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Machine-Learned Interatomic Potential Development for W-ZrC for Nuclear Fusion

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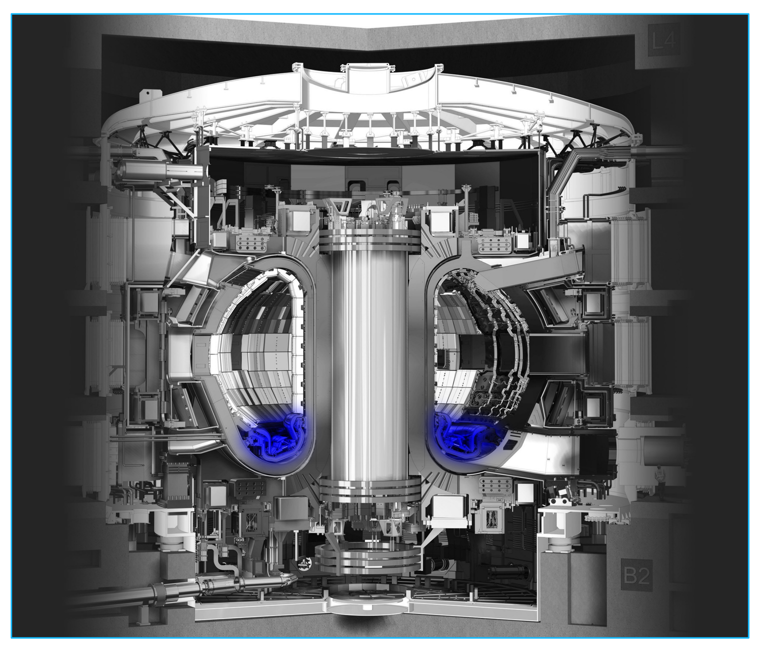
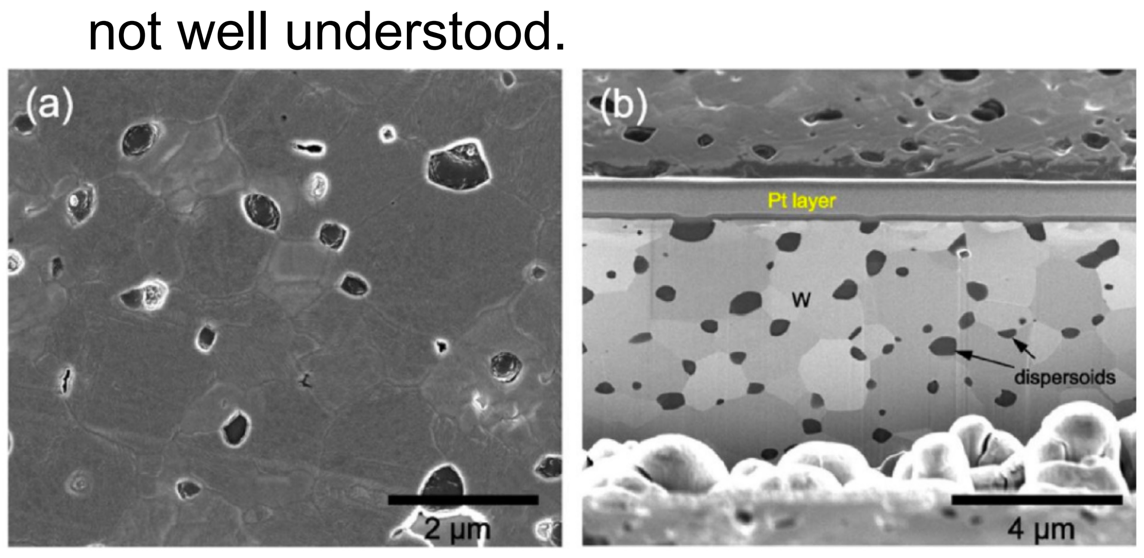
How can we predict fusion material performance?

- While tungsten (W) is the leading candidate divertor material for future fusion devices, it suffers from a high brittle-to-ductile transition temperature (>473 K)[2] and may undergo recrystallization and grain growth above 1000 K[3].
- Strengthening W with zirconium carbide (ZrC) can improve mechanical properties, but these mechanisms and effects on hydrogen fuel retention are not well understood.



