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Molecular Dynamics Simulations of Hydrogen and Nitrogen on Tungsten Surfaces

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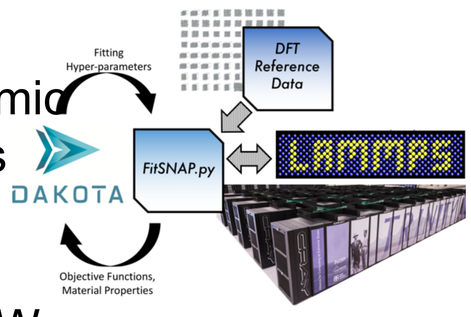
Motivation

- Divertor component will be subject to high fluxes of mixed ion species including hydrogen and nitrogen
- Hydrogen retention in reactor components is a concern
- Experiments of nitrogen implantation in tungsten has resulted in tungsten nitride formation which increases hydrogen retention[1]
- Critical to understand how tungsten nitrides form and increase hydrogen retention

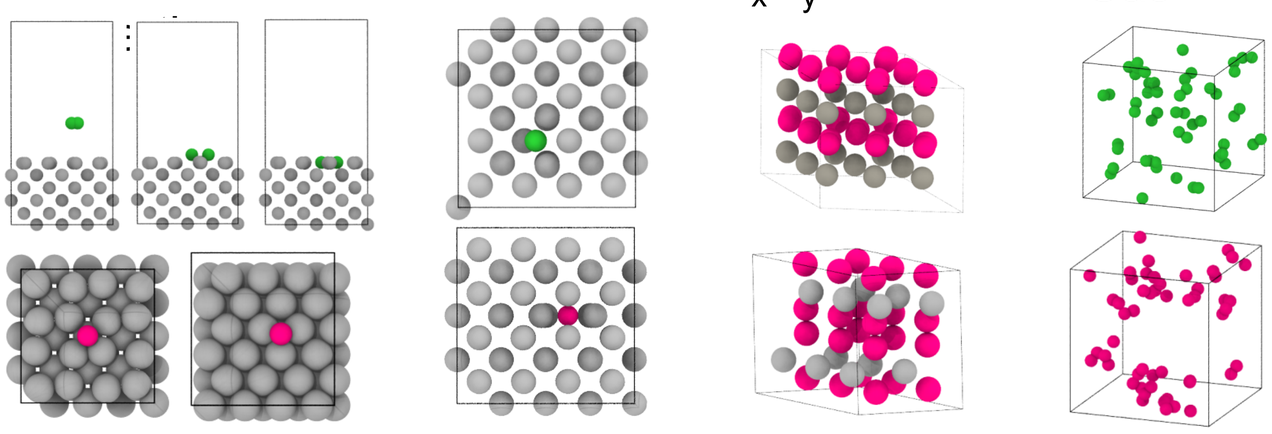
SNAP Potential Development

- Few existing potentials for W-H and W-N with limited accuracy
- SNAP[2] is a machine learned interatomic potential trained to DFT data and has improved accuracy[3] compared to traditional potentials
- Extension of W[4,5] SNAP to W-H and W-N
- However, very limited experience in machine learned potentials for gas-metal interactions



DFT Training Data

W: Grey H: Green N: Pink



Fitted Properties

- SNAP can reproduce both gas-phase and condensed-phase chemical interactions
- One set of descriptors for very different atomic species

Formation Energies

* units in eV	H DFT	H SNAP	N DFT	N SNAP
E_f^{Dimer}	-4.75	-3.27	-9.79	-9.73
E_f^{Tet}	0.88	0.83	1.85	1.39
E_f^{Oct}	1.26	1.35	1.11	1.05
E_f^{Sub}	4.08	3.93	4.72	4.20

