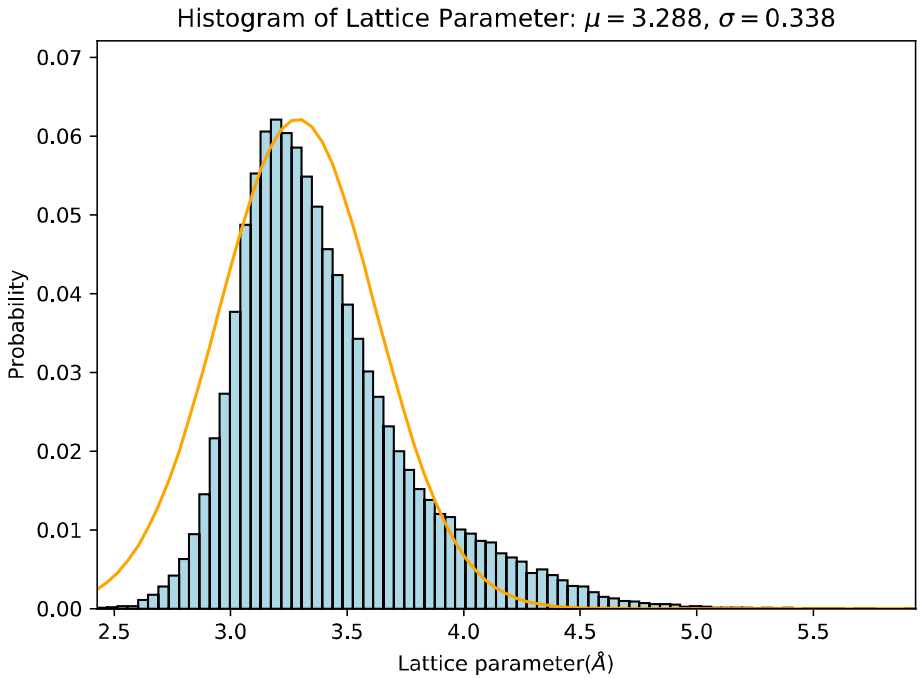
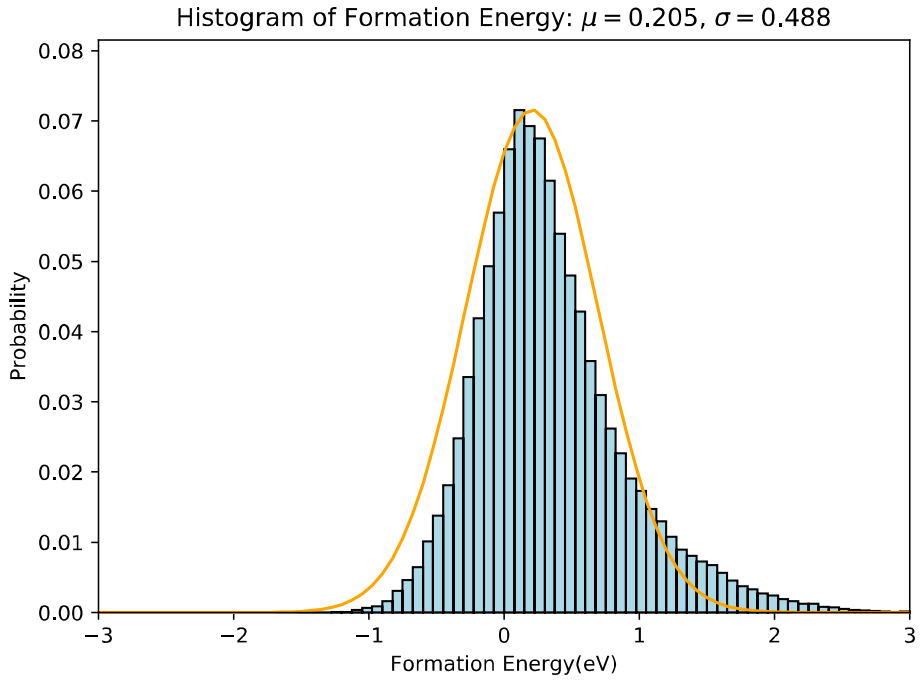
**Supporting information**




(a)




(b)

Fig.S1 Histograms of (a) lattice parameter and (b)enthalpy of formation of all the full-Heusler compounds in OQMD training set.

