IDENTIFICATION OF STABLE NEAR SURFACE ALLOY SYSTEMS USING DENSITY FUNCTIONAL THEORY AND DATA SCIENCE

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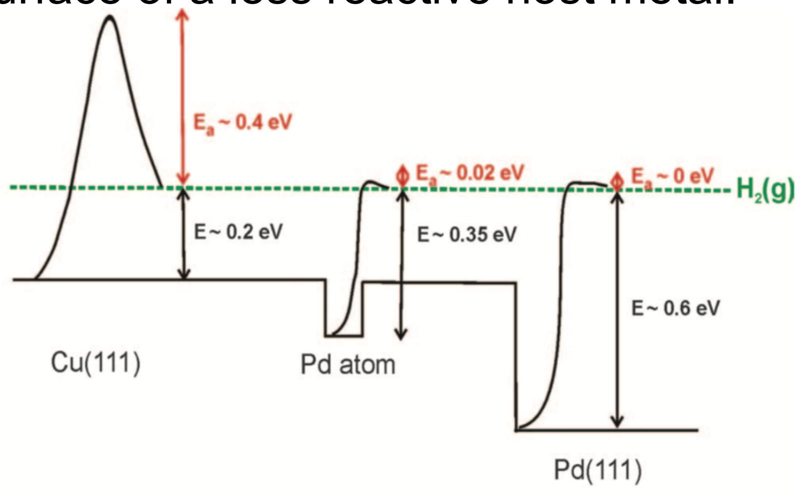
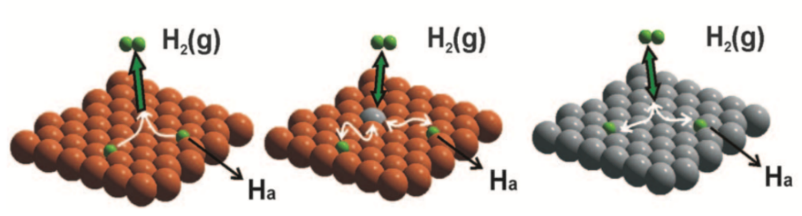
Background

Recently, a new class of catalysts, called single-atom alloy (SAA), has been discovered, synthesized, and studied. These heterogeneous catalysts contain a single, highly active promoter metal that sits within the surface of a less reactive host metal.





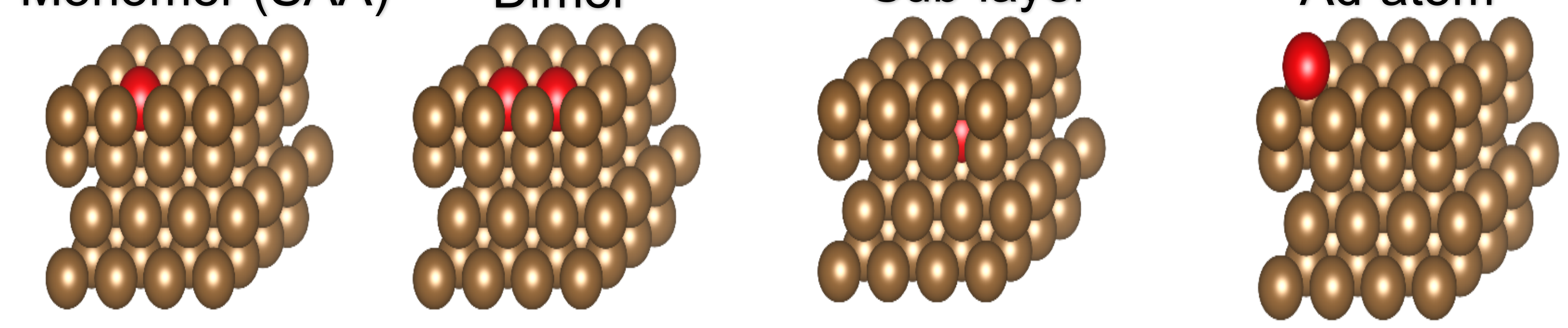
Our research group has also found multiple varieties of SAAs that are useful and practical for many industrial processes, trying to the relation between the alloy's stability and its component's properties.
These guidelines will provide fundamental insight into the formation of stable surface structures of binary alloys where one component is a minority species. In the near future, this work will help scientists and researchers to focus their efforts on stable SAAs in their quest to develop new catalyst for industrial applications. In the distant future, this work may also contribute to understanding dynamic restructuring of active catalytic sites when they are exposed to a reactive environment, for example an oxidizing or reducing atmosphere.