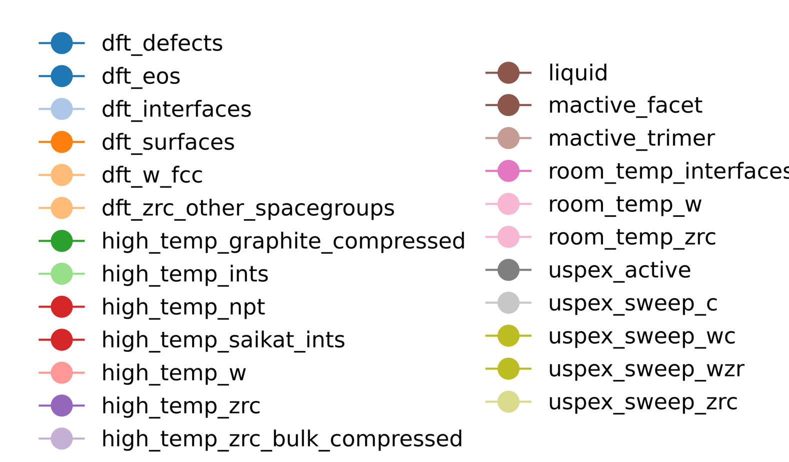
The divertor in a fusion reactor will control the waste and withstand the highest heat loads of the machine[1].

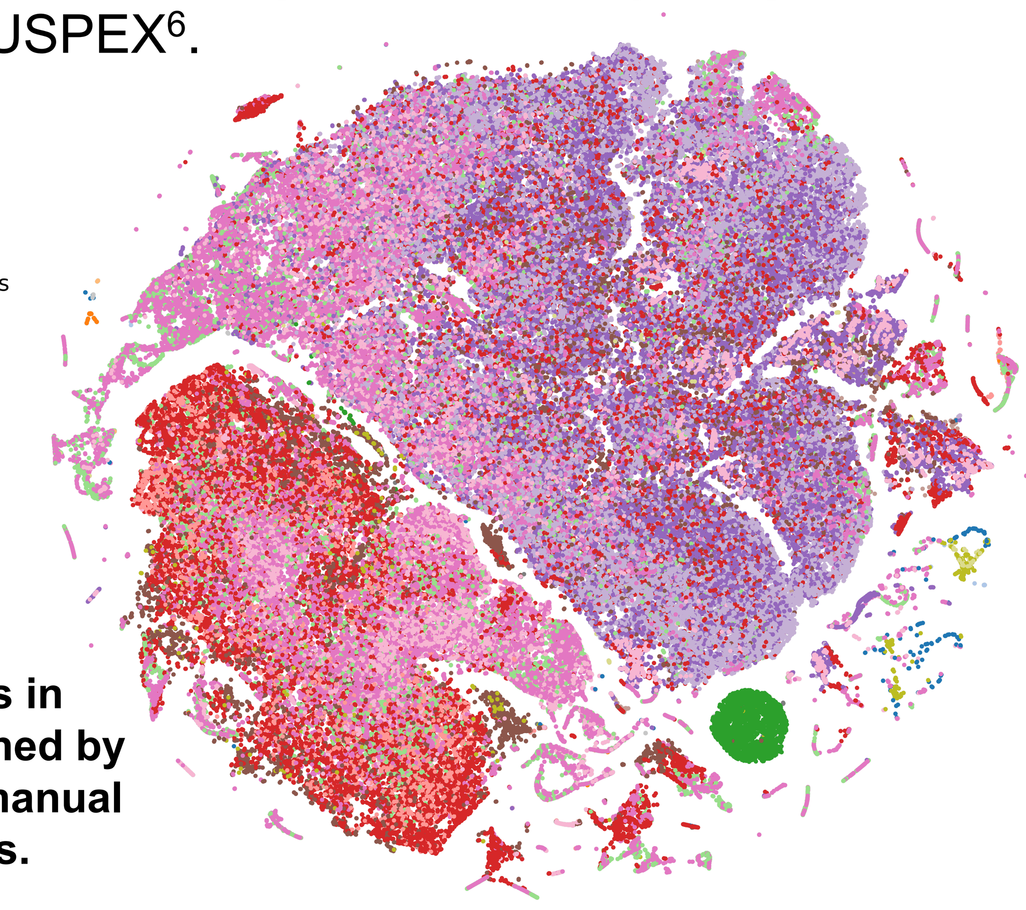


SEM of ZrC dispersoid strengthened W

What kind of training data do we need?

