# Using Machine Learning for Advanced Materials: The Case of High-Entropy Alloys

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High-Entropy Alloys (HEAs) are a novel class of materials involving many principal elements. They offer a broad range of applications beyond traditional low-entropy alloys, by combining unique properties like strength, ductility, corrosion resistance, thermal stability, etc. [1,3], as well as fine-tuned catalytic behavior [4,6], all in one material. However, these unique properties derive from specific elemental compositions, stoichiometries and geometries, and so are not easily predicted due to their vast space of complex, combinatoric possibility.

Therefore, many have turned to machine learning (ML) methods utilizing neural networks (NNs) to learn chemical patterns in experimental and theoretical data and hence infer predictive design with significant accuracy [7,9]. Yet the bottleneck for data-driven predictive models is of course data acquisition.

Due to the immense scale of the combinatoric space available to HEAs, no straightforward method exists for exploring these possibilities exhaustively. ML methods work to reduce this possibility space given specific design parameters, however, only recently have more advanced techniques been applied together with NNs to further improve efficiency [10,12].

To this end, our work addresses this bottleneck. It expands upon the research from a theoretical standpoint, by demonstrating how one can engineer a feedback loop between structures generated and structures validated within an active learning algorithm (ALA) [13]. As proof-of-concept we focus on high-entropy clusters HECs, rather than bulk or substrate alloys, which have advantages in their high surface-to-volume ratio, allowing for a wide range of coordination and hence reactivity for novel catalytic design [14,16]. The ALA combines a genetic algorithm (GA) for generating novel structures and density functional theory (DFT) for validating said structures. We explore 6 elements, Ag, Au, Cu, Ni, Pd, Pt, and show that one can reliably predict HEC energies and forces at the quantum level using deep convolutional NNs in a highly efficient and automatic method.

## References

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## Figures

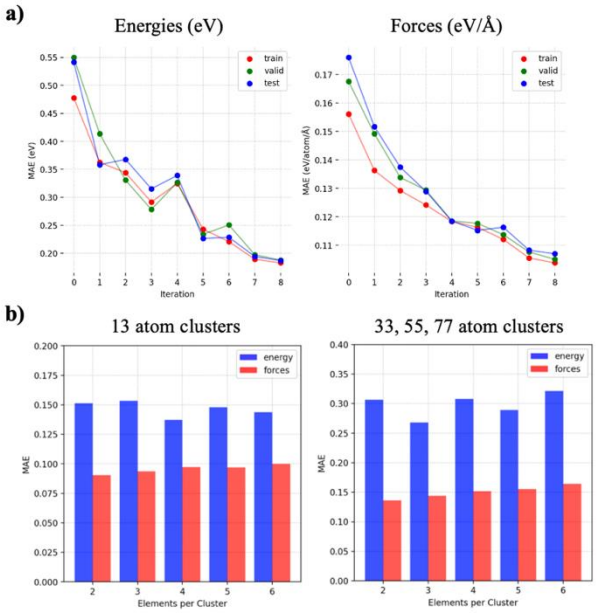


***Figure 1.*** *(a) Mean absolute error on prediction loss for all datasets, energies, and forces. (b) Low-to-high entropy predictive extrapolations.*

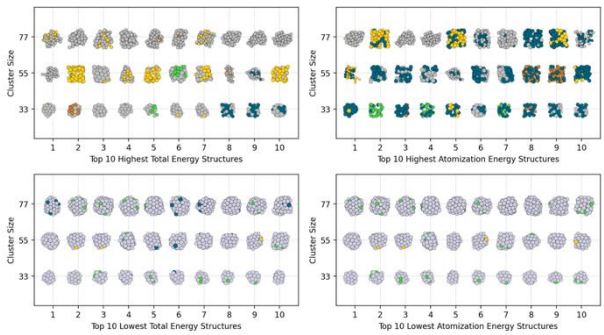


***Figure 2.*** Generated and validated clusters showcasing geometric, compositional, and stoichiometric preferences.