Method

- We used the Density Functional Theory (DFT) and Atomic Simulation Environment (ASE) to calculate the energies of promoter host combinations of all 30 d-block elements, containing 900 combinations.
- In the calculations for the close packed bcc(110), hcp(0001), and fcc(111), we included 64 atoms with the projector augmented wave (PAW) potentials (sv, pv or d) in the self-consistent iterations.
- Using open source machine learning framework Tensor Flow, we created an artificial neural network (ANN) of one input layer, 2 hidden layers with 10 nodes and one output layer.

Promoter Host Combinations

Monomer (SAA) Dimer Sub-layer Ad-atom



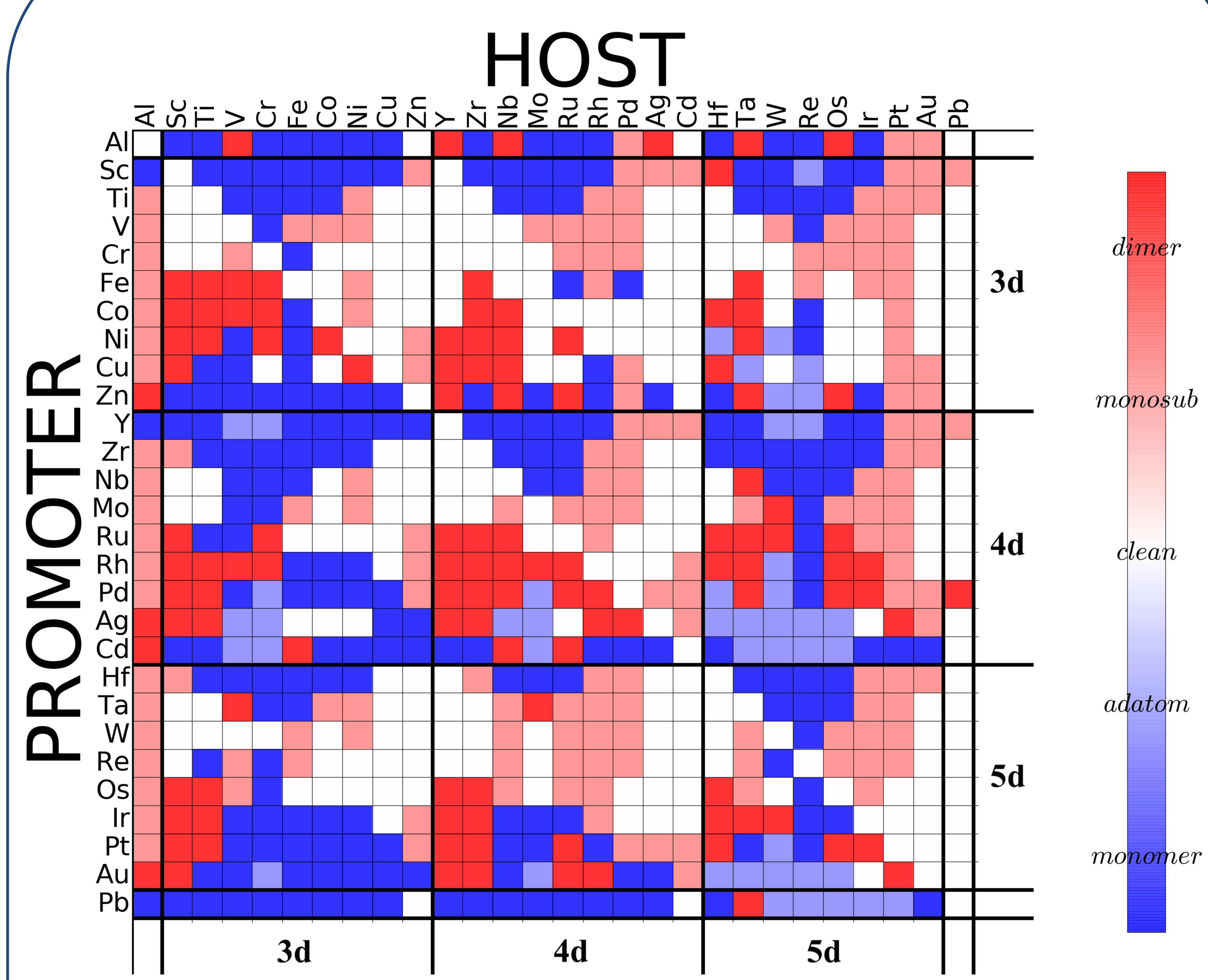
Energy per atom for the system

Monomer / Sub-layer
$$\frac{Energy}{Atom} = E_{host/promoter} + E_{host/bulk} - \left(E_{host/clean} + E_{promoter/bulk}\right)$$