- The W-ZrC training set includes DFT calculations of W and ZrC bulk and surfaces, as well as expected interfaces.
- To improve the performance of the potential, we included Ab initio Molecular Dynamics (AIMD) simulations from 300 – 5000 K.
- To constrain the potential to physical behavior, we added manual active learning structures and structures generated using the genetic algorithm structure predictor USPEX[6].

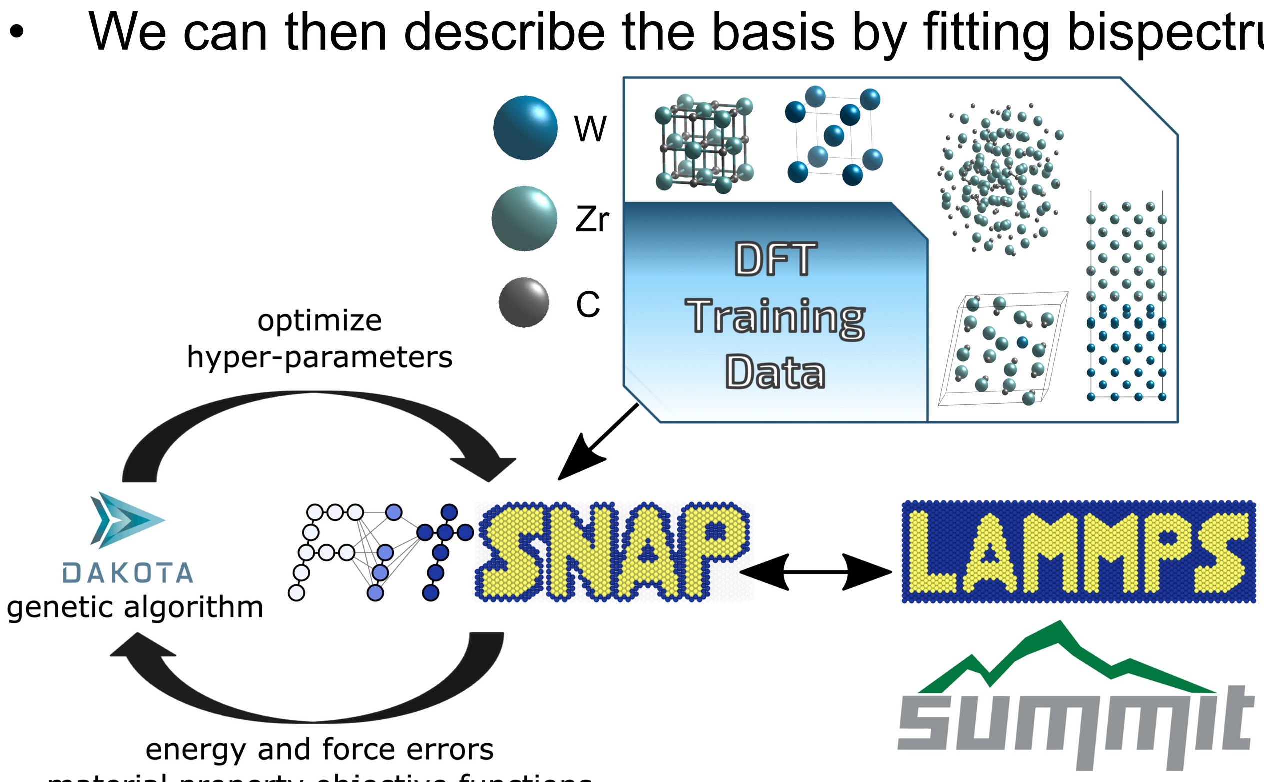




t-SNE visualization of training data bispectrum components and energies in 2D. More configuration space is reached by including a variety of AIMD, liquids, manual active learning, and USPEX structures.

