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Towards Accelerated Design of Multi-Principal Element Alloys with Optimized Hardness and Elongation Features by an Ensemble of Neural Network

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Introduction

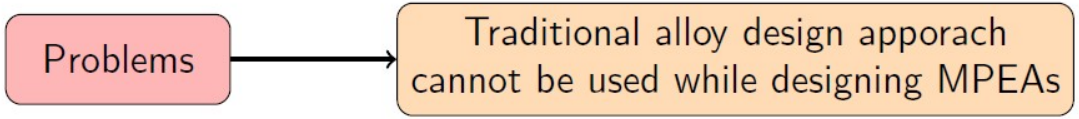
HEA
High Entropy Alloys

5 or More Principal Elements

MEA
Medium Entropy Alloys

3 or 4 Principal Elements

Problem Statements



Literature Review

Paper	Review
[1]	Machine Learning technique to obtain new MPEAs with high hardness value in *Al-Co-Cr-Cu-Fe-Ni* alloy.
[2]	Used artificial neural network to predict the hardness of *AlCoCrFeMnNi* on **91 dataset**.
[3]	Machine Learning approach to evaluate the hardness by Random forest regression on **290 Cast MPEAs**.

(1) Wen, C., Zhang, Y., Wang, C., Xue, D., Bai, Y., Antonov, S., Dai, L., Lookman, T.,and Su, Y. (2019). Machine learning assisted design of high entropy alloys with desired property. *Acta Materialia*, 170:109–117.

(2) Chang, Yao-Jen, et al. "Prediction of the composition and hardness of high-entropy alloys by machine learning." *Jom* 71.10 (2019): 3433-3442.

(3) Xiong, J., Shi, S.-Q., and Zhang, T.-Y. (2021). Machine learning of phases and mechanical properties in complex concentrated alloys.