Dimer
$$\frac{Energy}{Atom} = E_{host/promoter} + 2 * E_{host/bulk} - \left(E_{host/clean} + 2 * E_{promoter/bulk}\right)$$

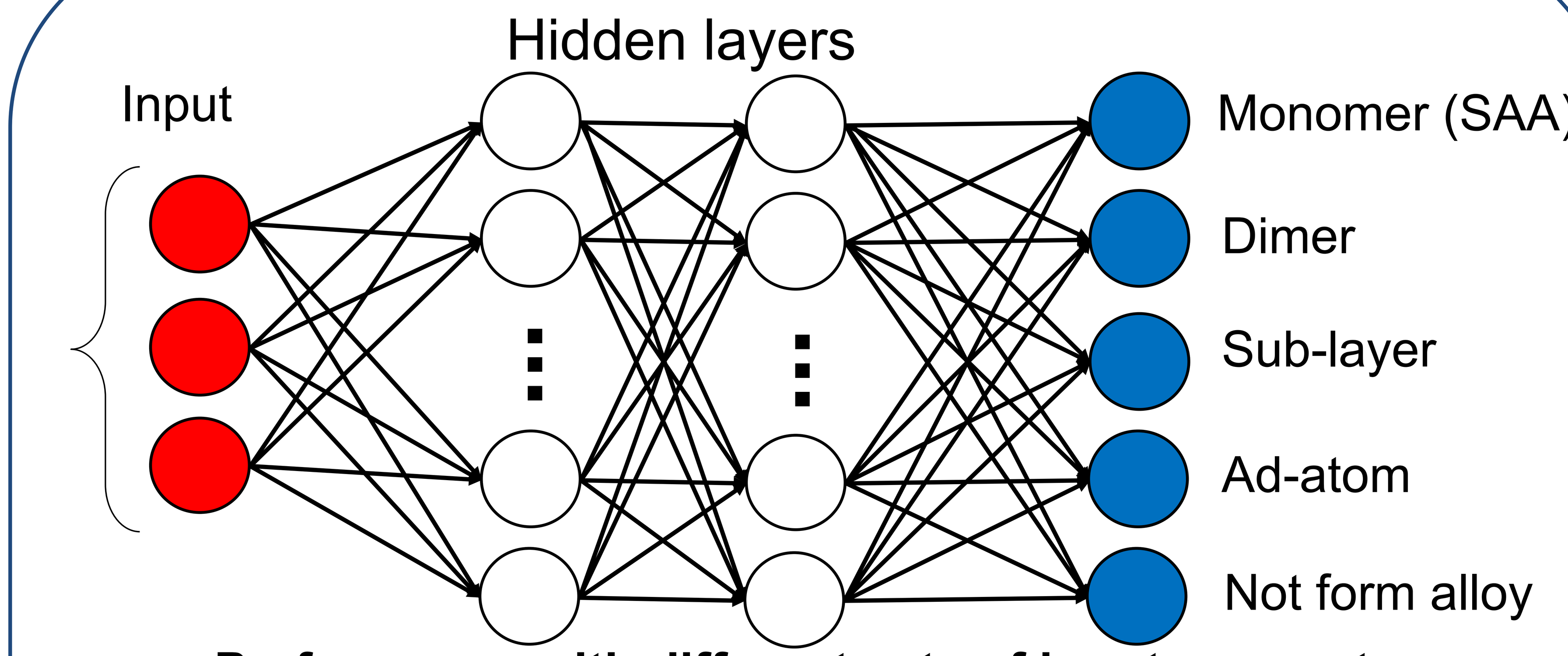
Ad-atom
$$\frac{Energy}{Atom} = E_{host/promoter} - \left(E_{host/clean} + E_{promoter/bulk}\right)$$

