Supplementary information for 'Element-wise representations with ECNet for material property prediction and applications in high-entropy alloys'

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(Dated: May 25, 2022)

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The readout feature vectors for Co_3Cr binary alloy are listed for understanding the ECNet model. Here, we use the three-target learning model as the parent model, which is trained from total energy, mixing energy and formation energy. Figure S1 illustrate the three outputs of the BCC Co_3Cr alloy after three successive interaction blocks in the ECNet model. In comparison, Figure S2 shows the two readout feature vectors after the same neural network layer (IB3). The element-wise features for the FCC and BCC Co_3Cr alloy show nearly the same characteristics. To quantify the difference, we also compare the Frobenius norm of the feature matrix $\|X\|_F$ and the structural matrix $\|S\|_F$. The differences between the FCC and BCC quasi-random structures for the feature matrix and the structure matrix are represented as $\|\Delta X\|_F$ and $\|\Delta S\|_F$, respectively. We notice that $\|X\|_F^{BCC}$ and $\|X\|_F^{FCC}$ are 4.51 and 9.76, respectively. The F norm of feature difference matrix is 9.71, and the relative difference ($\|\Delta X\|_F/\|X\|_F^{FCC}$) is 0.99. However, the $\|S\|_F^{BCC}$ and $\|S\|_F^{FCC}$ are 29.57 and 17.97, respectively. The F norm of structure difference matrix is 27.38, and the relative difference ($\|\Delta S\|_F/\|S\|_F^{FCC}$) is 1.52. The relative difference in feature vectors is closer to original structural difference, compared to the first block with value of 0.71. Generally, the relative structural matrix norm shift is almost consistent with those in feature matrix.

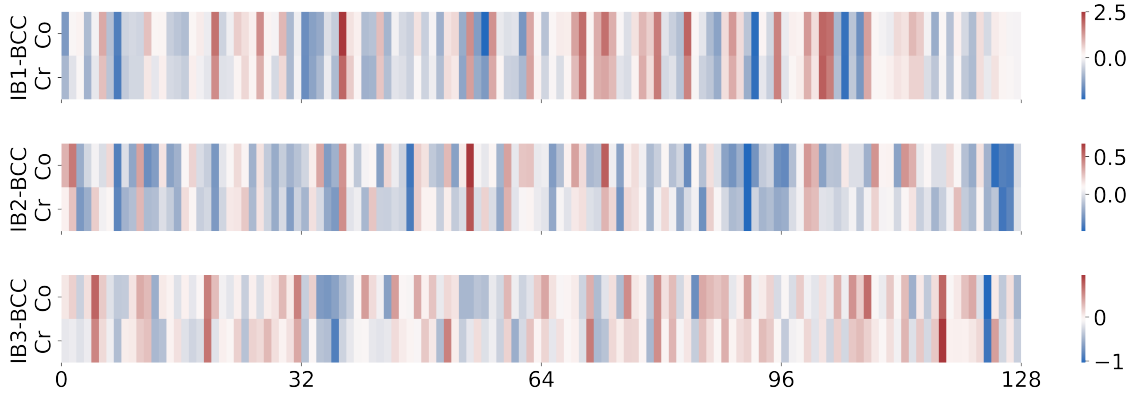

FIG. S1. Element-wise feature vectors. Three outputs after three successive interaction blocks in the ECNet model for the Co_3Cr alloy. This features are based on the model that trained from magnetic properties in the alloy dataset.

To further understand the underlying physics in the ternary system, we show the predicted formation energies for Fe-Co-Ni and Fe-Co-Pd ternary alloys. For the Fe-Co-Pd alloy system, we can observe that the distributions of the stability for Fe-Co-Pd are almost similar between the FCC and BCC phase, while those of Fe-Co-Ni show significant difference between the

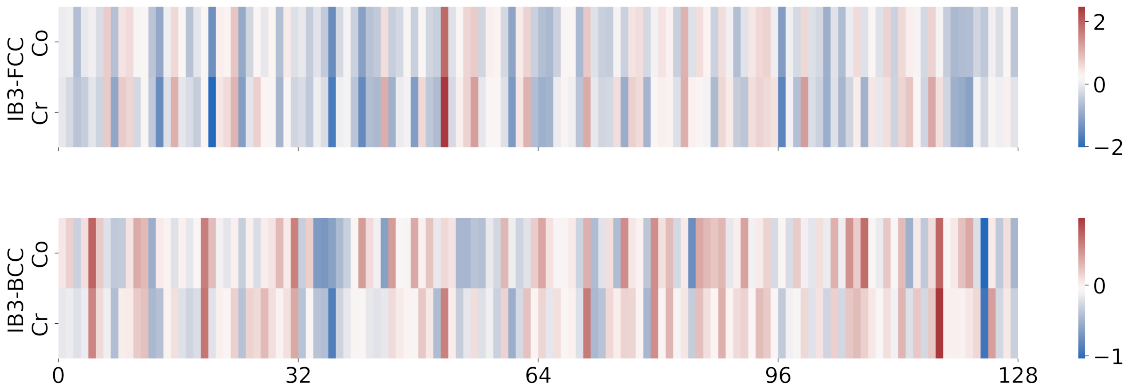

FIG. S2. Element-wise feature vectors. The outputs after the third interaction block in the ECNet model for the Co_3Cr alloy in FCC and BCC phase. This features are based on the model that trained from magnetic properties in the alloy dataset.

FCC and BCC solid solution phases.