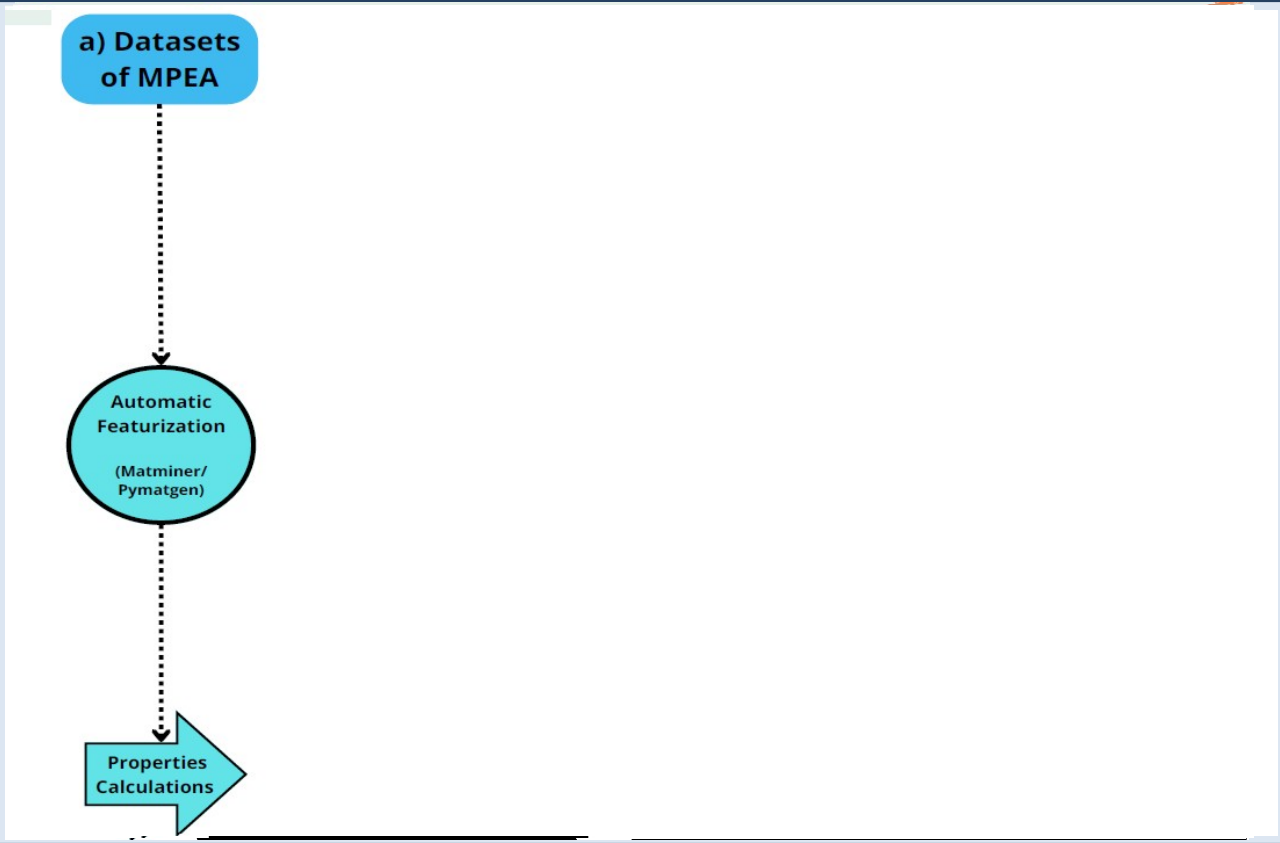
Research Gap

Originality of Research

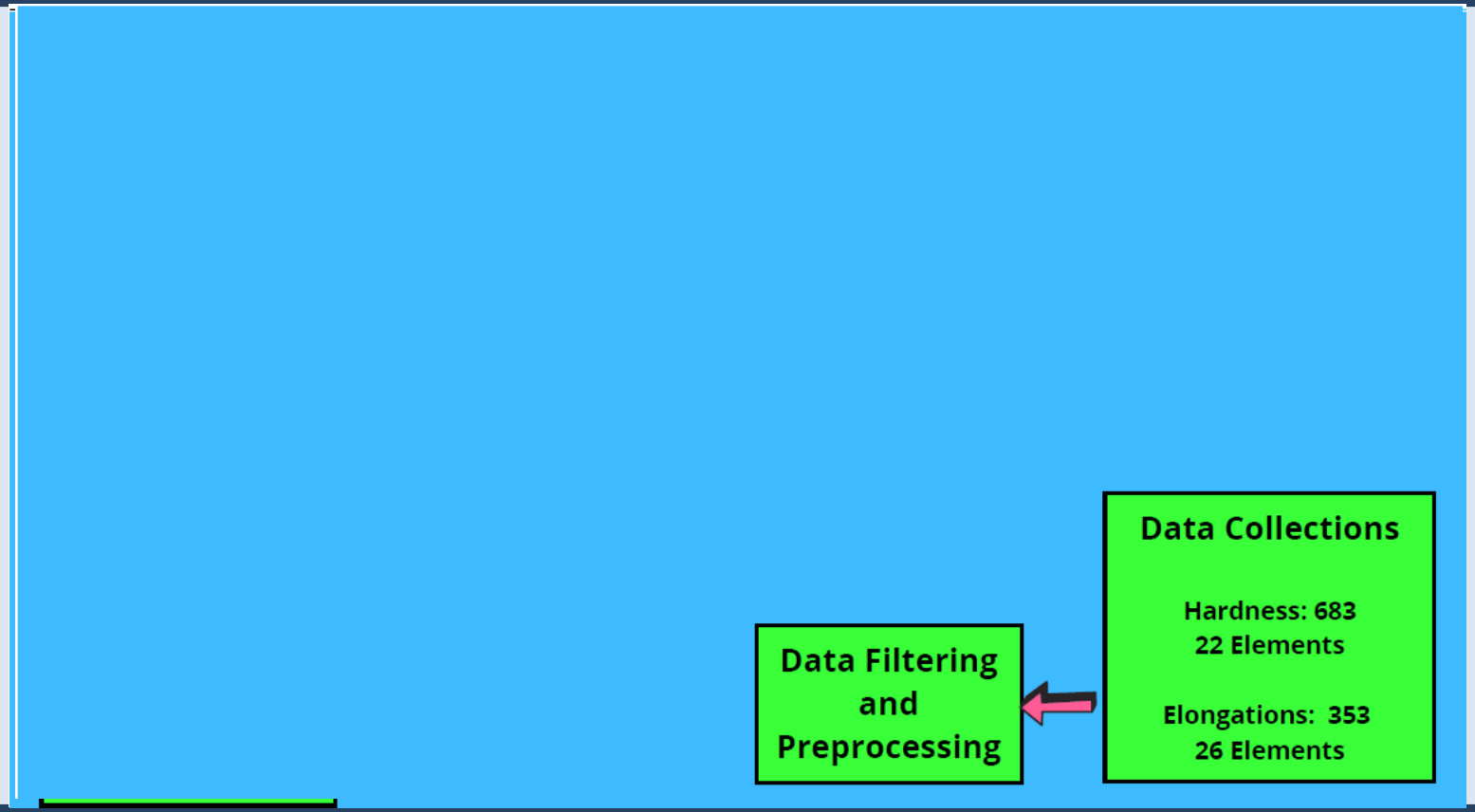
Study on opposite natured properties

What's new in this work?

Research Flow



Model Development



Methodology: Hyper-Parameter Tuning

Hyper-parameters are used to evaluate

- Weights
- Bias

SN			Hyper parameters
1	Epochs	=	[100, 150, 200]
2	batch size	=	[2,4,6]
3	layers	=	[4,6]
4	neuron size	=	[32,48,64]
5	optimizer	=	['SGD','RMSprop', 'Adam', 'Nadam']
6	activation	=	['relu', 'selu', 'LeakyReLU', 'PReLU']
7	loss function	=	[mse, msle, huberwith alpha=1.5]
8	drops	=	[0.05,0.075,0.08,0.1,0.15,0.2]
9	learning rate	=	[0.0001,0.00025,0.000375,0.0004,0.0005, 0.00075,0.001,0.005,0.01]
10	Regulirazation	:	[L1,L2 & L2]
	For weight initialization		
11	weight constraint	=	[1,2,3]
12	init weights	=	['uniform', 'normal', 'he_uniform']