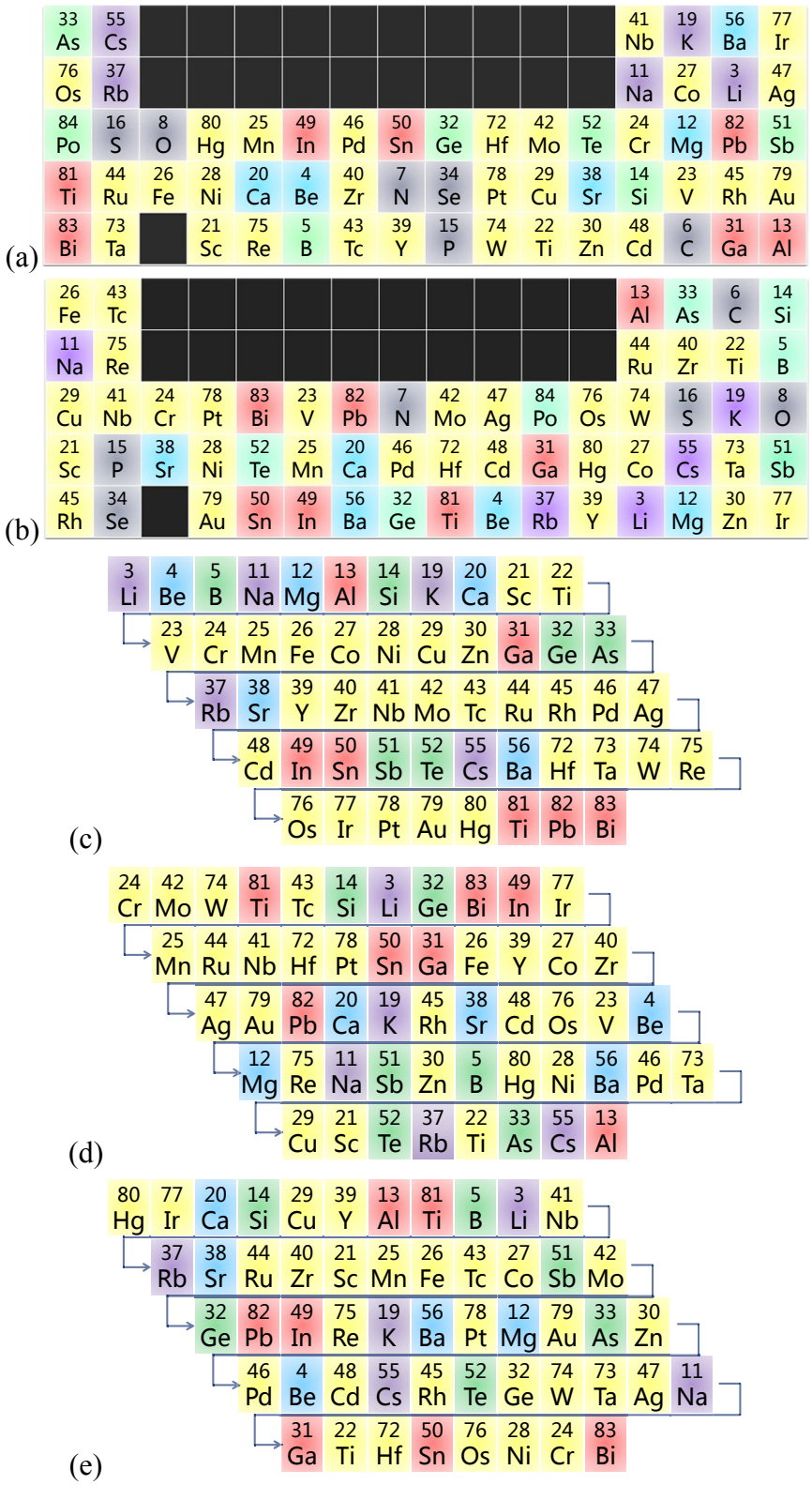
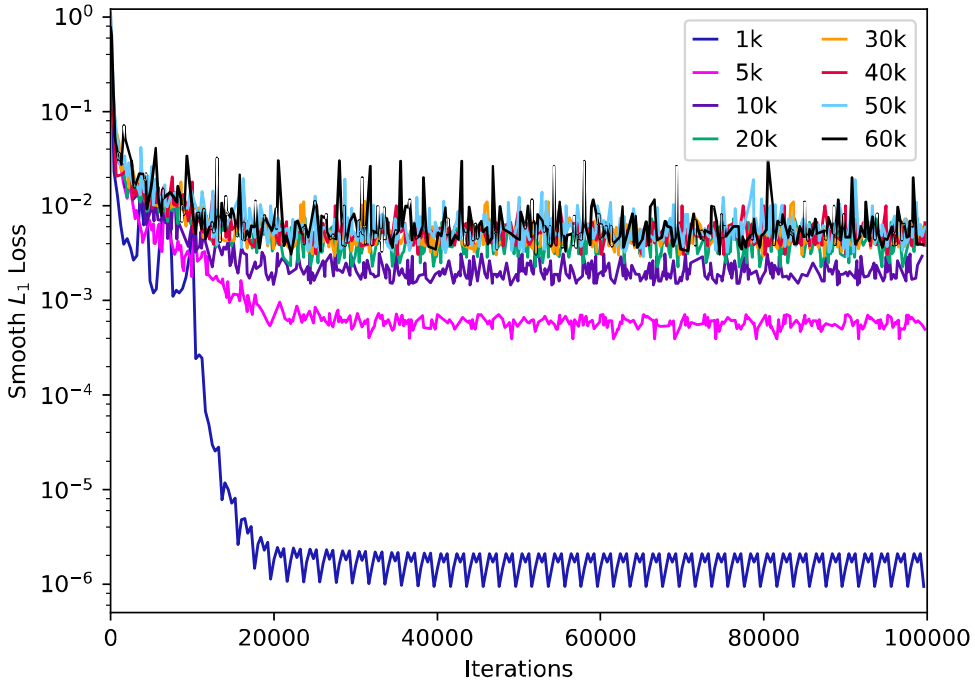