W_xN_y Cohesive Energies

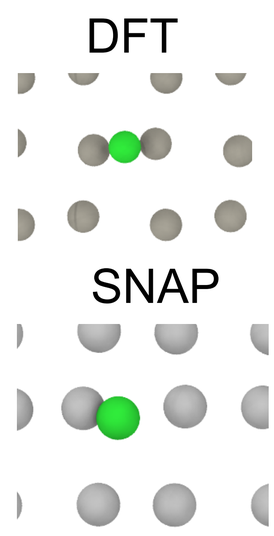
* units in eV	P$\bar{6}$2m (WN_2)	P6m2 (WN_2)	NiAs (WN)	WC (WN)	$MoSi_2$ (W_2N)
DFT	-1.82	-0.91	-0.84	-0.23	-0.03
SNAP	-2.13	-1.45	-0.46	-1.16	0.36

H and N Adsorption Sites on (100) W

- Experiments using the Angle-Resolved Ion Energy Spectrometer (ARIES) device at Sandia can provide information about surface adsorption sites
- ARIES results were compare with the SNAP potentials developed for W-H and DFT training data

Hydrogen	Ads. Site	Height (Å)	E_{ads} (eV)
DFT	Bridge	1.37	-1.2
SNAP	Bridge	0.78	-2.9
ARIES	Bridge	1.0	-

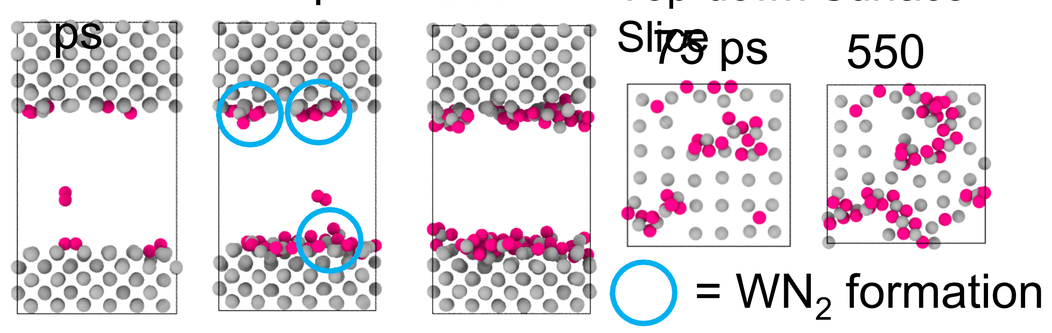
Nitrogen	Ads. Site	Height (Å)	E_{ads} (eV)
DFT	Hollow	0.67	-2.1
SNAP	Hollow	0.84	-3.9



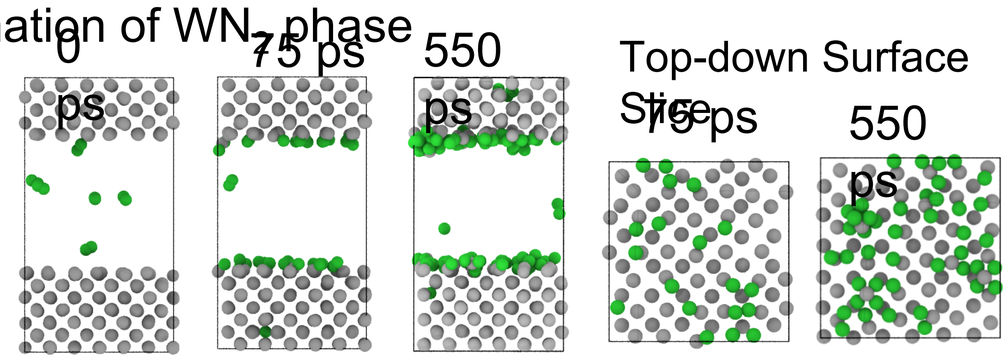
* See poster by C-.S. Wong et al. for more on experimental results

Surface Dynamics at 1000 K

- Simulations of periodic W slab with dimer gas insertion at



- H_2 continually adsorbs to surface and initially at hollow site
- Formation of WN_2 phase



- H_2 continually adsorbs to surface
- H resides at offset bridge site
- Some diffusion into bulk, resides at tetrahedral sites

Conclusions

- SNAP potential for W-H and W-N have been developed that well reproduce key properties
- These potentials predict adsorption sites consistent with ARIES experiments for H on W surfaces
- H2/N2 adsorption on tungsten results in H surface layer with some diffusion to bulk or WN_2 formation

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