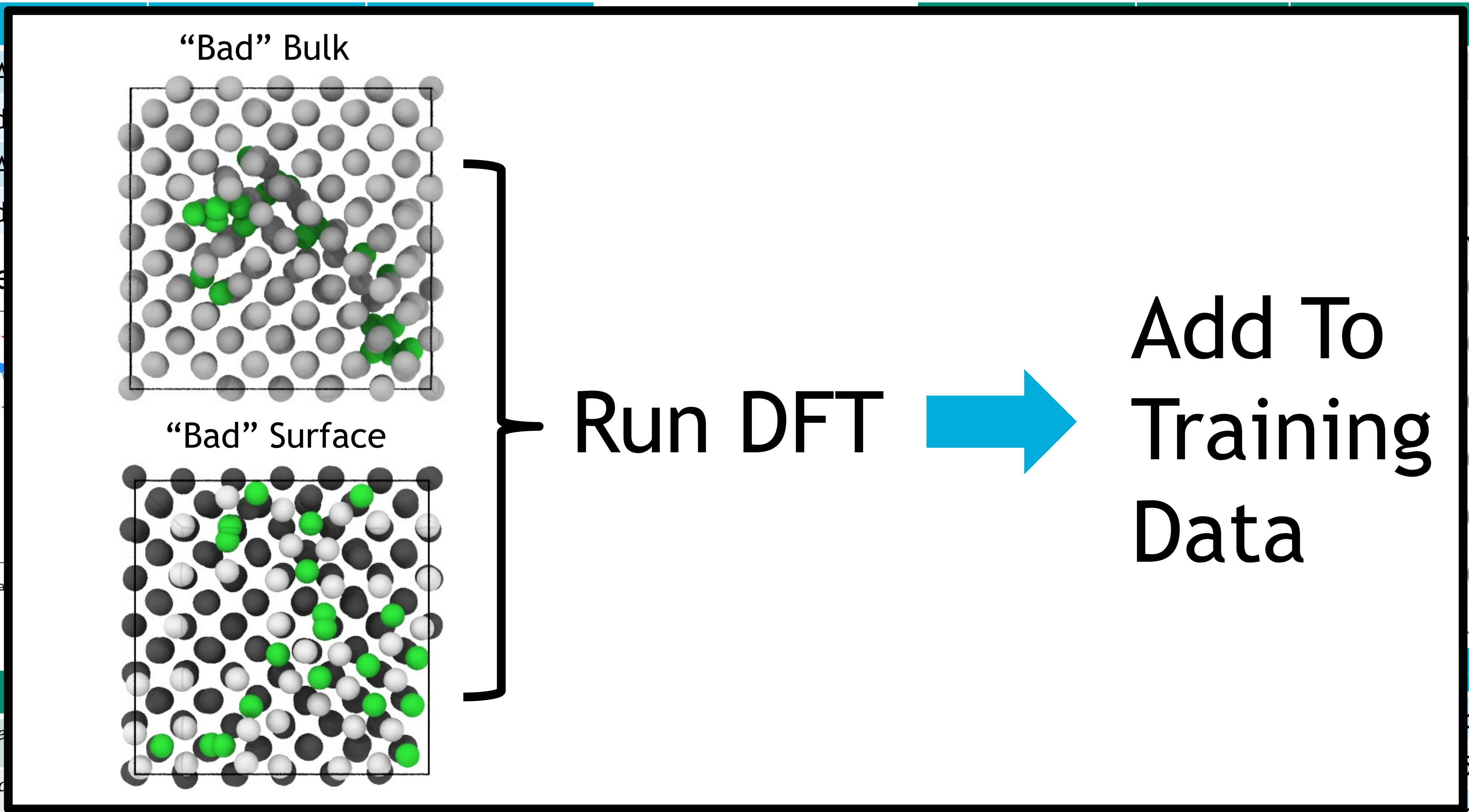
NEB Surface…



$E_f^{Te…}$		
$E_f^{Oc…}$		
E_f^{Sub} (eV)	4.08	3.87

Potential for H in Bulk





		…(eV)
		…ow
		…54
(100) Ads. Site	Hollow	Hollow
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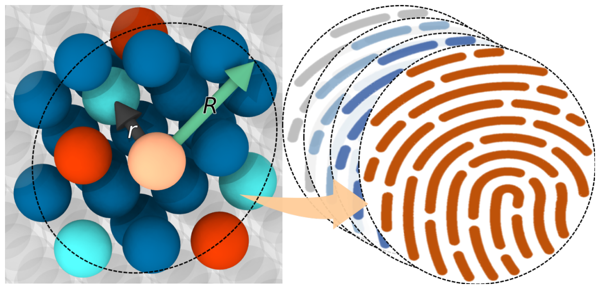
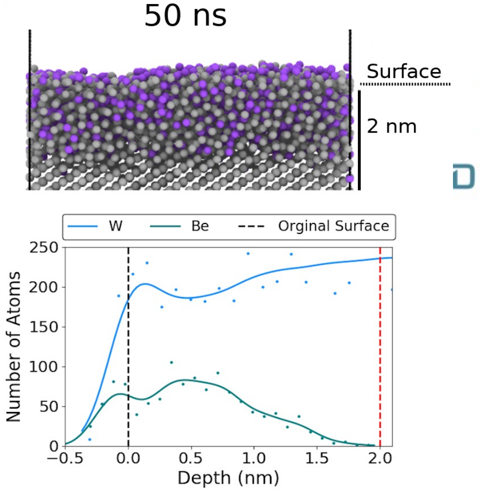
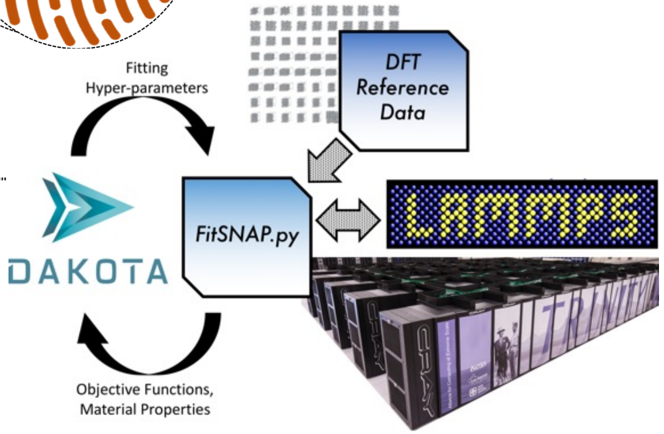
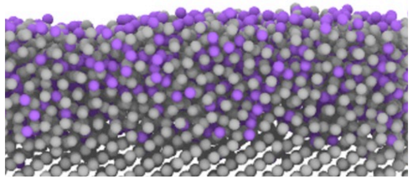
Summary

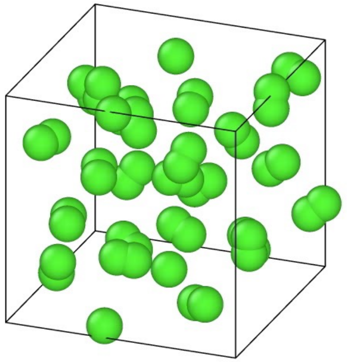
- SNAP is a versatile ML interatomic potential that has been applied to a variety of materials including materials for fusion energy
- A W-Be SNAP potential has been developed and used to study Be implantation in W and extended to simulation He implantation W-Be materials
- The current SNAP potential 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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mcusent@sandia.gov