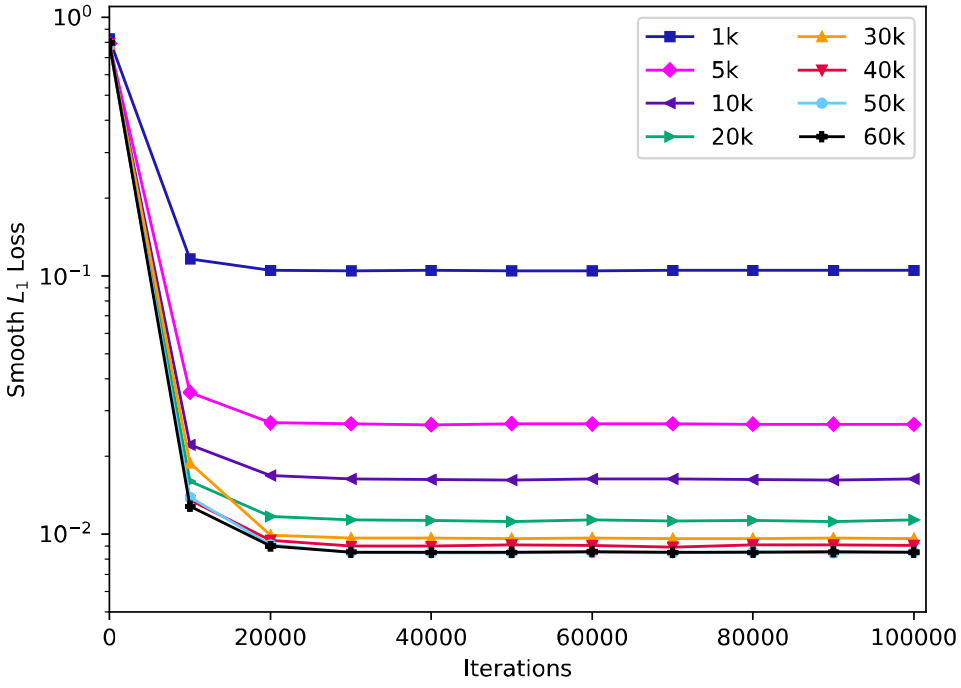



