SAND2022-7338C

Sandia National Laboratories

Exploring refractory complex concentrated alloy behavior in the fusion reactor environment with a machine-learned interatomic potential

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PSI-25 2022

June 13-17, 2022

U.S. DEPARTMENT OF ENERGY NNSA

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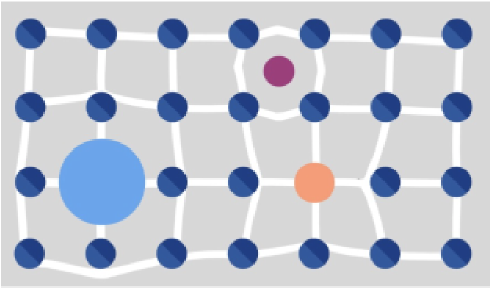
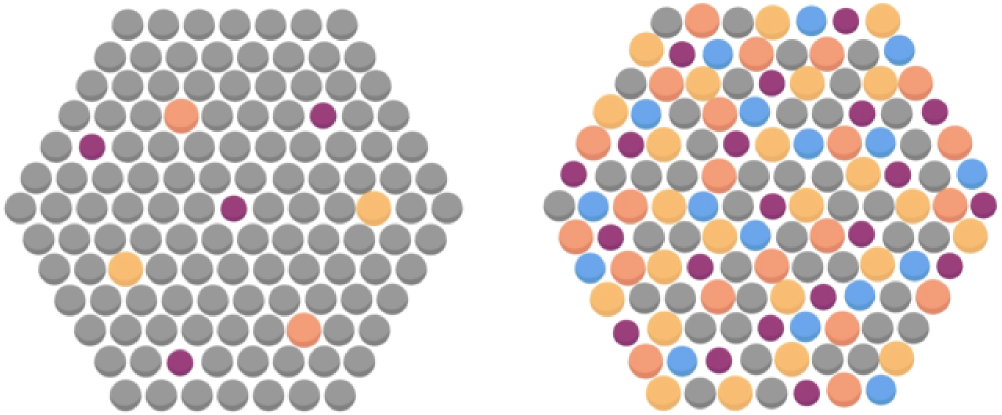
Complex concentrated alloys (CCAs)



