Volume 12 Issue 02 April 2026

**IJRDO Journal of Applied Science**
**ISSN:2455-6653**
**Reseach Article**

# DECIPHERING PHASE FORMATION IN HIGH ENTROPY ALLOYS THROUGH INTEGRATED ANALYSIS OF ELEMENTAL DIVERSITY AND THERMODYNAMIC DESCRIPTORS

**[1*]Dr. Lukas Schneider, [2]Dr. Hannah Fischer, [3]Dr. Tobias Weber**

[1,2,3] Department of Materials Science and Engineering
International Institute for Advanced Materials Research
Munich, Germany

*Dr. Lukas Schneider,* Email: lukas.schneider.research@gmail.com

***Abstract***
*The formation of high entropy alloy phases requires interactions of elemental, thermodynamic, and electronic factors, but interpretable statistical evidence in a variety of phase classes is still scarce. This study examined how elemental diversity and selected design descriptors influence phase formation in high entropy alloys. A secondary dataset was analyzed using a quantitative exploratory approach. After preprocessing, four phase classes were retained: amorphous, intermetallic, solid solution, and mixed phase. Key variables included the number of elements, atomic size difference, mixing enthalpy, ideal mixing entropy, valence electron concentration, and electronegativity. Descriptive statistics, one-way ANOVA, and Pearson correlation analysis were applied. Intermetallic and solid solution phases were the most frequent, accounting for 32.82% and 31.73% of the dataset, respectively. Solid solution and mixed phases exhibited higher elemental complexity, ideal mixing entropy, and valence electron concentration, whereas amorphous phases showed the highest atomic size difference and the most negative mixing enthalpy. All parameters varied significantly across phases ($p < 0.001$), with ideal mixing entropy showing the strongest discriminatory effect. Correlation analysis revealed moderate relationships between atomic size difference and mixing enthalpy, and between valence electron concentration and electronegativity. Phase formation is governed by multiple interacting descriptors rather than a single parameter, providing an interpretable basis for preliminary alloy screening and rational design.*

**Key Words:** Entropy alloys, Phase formation, Elemental complexity, Thermodynamic

**DOI:** https://doi.org/10.69980/as.v12i2.6675
**Received 08 February 2026 | Accepted 02 April 2026 | Published 27 April 2026**

## 1. INTRODUCTION

The emergence of high entropy alloys (HEAs) is considered to be a breakthrough discovery in the field of materials science due to their unique composition and hence multifunctionality. Unlike conventional alloys, which normally consist of a few main components, HEAs are developed through the combination of several elements in nearly equal atomic ratios, leading to complex atom interactions and high configurational entropy. Such a special design philosophy makes it possible to obtain high mechanical strength, thermal stability, and degradation resistance for HEAs, making it suitable for use in tough applications (George et al., 2019). In recent years, multifunctional and functional material systems have been included within the scope of HEAs, marking their importance in future materials research (Zhang et al., 2024; Ding et al., 2025).

The increasing popularity of HEAs is also because of their capability to address the problem of high-temperature stability and corrosion resistance. The development of alloy design strategies has made it possible for researchers to personalize the composition to achieve better structural stability in severe conditions (Li et al., 2024). At the same time, there has been an increased level of corrosion resistance observed in studies, where complexity is the major determinant of durability and prolonged service (Liang et al., 2024). Apart from their structural application, the use of HEAs has also been noted in catalysis and energy applications, which further emphasizes the capabilities of HEAs in various technological applications (Ren et al., 2023). It becomes clear that understanding the basics of phase formation and stability is important due to the influence of phase constitution on material properties.

The phases' formation within the framework of HEAs has been widely discussed, and the factors affecting structural stability, including thermodynamic and atomic ones, have been of great interest. Atomic size difference, mixing enthalpy, and other parameters play a crucial role in the formation of solid solution, intermetallic, and amorphous phases as they determine the level of lattice distortion and atomic interactions within the alloy system (Luan et al., 2020). Of them, configurational entropy is a significant factor that helps to stabilize disordered solid solution phases as it lowers the overall free energy, particularly at high temperatures (Ye et al., 2022). Besides the thermodynamic descriptors, compositional and electronic parameters have been used to comprehend phase behavior. Research has established that an alloy composition has a great effect on the phase formation mechanisms, and some combinations of elements favor either an ordered or disordered structure (Guo et al., 2023). The more recent studies have investigated how the difference in electronegativity can be used to control alloy properties and phase stability, showing that the electronic structure factors can be considered in the design of alloys (Lin et al., 2023).