Results

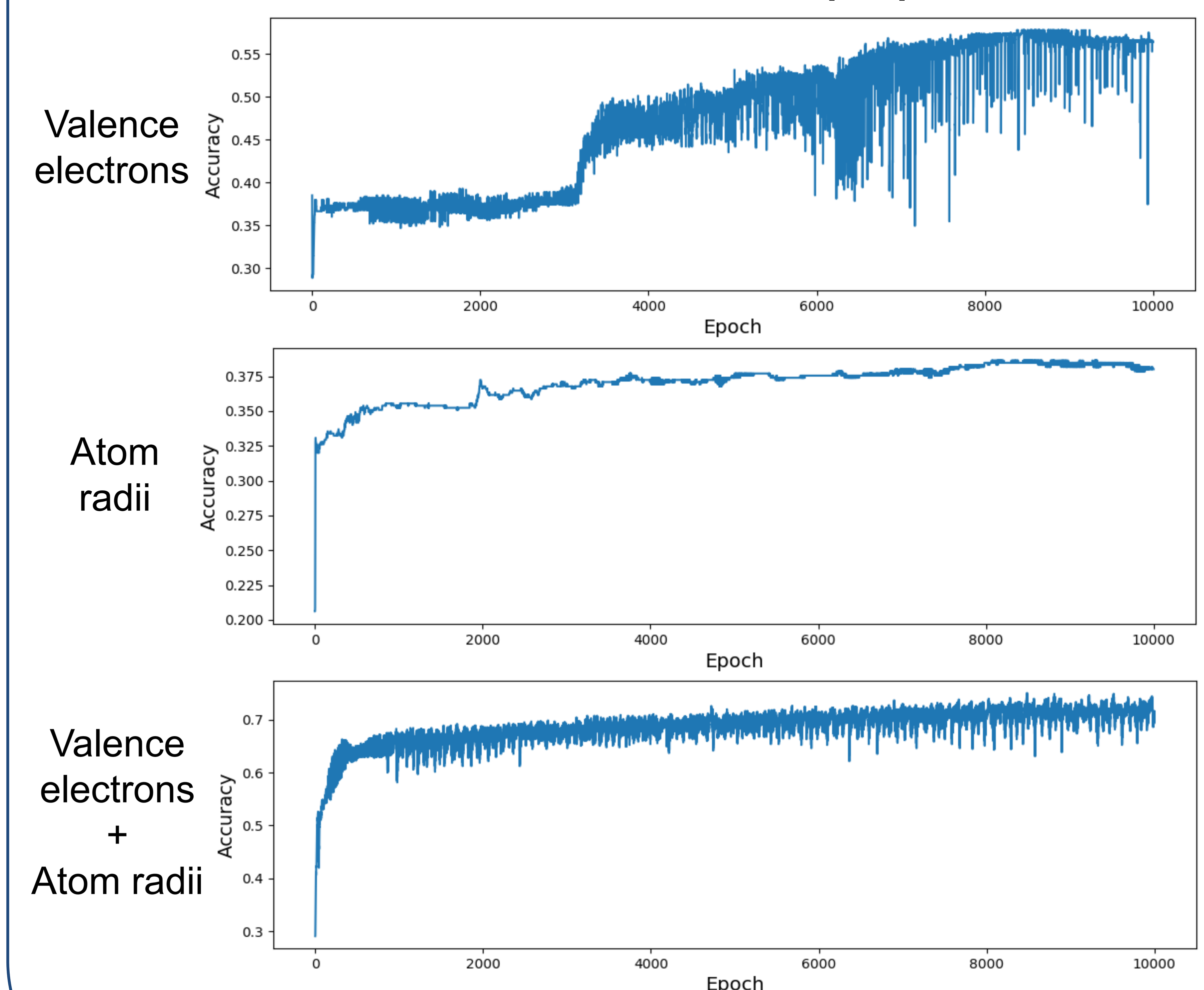


Stability of metal promoter-host systems in different configuration based on the surface energies. Host and promoter elements are ordered first by period then by group numbers.

Machine Learning Algorithm and Results



Performance with different sets of input parameters



Epoch is one complete presentation of the data set to be learned to a learning machine

Conclusions

- The stability of the alloy has a strong relation to the the number of valence electrons and atom radii of the components in the alloys. Using these 2 properties, we have reached the accuracy of 75%, which is an acceptable value.
- Future algorithms and methods are going to be tested to carry out a better result. Possible improvement is to use the full electronic density of the promoter and host with the suitable adjustment in step size and number of layers to enhance the accuracy and avoid overfitting.

Acknowledgement

- This research was supported by the Summer Undergraduate Research Fellowship (SURF).
- Computational resources from UH CACDS is gratefully acknowledged.

Reference

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