https://doi.org/10.21203/rs.2.15081/v1

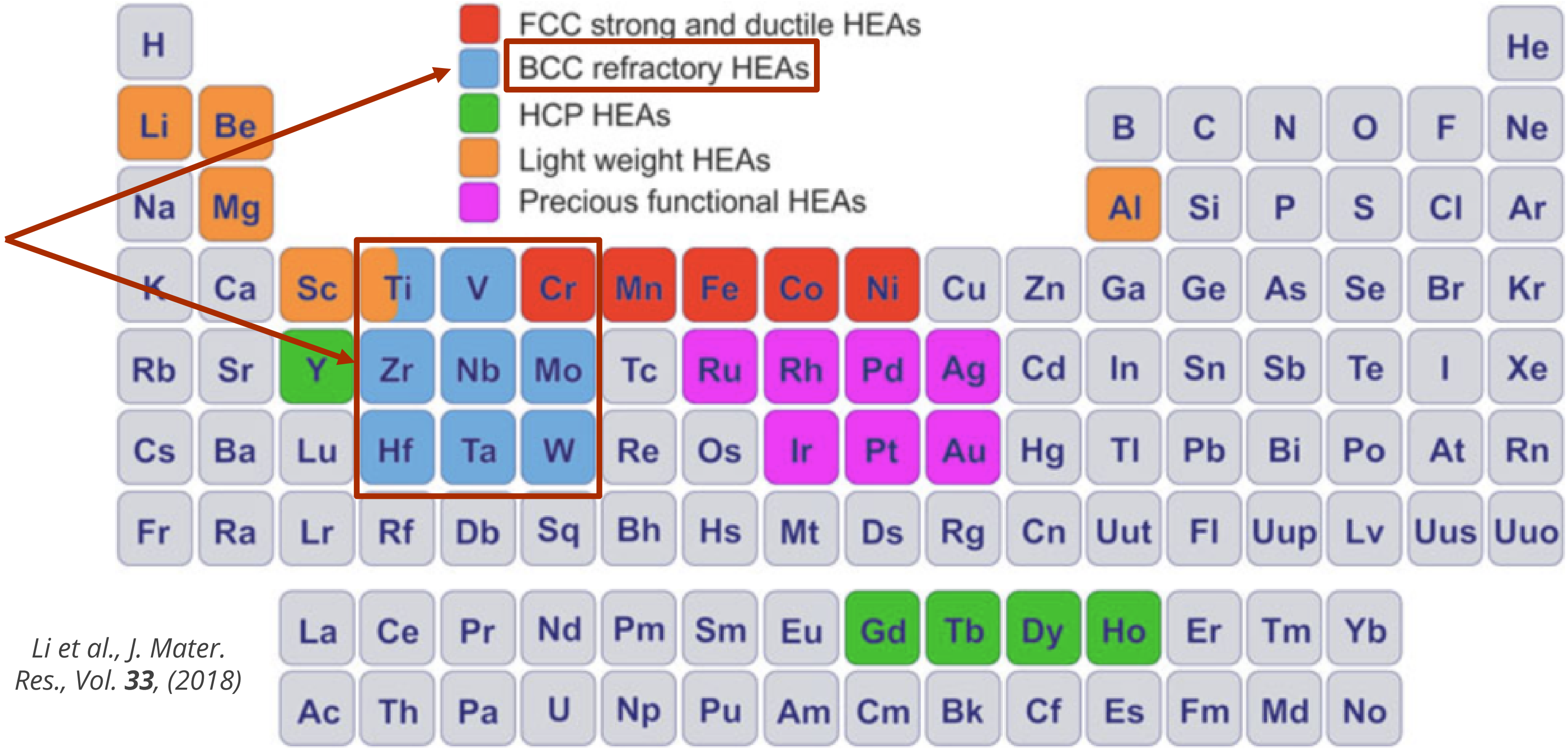


Conventional alloy High-entropy alloy

CCA: Alloy with high concentrations of 3 or more elements that can coexist without extreme phase separation

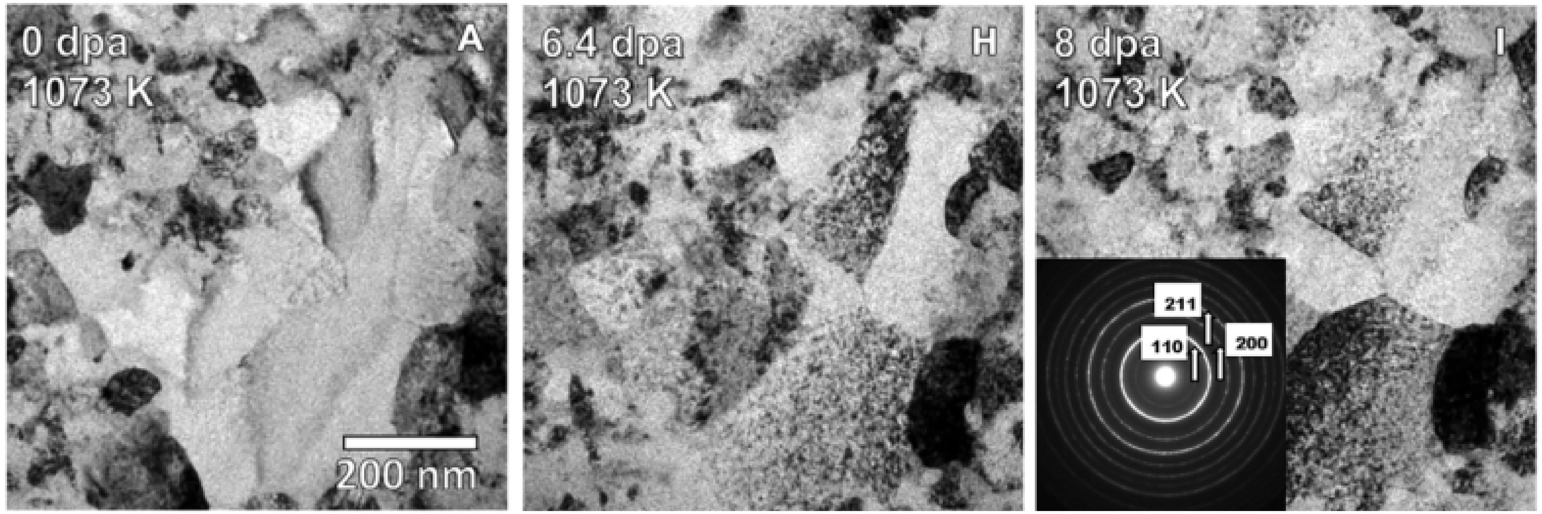
AKA: high-entropy alloy (HEA), multi-principal element alloy (MPEA)

Refractory CCAs (RCCAs)