RandomSearchCV

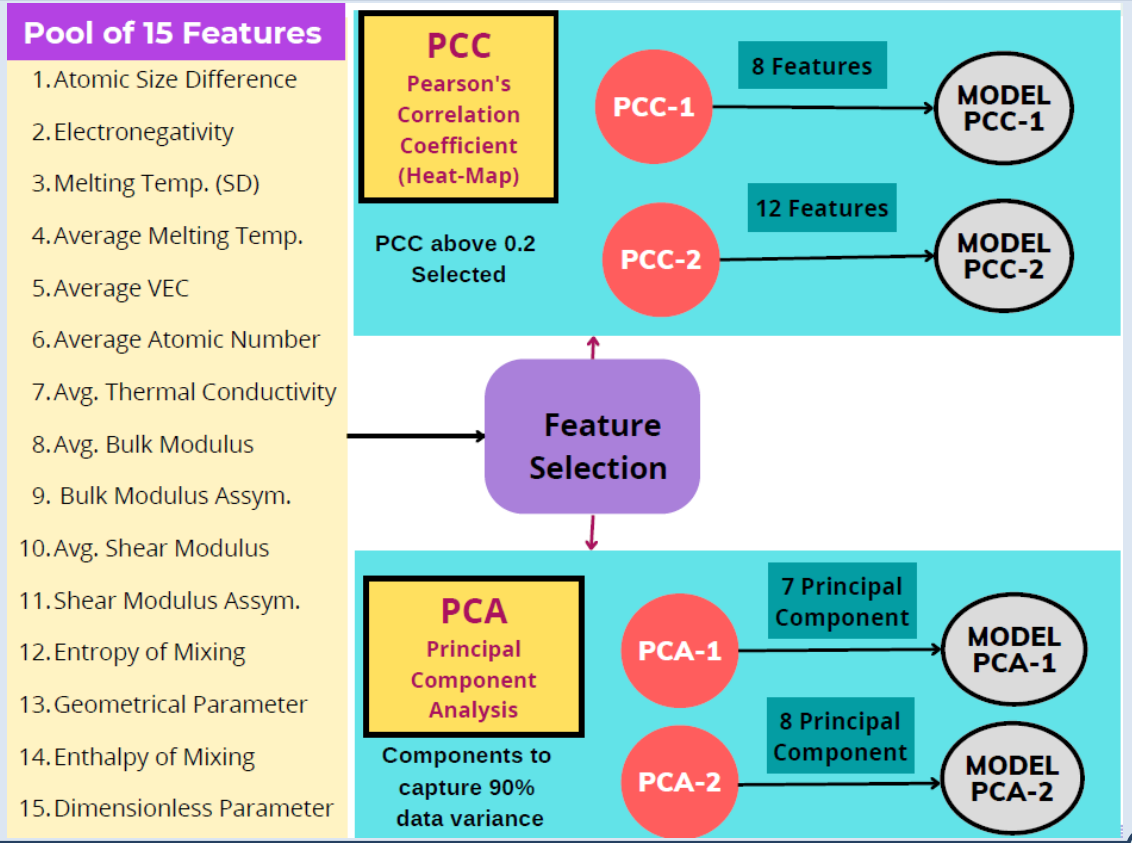
300 Hyper-Parameter Configurations

Model Inputs: Feature Selection Flowchart

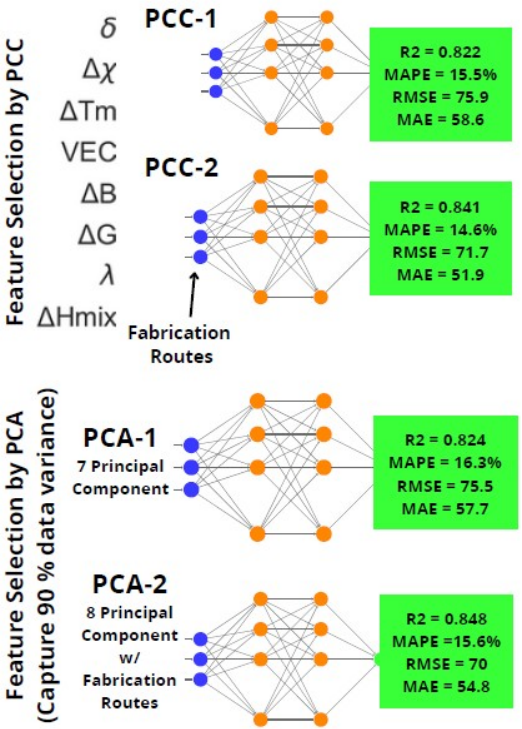
2 Feature sets from PCC (with and without Fab routes)

2 Feature sets from PCA (with and without Fab routes)

4 Models built from 4 different feature sets



Results: Ensemble of 4 Models



Material Design: Approach

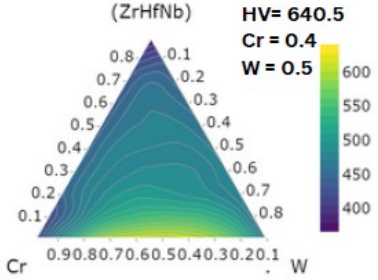
Material Design: Significance

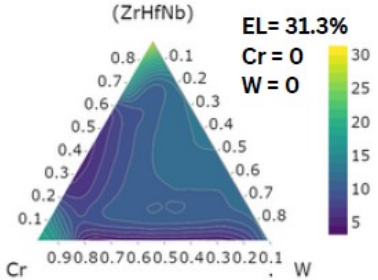
To check effect of doping, it would require fabrication of thousands of alloys physically.

Experiments can only study effect of variation of a single element.