Fig.S2 Representations used as comparisons to the periodic table. (a,b) Random-element-positioning using the layout the periodic table. (c) Elements were aligned in one line in descending order according to Mendeleev numbers. (c,d) The elements were totally randomized in one line.

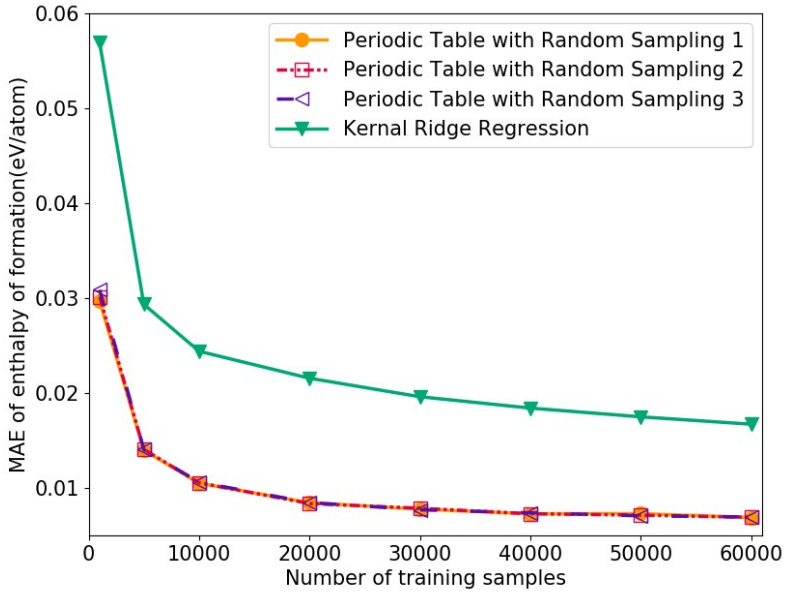



(a)

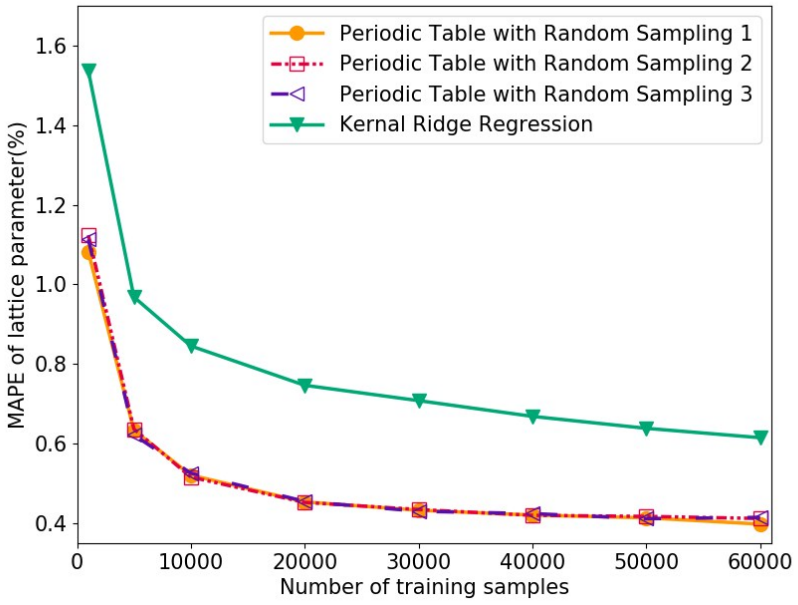



(b)

Fig. S3 (a) Training loss and (b) Test loss with different training sample size.




(a)




(b)

Fig.S4 Comparison of test errors of CNN and kernel ridge regression (KRR) as a function of training set size. The KRR used radial basis function (RBF) as the kernel function, and was trained using 5-fold cross validation. The parameters were optimized using grid search. The search space was [0.01, 0.1, 1, 10, 100] for gramma parameter in RBF, and [1, 0.1, 0.01, 0.001] for lamda parameter in KRR.