Li et al., J. Mater. Res., Vol. ***33****, (2018)*

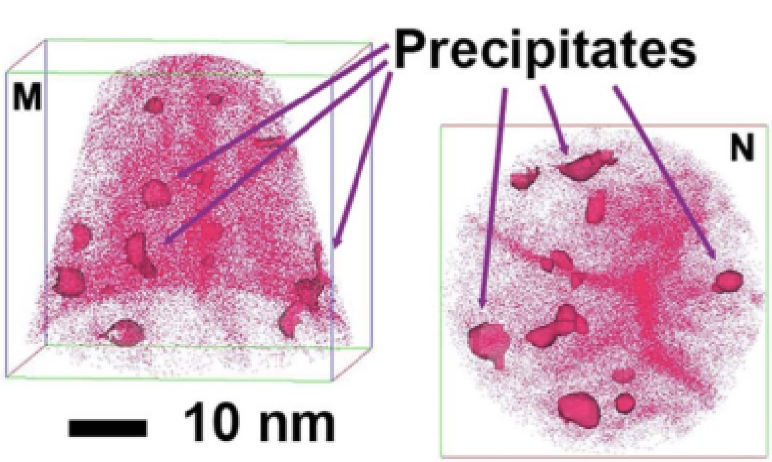
RCCAs in fusion reactor conditions

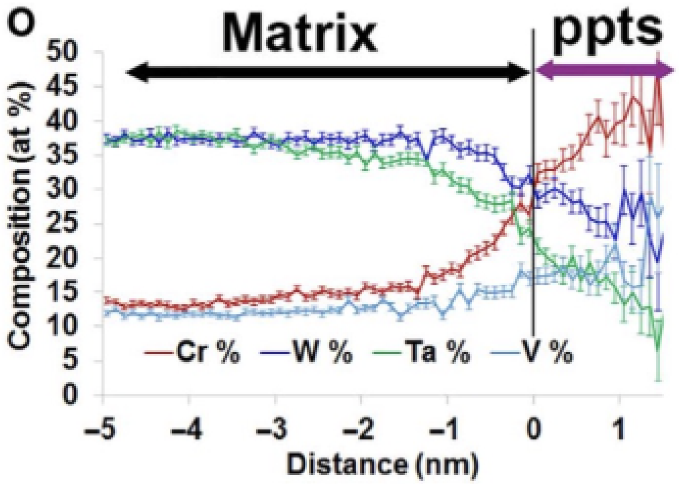


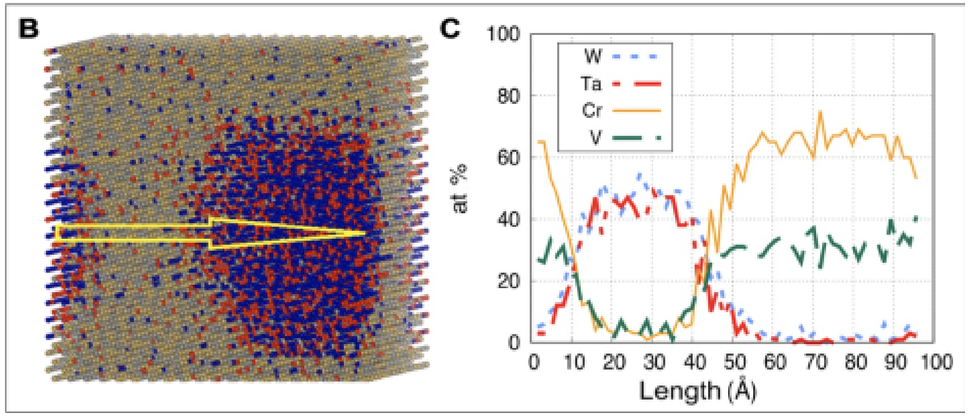
$Cr_{15}Ta_{36}W_{38}V_{11}$ (BCC)

Radiation damage → precipitate formation, increased hardness, lack of dislocation loops