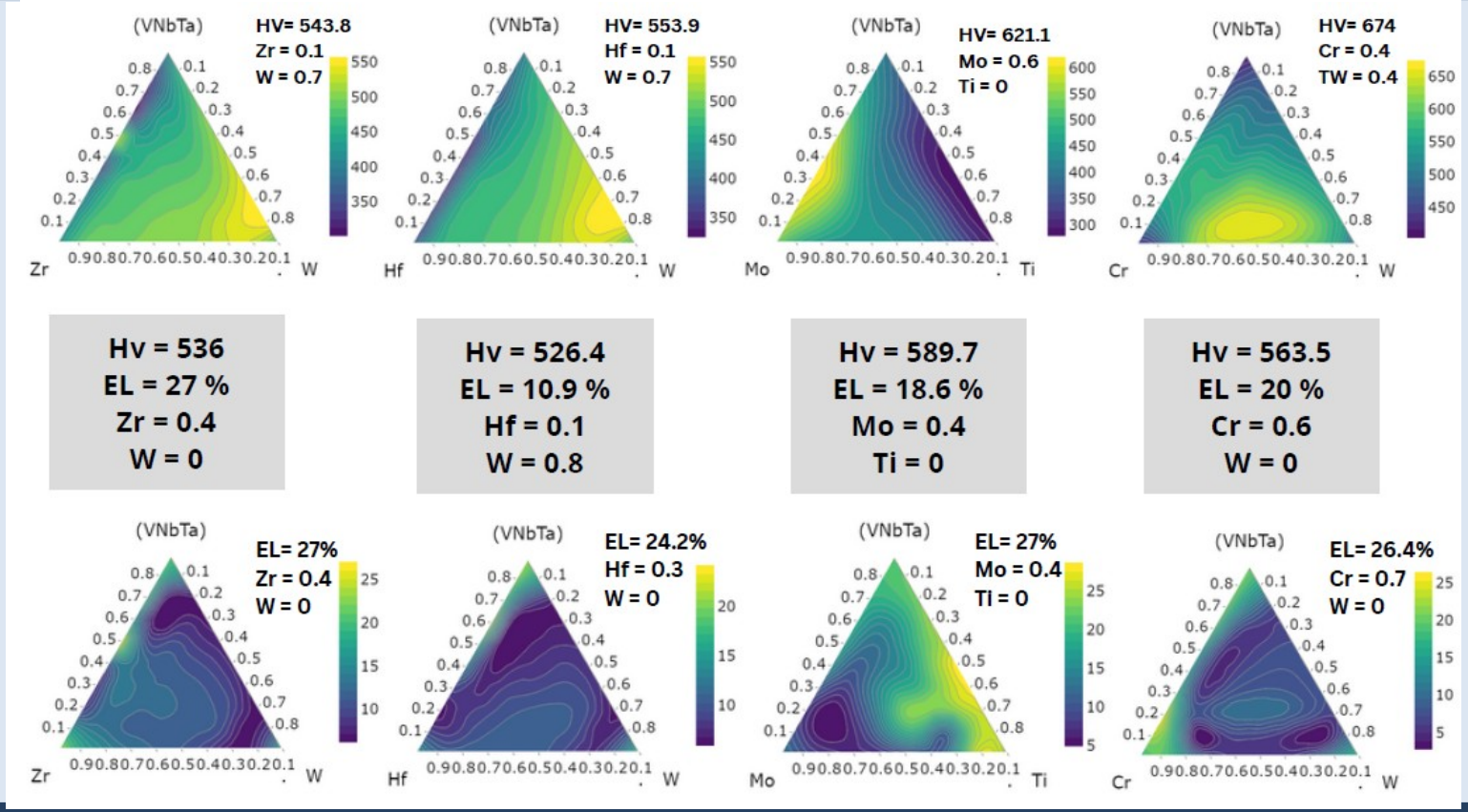
Not Possible to study the effect of two dopants in a base system.