Using first-principles to train a classical interatomic potential

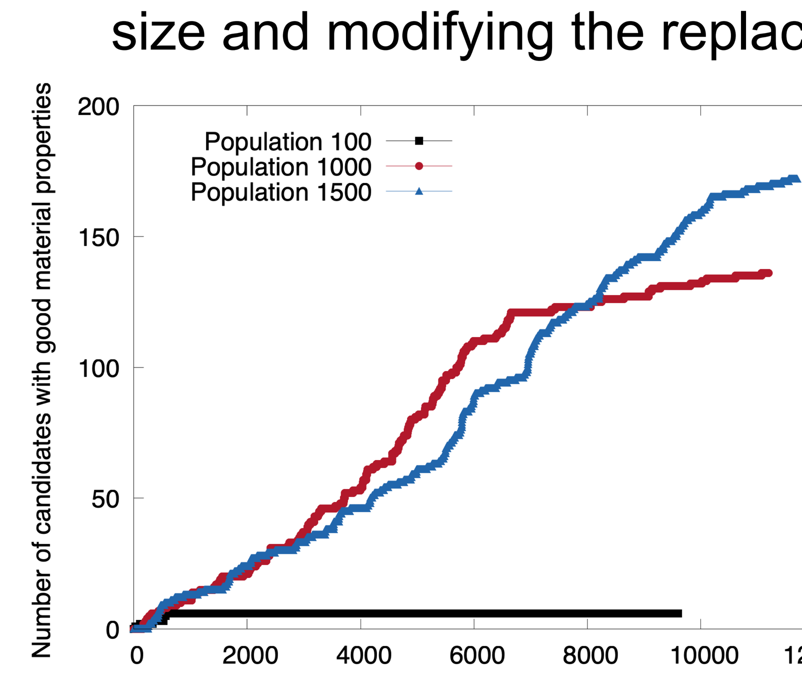
- We leverage machine learning to train a Spectral Neighbor Analysis Potential (SNAP) on DFT data[4].
- Each neighboring atom position is mapped to a point on a 3-sphere along with its corresponding energy.
- We can then describe the basis by fitting bispectrum components.



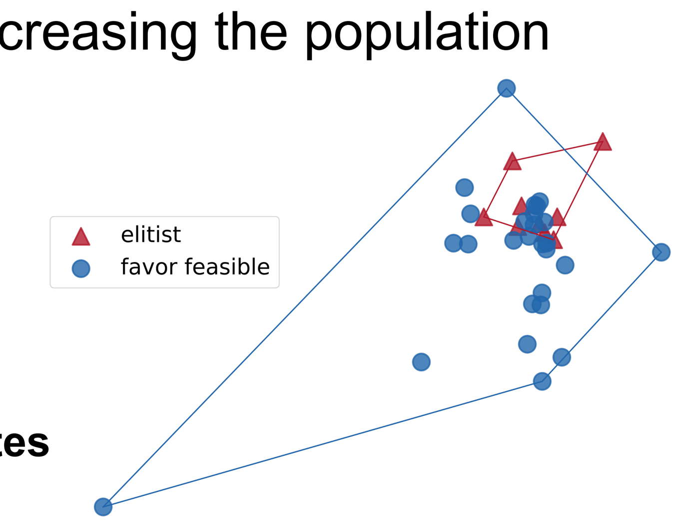
FitSNAP[5] fits bispectrum components based on the training set, hyper parameters, and group weights. Dakota searches the variable phase space towards the best performing potentials.

Optimizing potential hyper-parameters

- Finding optimal potentials requires searching over a hyper-parameter and group weight phase space that can easily be 20+ dimensions.
- To best search this variable space, we want to maintain diversity in the candidate potential population during the genetic algorithm[7].
- Better quality candidates can be found by increasing the population size and modifying the replacement type.