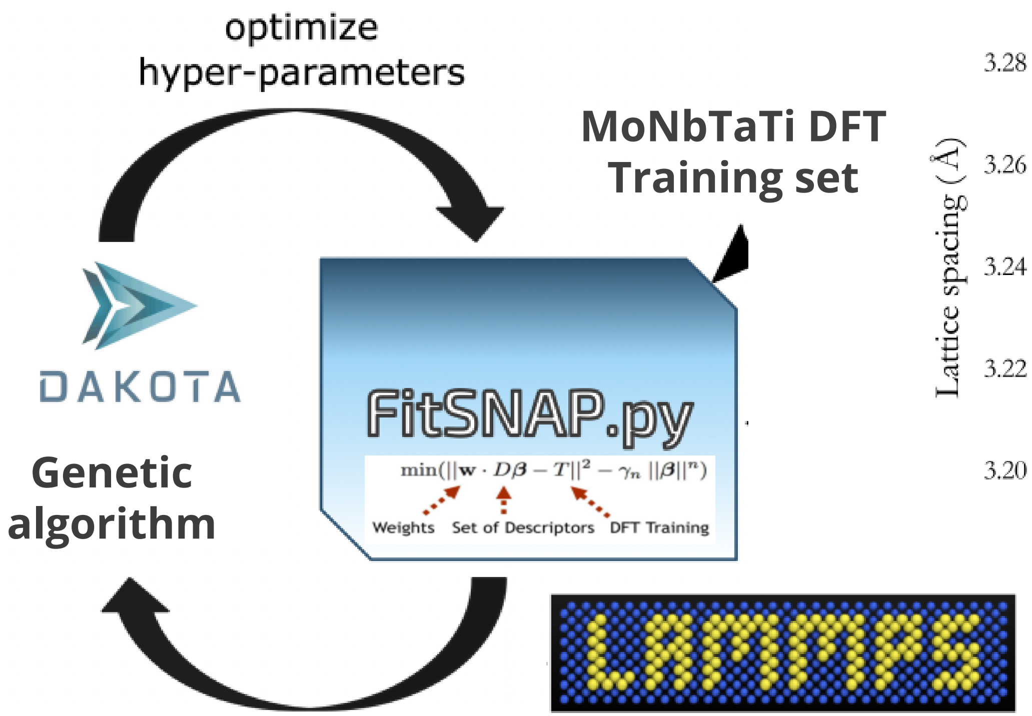
El-Atwani et al., Sci Adv. 2019 ***5***



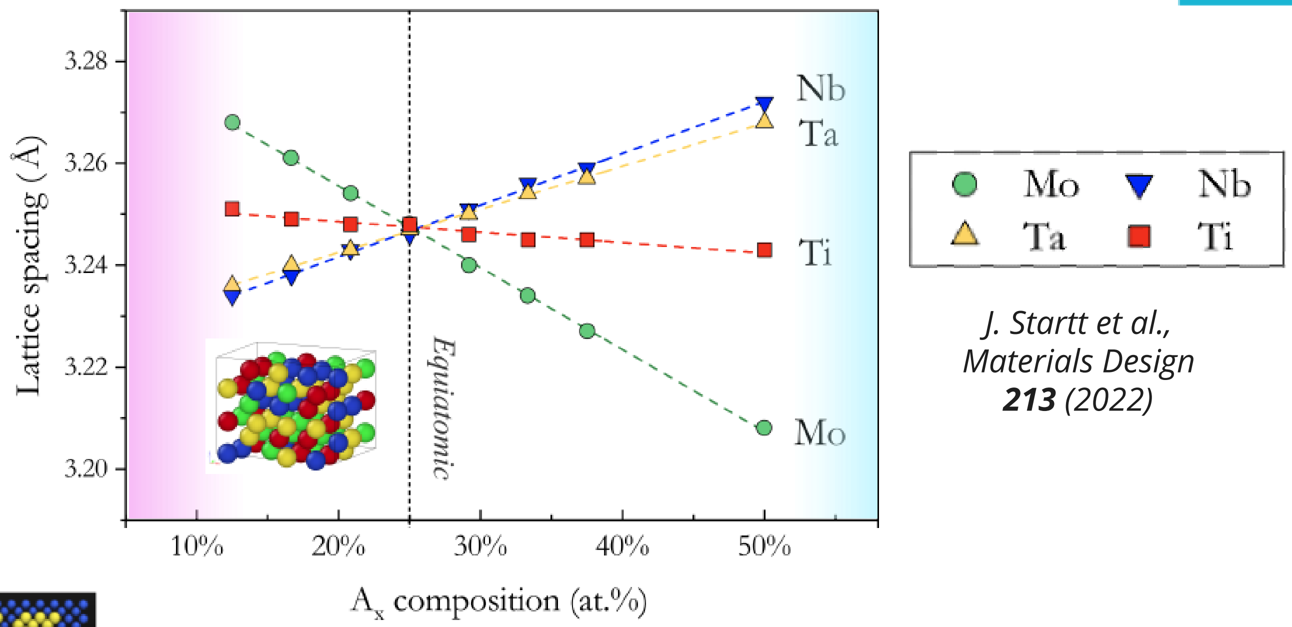




MoNbTaTi: a new RCCA machine-learned interatomic potential

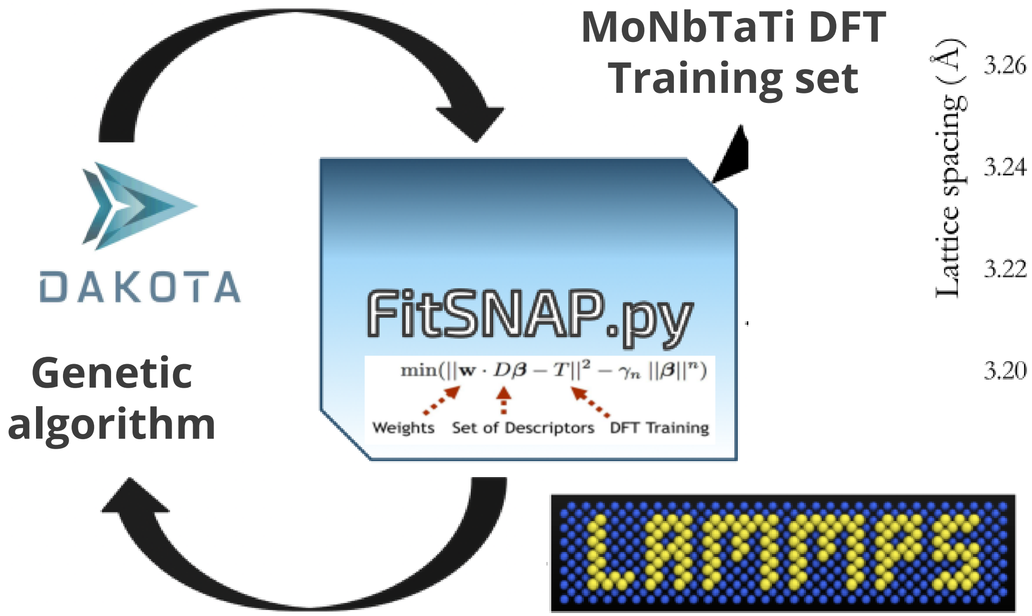


Outputs MLIAP:
Spectral Neighbor Analysis Potential (SNAP)