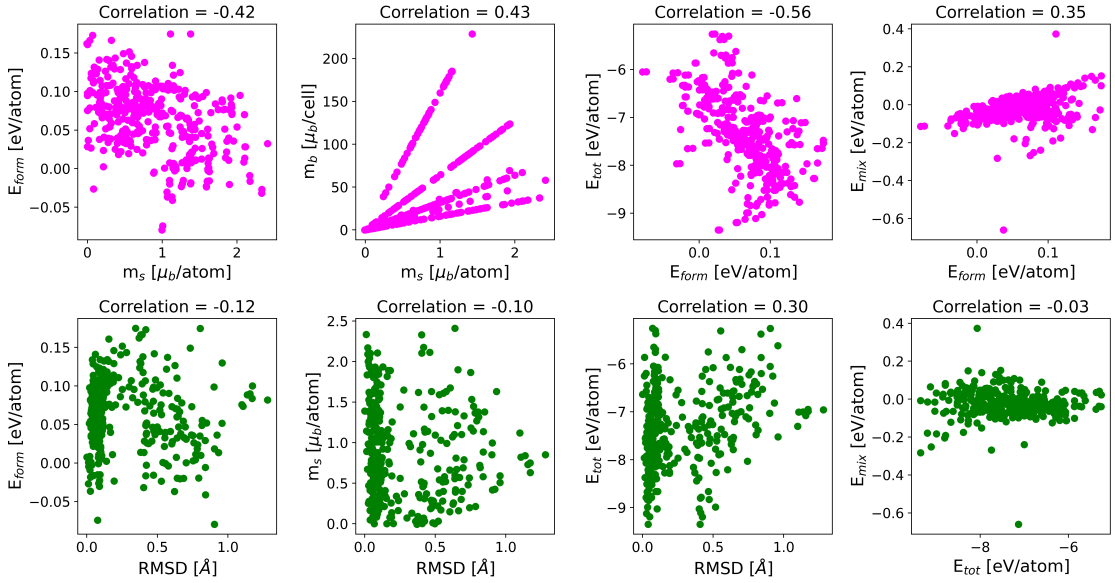

FIG. S3. The parity correlations between two different properties in the alloy data set.

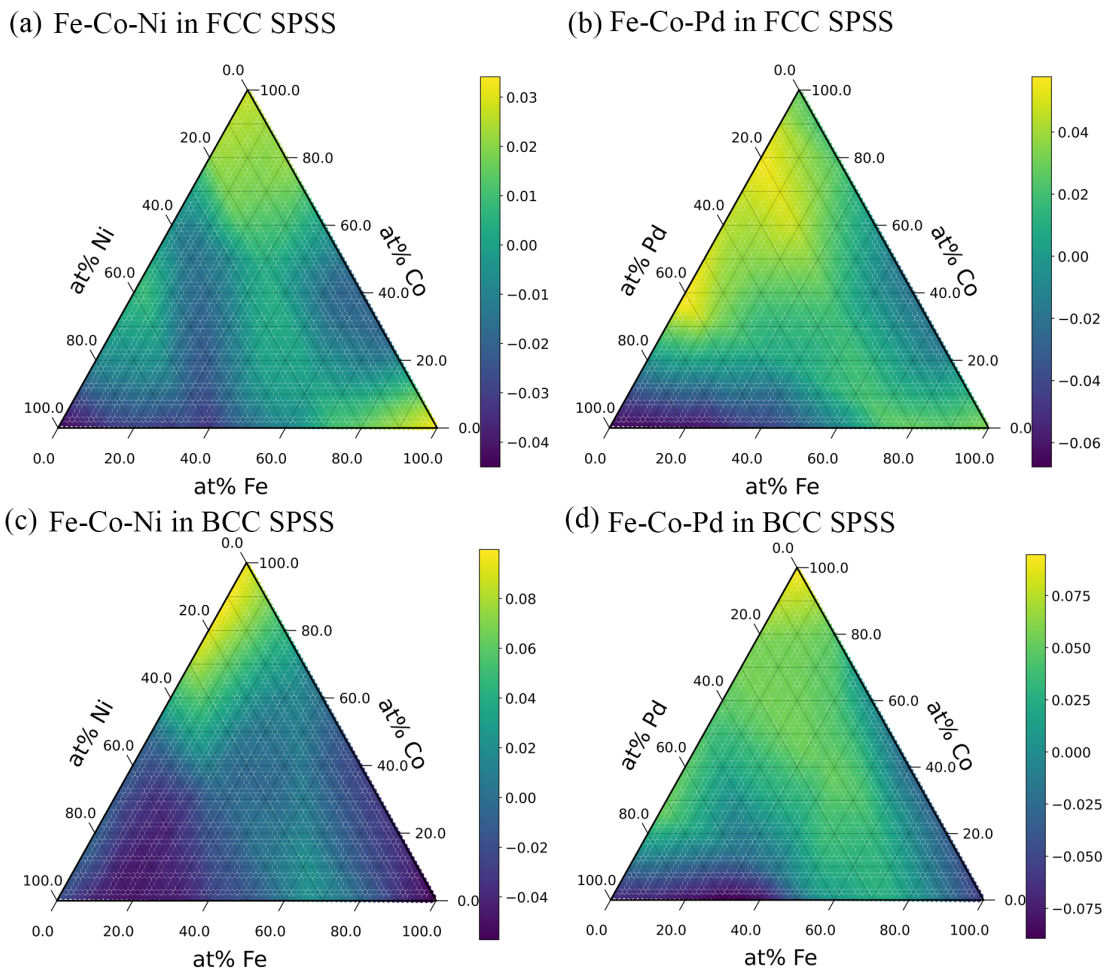

FIG. S4. (a) and (c) are the predicted formation energies at 0K for the Fe-Co-Ni alloys in FCC and BCC single-phase solid solution (SPSS), respectively. (b) and (d) are the predicted formation energies at 0K for the Fe-Co-Pd alloys in FCC and BCC SPSS, respectively.