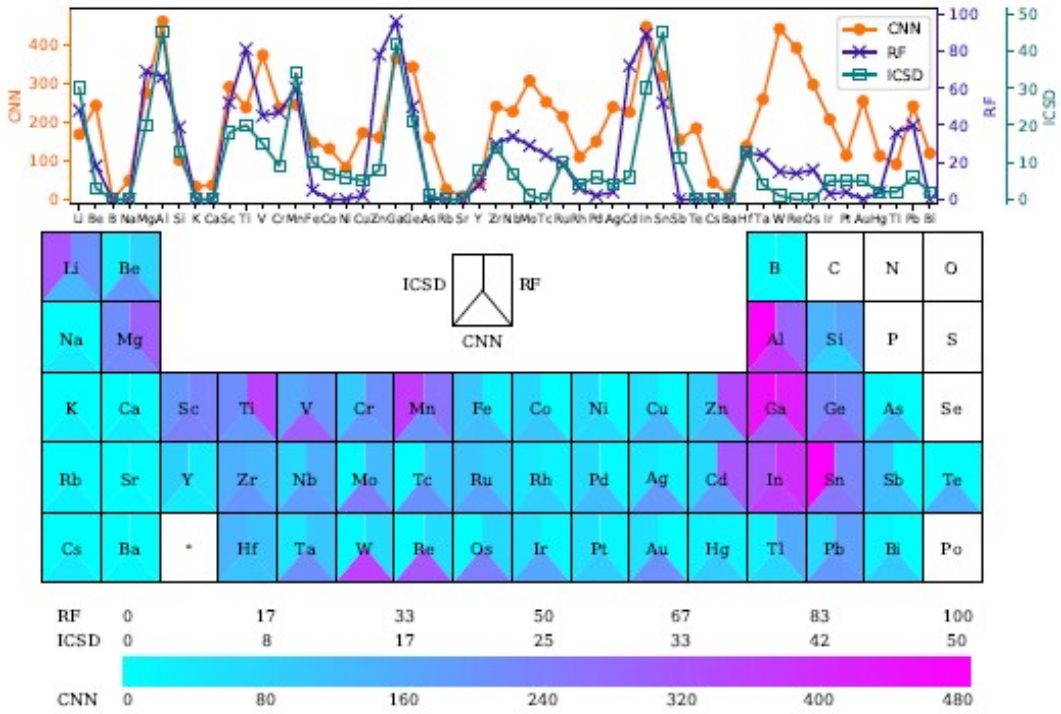



Fig. S5 Number of stable $X_2YZ$ full-Hesuler compounds which have corresponding elements on *YZ* sites (Y and Z are equivalent sites), shown in (a) line chart and (b) periodic table. The experiential data from ICSD and random forest (RF) results from Ref 8 were also shown.