J. Startt et al., Materials Design ***213*** *(2022)*

MoNbTaTi: a new RCCA machine-learned interatomic potential



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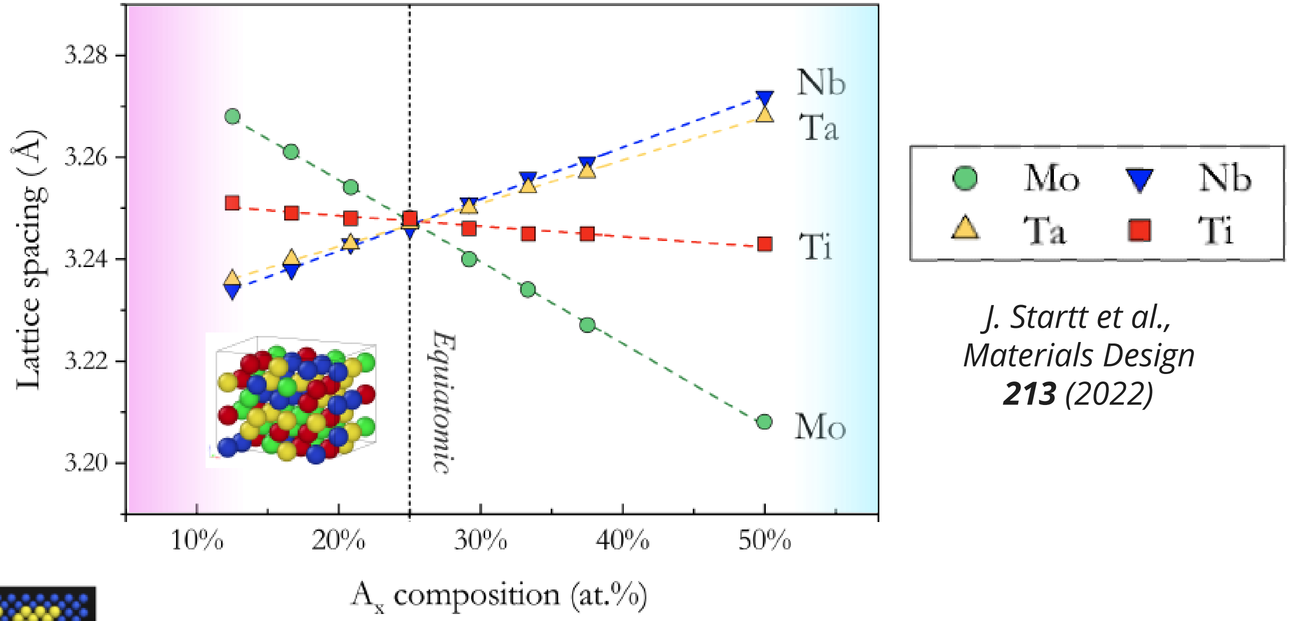
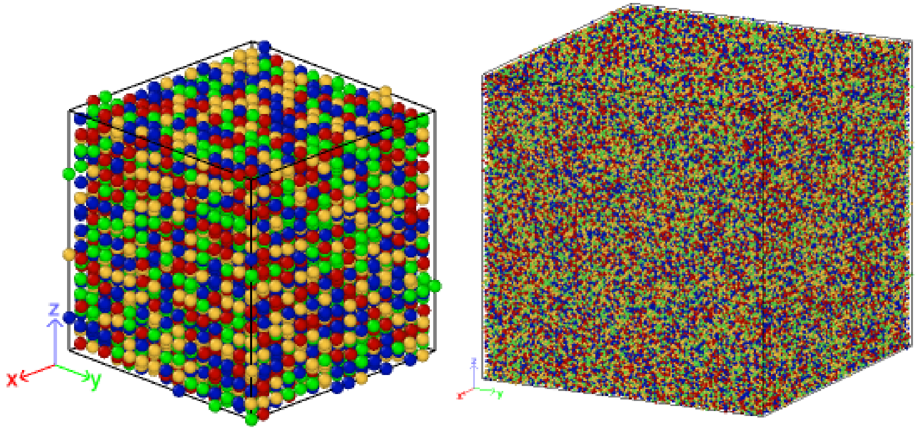