EXASCALE COMPUTING PROJECT

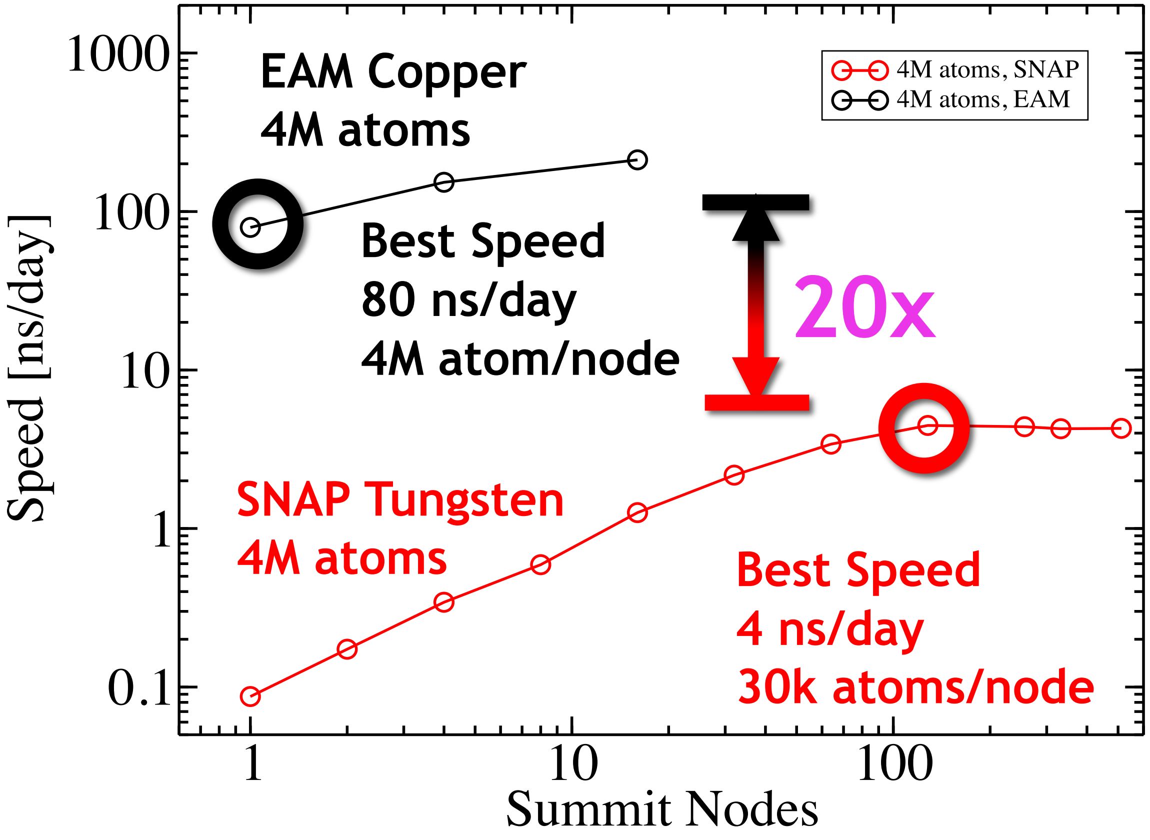
Office of Science

Backup Slides

MD Approximations Change Over Time

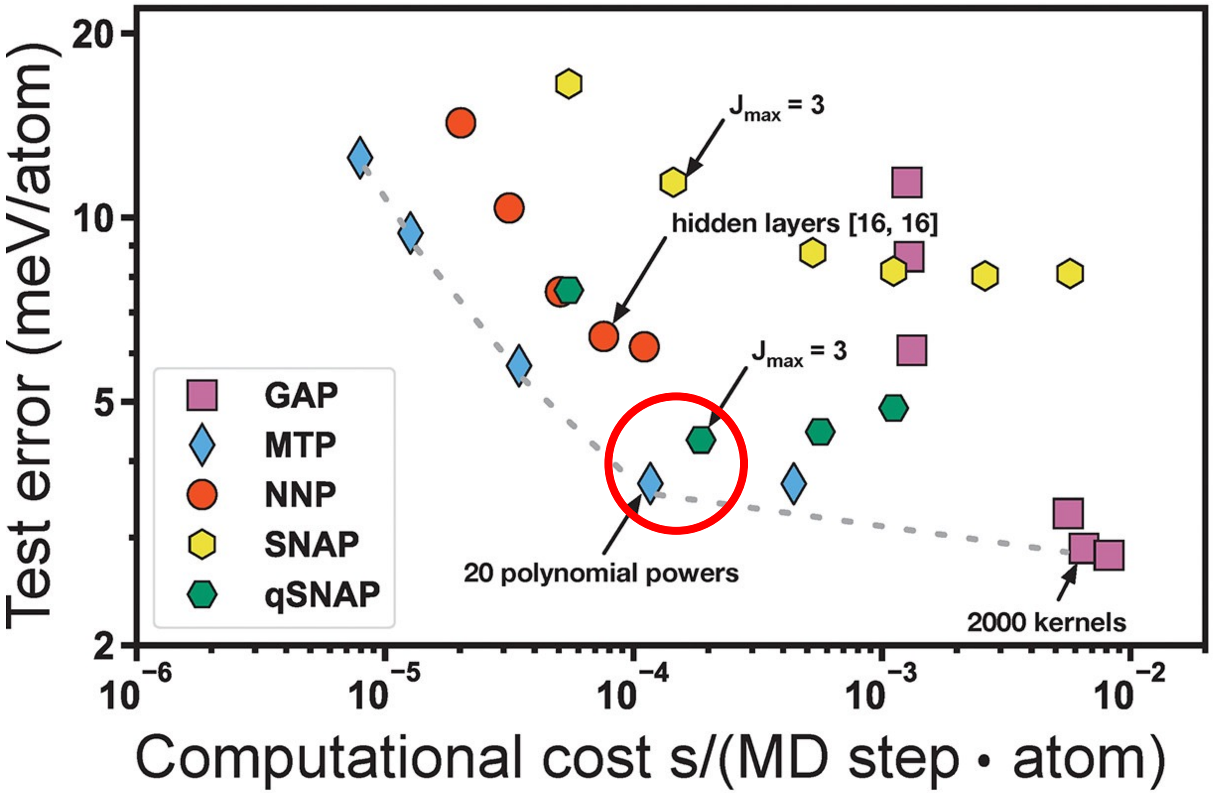
Twobody (B.C.)	Manybody (1980s)	Advanced (90s-2000s)	Big Data / Deep / Machine Learning (2010s)
Lennard-Jones, Hard Sphere, Coulomb, Bonded	Stillinger-Weber, Tersoff, Embedded Atom Method	REBO, BOP, COMB, ReaxFF	GAP, SNAP, NN,…

GPU Timings



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

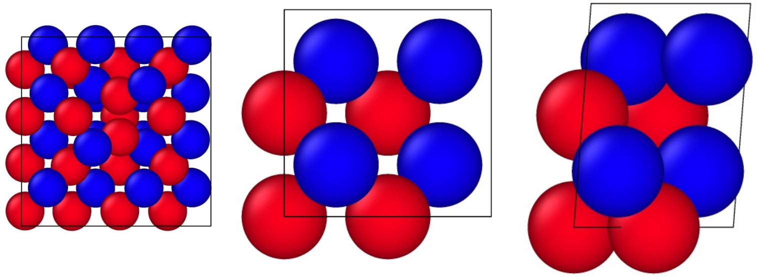
Resources are limited, which is your best choice?



What Makes a Machine Learned Interatomic Potential?

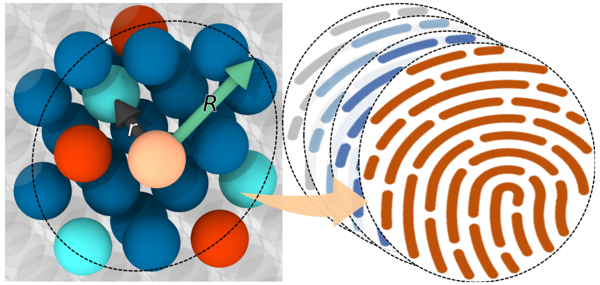
Training Data

- 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

Testing Potentials: Hydrogen Implantation in Tungsten

- Interested in studying hydrogen implantation in tungsten and how it interacts within the material, especially with other plasma species or defects
- Initial testing of W-H SNAP potentials for hydrogen implantions
- 100 eV H implanted every 10 ps at 1000 K for (100) W surface
- Hydrogen correctly initially resides at tetrahedral interstitial site
- Diffusion barrier is somewhat high so diffusion is lower than expected
- EAM does not predict correct surface behavior and desorbs as H atoms as opposed to H_2 molecules