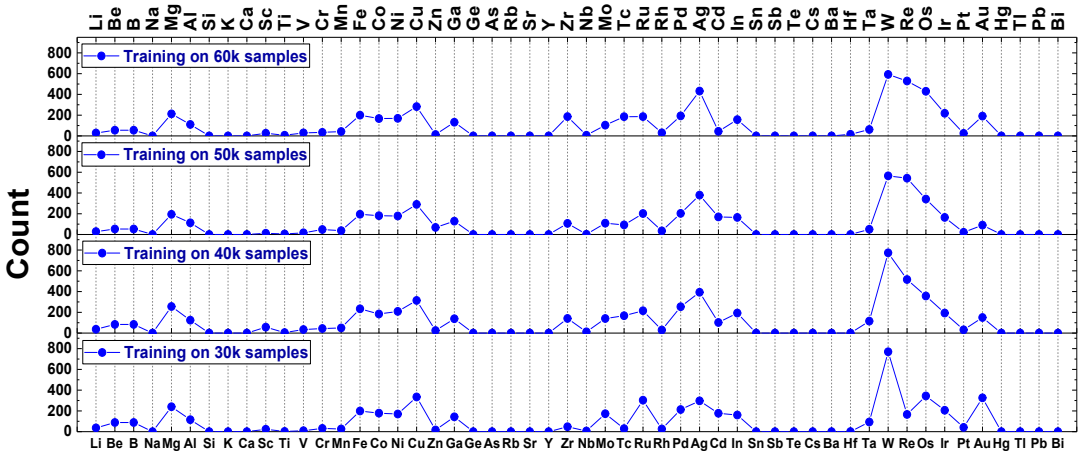
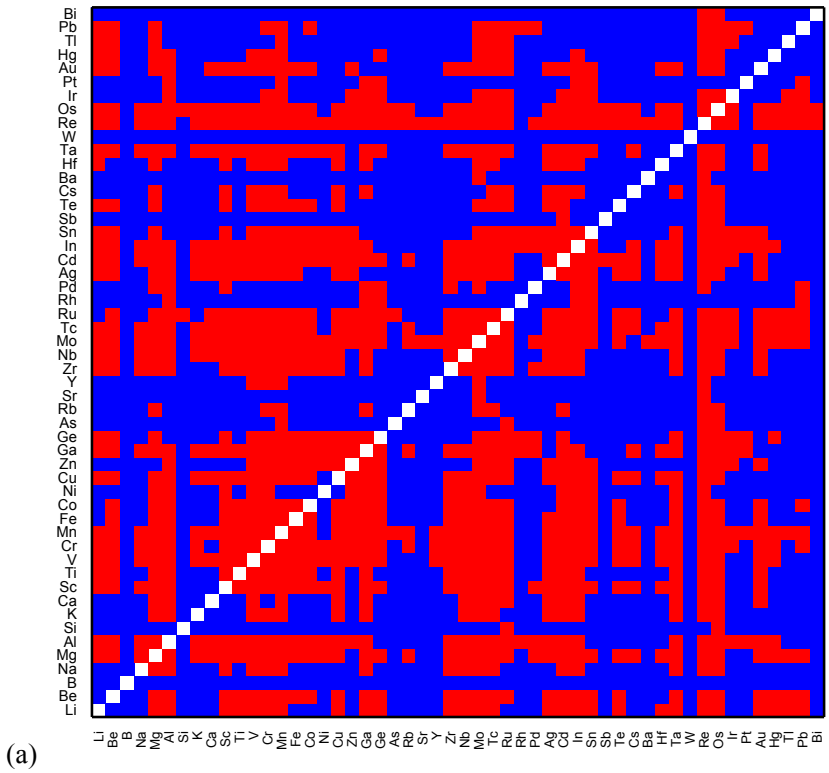
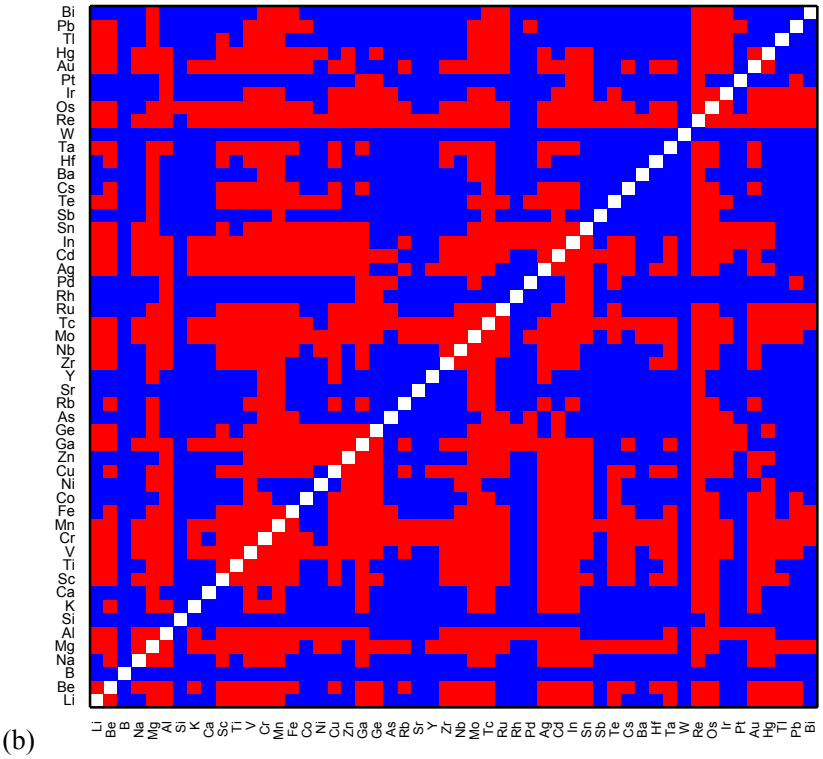



Fig.S6 Comparison of stability prediction results using different OQMD training set size. The numbers are for predicted stable $X_2YZ$ full-Hesuler compounds which have corresponding elements on X site.