J. Startt et al., Materials Design ***213*** *(2022)*

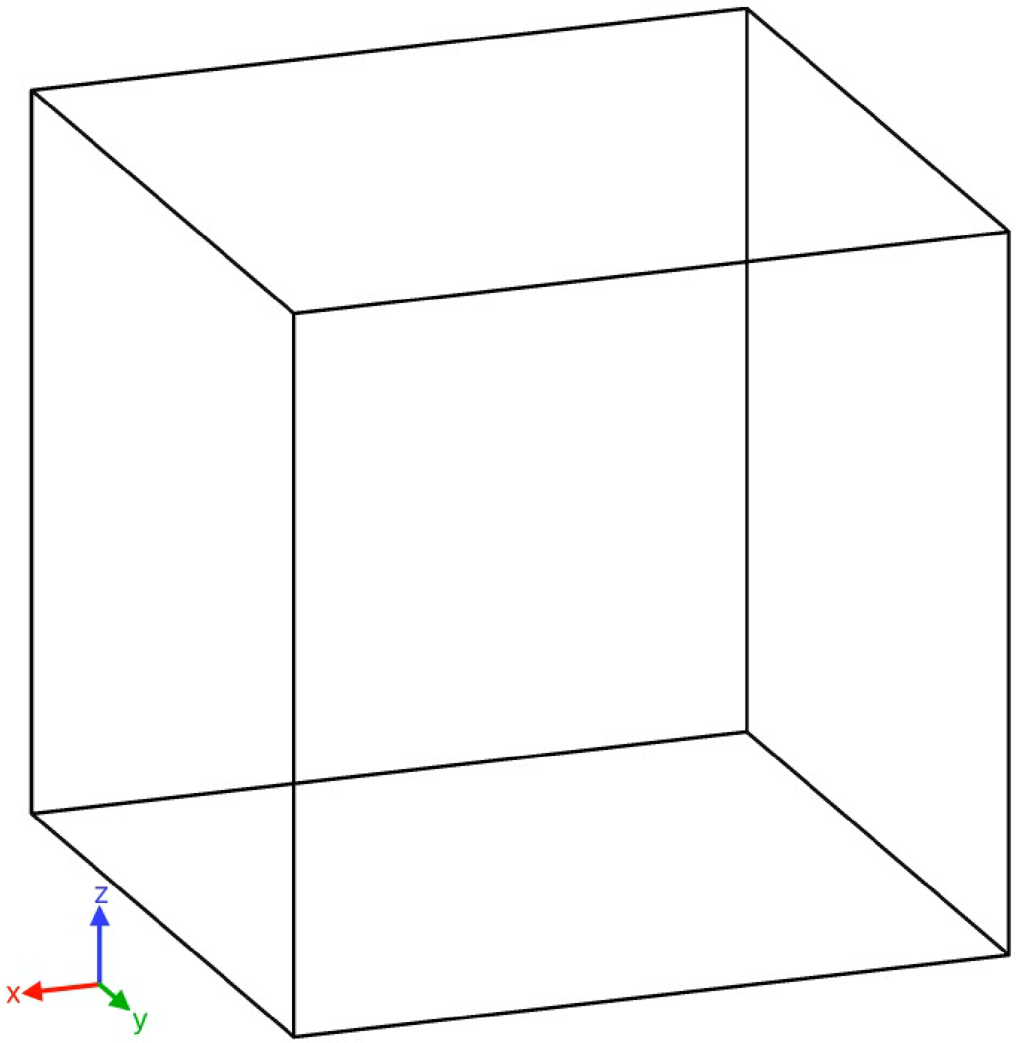


Property	SNAP New MLIAP	New DFT (not in training)	|SNAP - DFT|
B (GPa)	175.6	165.7	**6.0 %**
G (GPa)	42.7	43.6	**2.1 %**
E (GPa)	118.5	120.1	**1.3 %**

Initial results: MD SNAP errors agree very well with DFT on new structures

→ Explore multiple compositions in fusion reactor environment!