Total evaluated candidates vs. quality candidates with varying population sizes



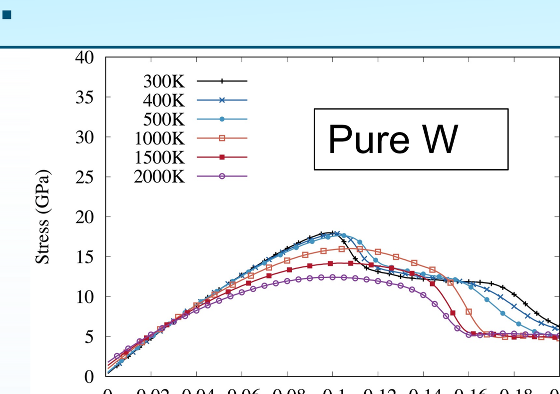
t-SNE visualization of quality candidates produced by two different replacement types

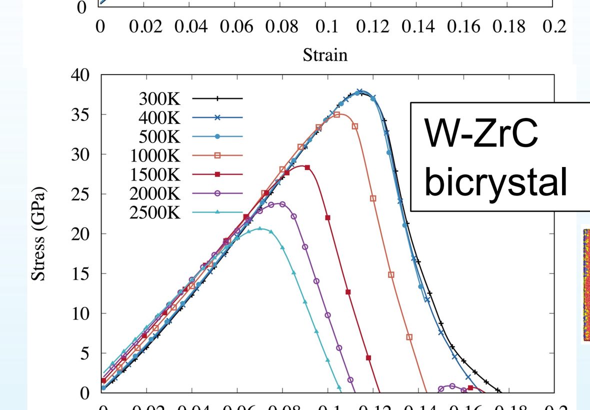
With diverse training data and an optimized search over hyper-parameters, we can now study ZrC strengthened W thermomechanical properties.

- The W-ZrC SNAP potential yields material properties in good agreement with DFT values for lattice parameter, *a* (Å), bulk modulus, *B* (GPa), and surface energies, E_{surf} (eV/Å).
- Using the W-ZrC SNAP potential we can run millions of atom simulations at divertor temperature ranges (~373 – 2573 K[8]).

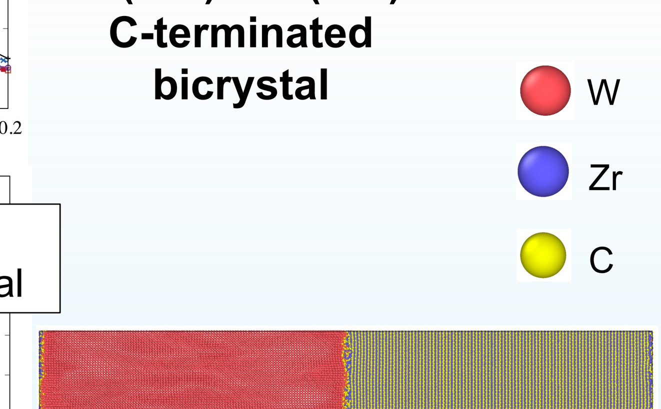
Material properties predicted by DFT vs. SNAP

	a_W	a_{ZrC}	B_W	B_{ZrC}	E_{surf} W (100)	E_{surf} W (110)	E_{surf} ZrC (200)	E_{surf} ZrC (110)
DFT	3.18	4.70	301.4	216.0	4.13	3.18	1.63	3.31
SNAP	3.19	4.78	303.3	209.0	3.38	3.22	1.40	2.75

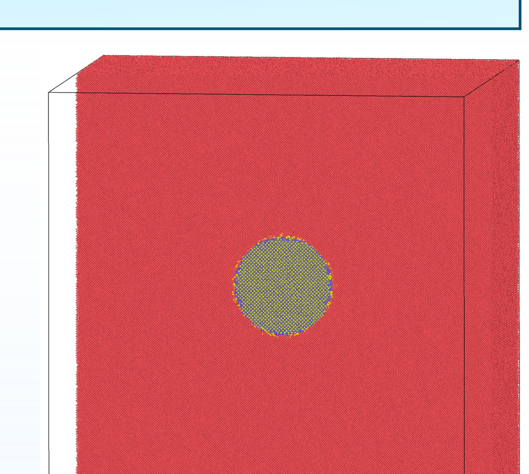




Tensile tests of pure W vs. a W(110)-ZrC(111) C-terminated bicrystal



Bicrystal at 300 K at 0.125 strain



Spherical ZrC in crystalline W at 1700 K (~10 million atoms, 56 nm per side)

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