(a)




(b)

Fig.S7 Heatmaps of stable $W_2YZ$ compounds predicted by CNN transfer learning, trained previously on (a) 50k and (b) 60k OQMD training sets, respectively. Red means the compound is stable in $L_{21}$ full-Heusler form.

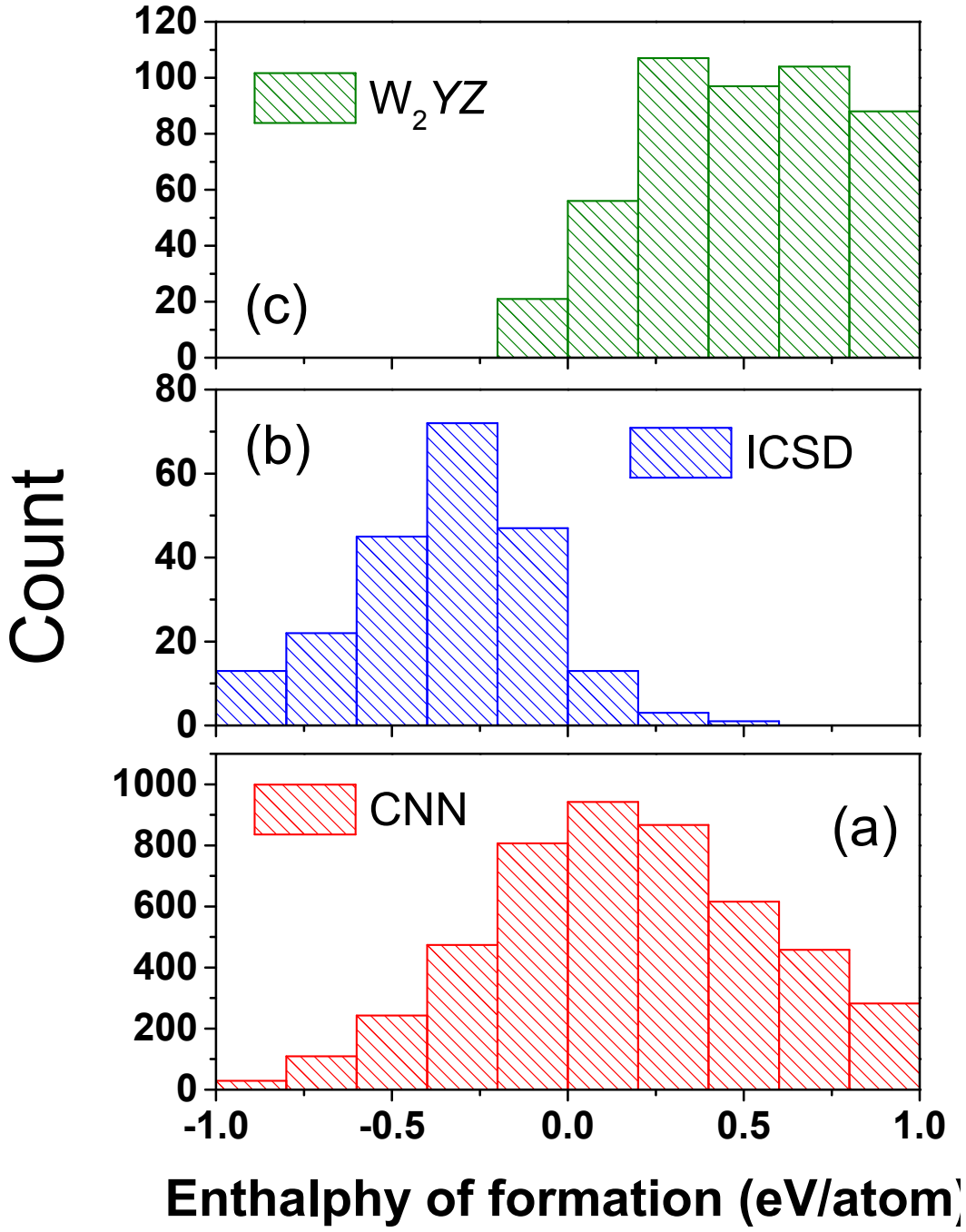



Fig.S8 enthalphy of formation distribution for (a) all 5088 CNN predicted stable compounds. (b) full-Heuslers compounds in ICSD (c) CNN prediction stable compounds containing tungsten on *X* site. The values of enthalpy of formation were taken from OQMD.