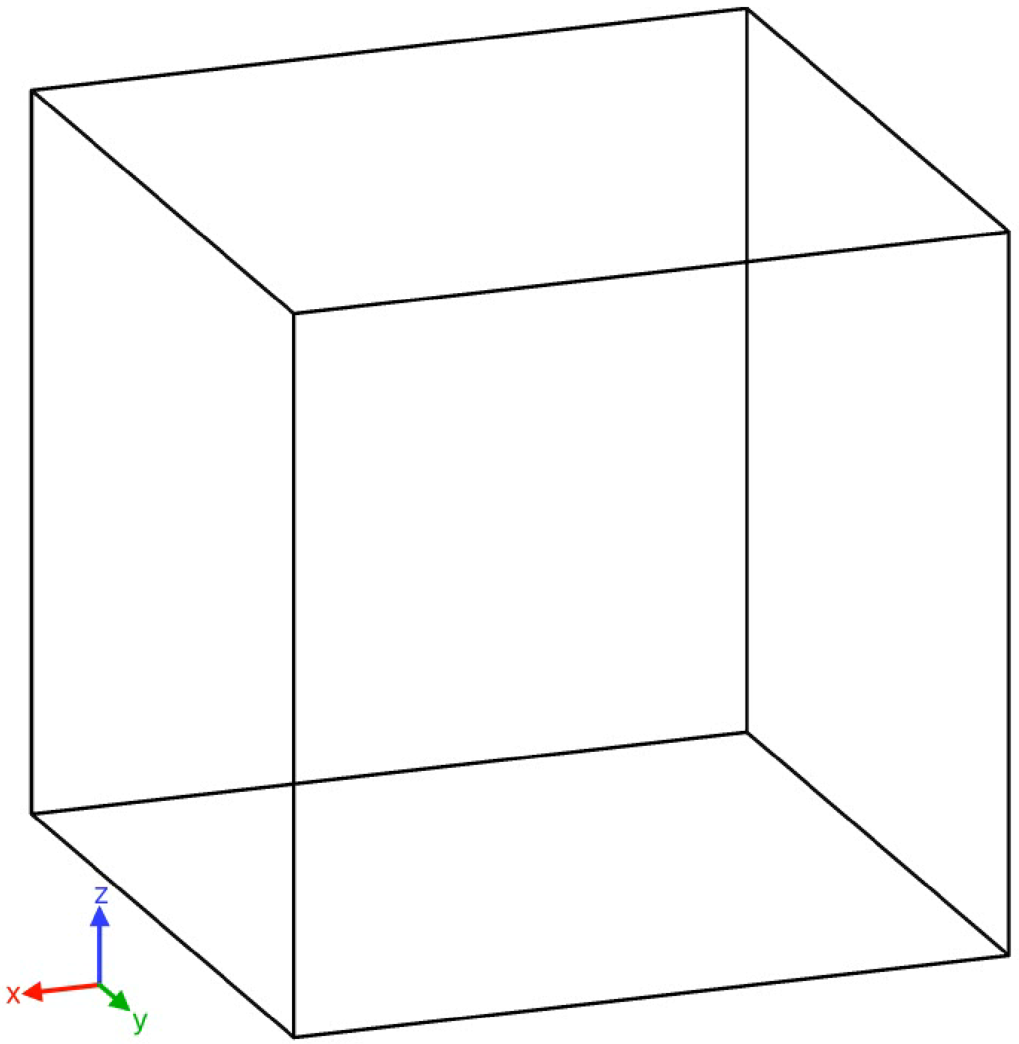
Radiation damage in MoNbTaTi



- SNAP potential stable in primary knock-on atom (PKA) simulations >20 kEV

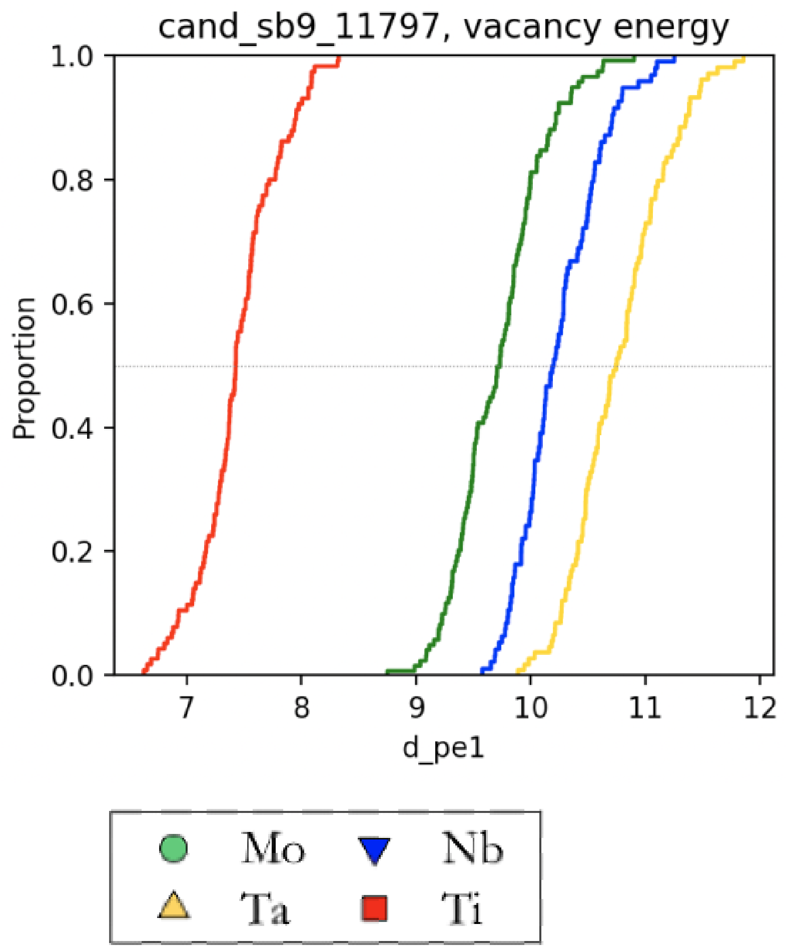
Point defects: Radiation damage (PKA)

Radiation damage in MoNbTaTi

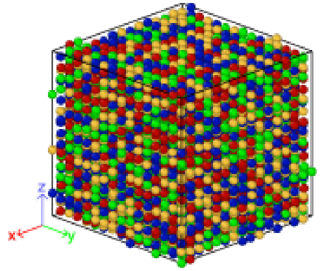


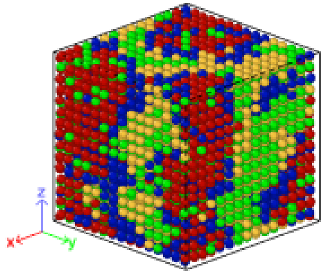
Point defects: Radiation damage (PKA)

- SNAP potential stable in primary knock-on atom (PKA) simulations >20 kEV
- Further characterization of radiation damage forthcoming

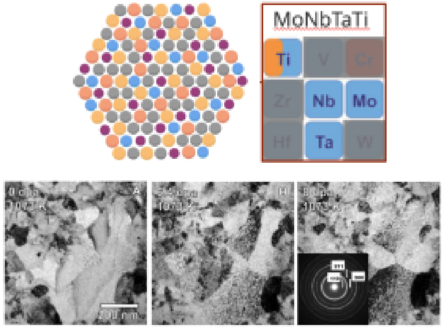


Next tests
Alloy chemistry:
Short-range order (SRO)