Material Design: *ZrHfNb* based Alloys

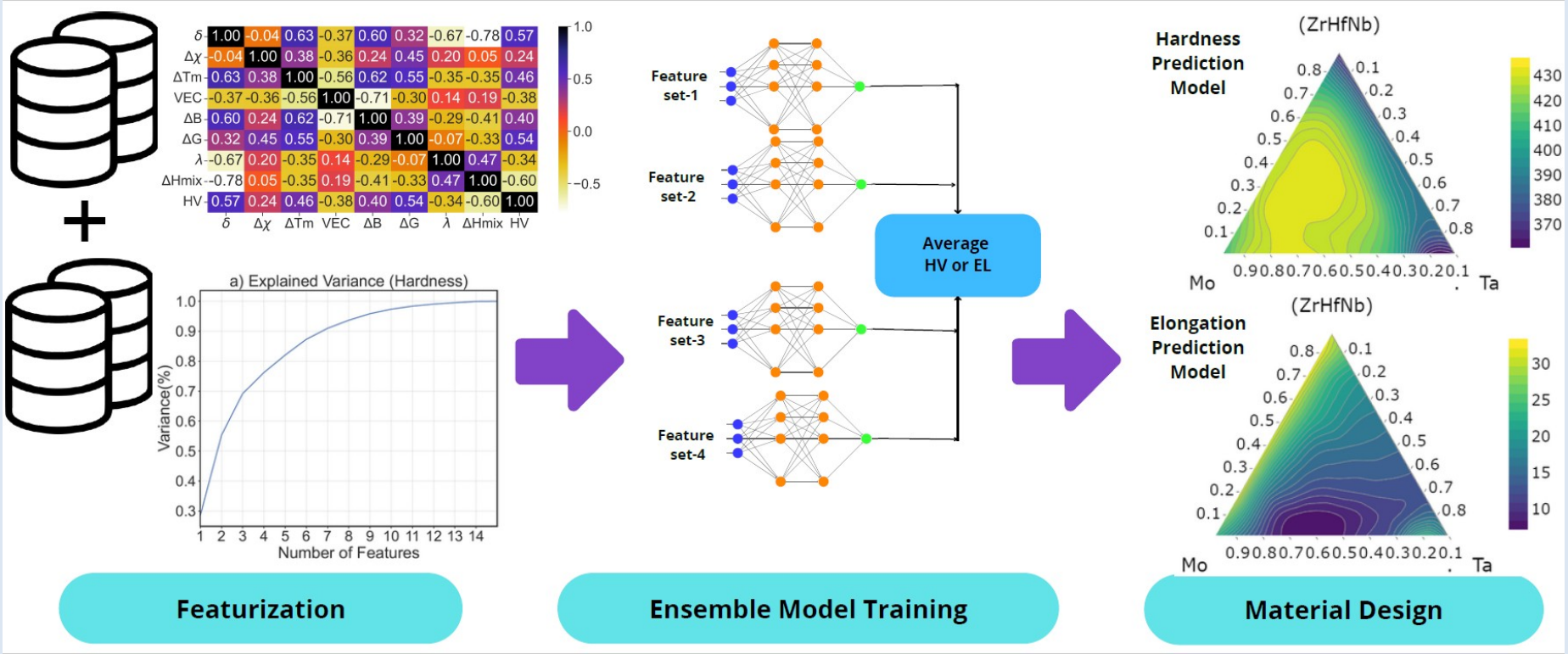




Material Design: *VNbTa* based Alloys



Conclusion


δ 1.00 -0.04 0.63 -0.37 0.60 0.32 -0.67 -0.78 0.57
Δχ -0.04 1.00 0.38 -0.36 0.24 0.45 0.20 0.05 0.24
ΔTm 0.63 0.38 1.00 -0.56 0.62 0.55 -0.35 -0.35 0.46
VEC -0.37 -0.36 -0.56 1.00 -0.71 -0.30 0.14 0.19 -0.38
ΔB 0.60 0.24 0.62 -0.71 1.00 0.39 -0.29 -0.41 0.40
ΔG 0.32 0.45 0.55 -0.30 0.39 1.00 -0.07 -0.33 0.54
λ -0.67 0.20 -0.35 0.14 -0.29 -0.07 1.00 0.47 -0.34
ΔHmix -0.78 0.05 -0.35 0.19 -0.41 -0.33 0.47 1.00 -0.60
HV 0.57 0.24 0.46 -0.38 0.40 0.54 -0.34 -0.60 1.00
δ Δχ ΔTm VEC ΔB ΔG λ ΔHmix HV
1.0 0.5 0.0 −0.5
a) Explained Variance (Hardness)
Variance(%)
Number of Features
Feature set-1
Feature set-2
Feature set-3
Feature set-4
Average HV or EL
Hardness Prediction Model
(ZrHfNb)
Mo
Ta
Elongation Prediction Model
(ZrHfNb)
Mo
Ta
Featurization
Ensemble Model Training
Material Design

Thank You