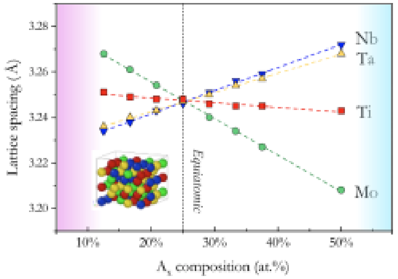




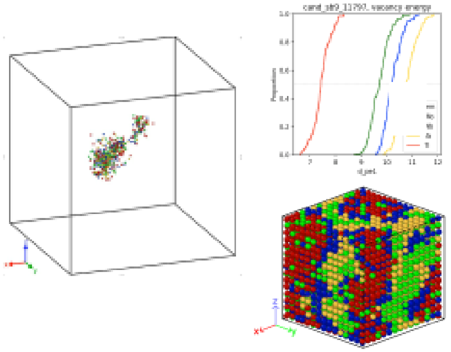
Summary



Refractory complex concentrated alloys (RCCAs) are promising materials for future fusion reactors. MoNbTaTi is a member of the RCCA family



Using FitSNAP and a genetic algorithm, we have successfully generated SNAP MLIAPs that can extrapolate successfully to new composition spaces on MD length and time scales



The new SNAP potentials can be used to explore how radiation damage evolves though changes in MoNbTaTi alloy composition and ordering

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