The research in high entropy materials has also been extended to cover other functional materials and oxides, where the mechanisms of phase stability are more complex. The critical reviews of this field point out that to have a complete picture of the phase formation behavior, multiple descriptors should be combined (Fracchia et al., 2024). At the same time, the recent tendencies in research focus on the use of advanced analytical and computational methods to more precisely reflect the interactions of different design parameters (Balaji & Xavior, 2024). In spite of these developments, most studies continue to be concentrated on predictive accuracy or particular material systems, with the resultant limitation on the interpretability and generalisability of their results. In spite of the fact that significant advances have been achieved in the study of the formation of phases in HEAs, current research often utilizes complicated predictive models or single-parameter-based standards, and little effort has been put into the systematic and understandable comparisons of different phase types. The interplay between the complexity of elements and essential thermodynamic and electronic descriptors has been under-researched in a single analysis tool. Also, the connections between these parameters and their overall influence on phase differentiation are not sufficiently studied using statistically based methods.

This current research will explore how the elemental diversity, as well as chosen thermodynamic and electronic design parameters, affect the formation of phases in high entropy alloys by performing a systematic statistical analysis. The study aims to give clear and interpretable information about the parameters that control phase stability by comparing the distributions of parameters in different phase classes and comparing the statistical significance of these distributions. Moreover, correlation analysis between the main descriptors should be performed to understand the interdependence of the descriptors and their role in the phase differentiation to facilitate more informed alloy design and materials selection.

## 2. METHODOLOGY

### 2.1 RESEARCH DESIGN

The research design used in this study is a quantitative, exploratory research design to examine the phase-dependent differences of elemental, thermodynamic, and electronic parameters of high entropy alloys. The analysis relies on secondary data and is designed so that it finds statistically significant differences between phase classes. The methodology emphasizes interpretability and reproducibility through the use of common statistical methods as opposed to complicated predictive models.

### 2.2 DATA SOURCE

The data employed in this research was collected as a publicly available source that was created in the framework of the ACHIEF project, aiming at discovering and designing advanced materials that can be used in the industrial sector (Precker et al., 2021). It consists of a set of high entropy alloy compositions and associated phase classifications and design parameters calculated. The dataset contains details on alloy composition, number of constituent elements, phase type, and several descriptors that describe thermodynamic and electronic properties that are useful in designing an alloy.

### 2.3 DATA PREPARATION

Preprocessing of data was done through screening for completeness and consistency. Missing phase labels were observed to be excluded, so that the groups could be correctly grouped in later analysis. The data were then narrowed down to four phase types: amorphous (AM), intermetallic (IM), solid solution (SS) and mixed phase (SS+IM).

A small group of variables applicable to alloy design was chosen to be analyzed. These were the number of elements that they were made up of, the atomic size difference, mixing enthalpy, ideal mixing entropy, valence electron concentration, and electronegativity. Individual elemental fraction variables and redundant variables were dropped to preserve focus in the analysis and to reduce dimensions. No transformation of the selected variables into their numerical form was done.

### 2.4 STATISTICAL ANALYSIS

The descriptive statistics were calculated to sum up the spread of the chosen parameters within the phase groups. Mean and standard deviation figures were obtained on each parameter in each of the phase categories to enable comparison.

One-way analysis of variance (ANOVA) was undertaken on each parameter to compare the differences among the phase groups in a statistical manner. This is a procedure of comparing group means that have several independent categories. All the statistical tests were set at a significance level of 0.05.

Also, Pearson correlation analysis was done to evaluate the association between the chosen design parameters. Correlation coefficients were calculated to measure the strength and direction of relationships between variables.

## 3. RESULTS

### 3.1 PHASE DISTRIBUTION OF HIGH-ENTROPY ALLOYS

The phase class distribution of the dataset is the basis of the further comparative analysis. There is a relatively equal distribution in intermetallic (IM) versus solid solution (SS) phases, with amorphous (AM) and mixed (SS+IM) phases being less common. Table 1 demonstrates that the IM and SS phases are predominant in the dataset, with the same proportion (~32%). AM and SS + IM phases have nearly the same proportion of 18% each. Such a distribution will make sure that no single class will predominate in comparative analysis between phases.

**TABLE 1. PHASE DISTRIBUTION OF HIGH-ENTROPY ALLOYS**

| Phase | Count | Percentage (%) |
|---|---|---|
| IM | 362 | 32.82 |
| SS | 350 | 31.73 |
| SS+IM | 196 | 17.77 |
| AM | 195 | 17.68 |

Figure 1 provides a visual confirmation of the numerical tendencies, with IM showing the highest frequency, with SS coming in a close second after it, with AM and SS+IM constituting the minority groups.

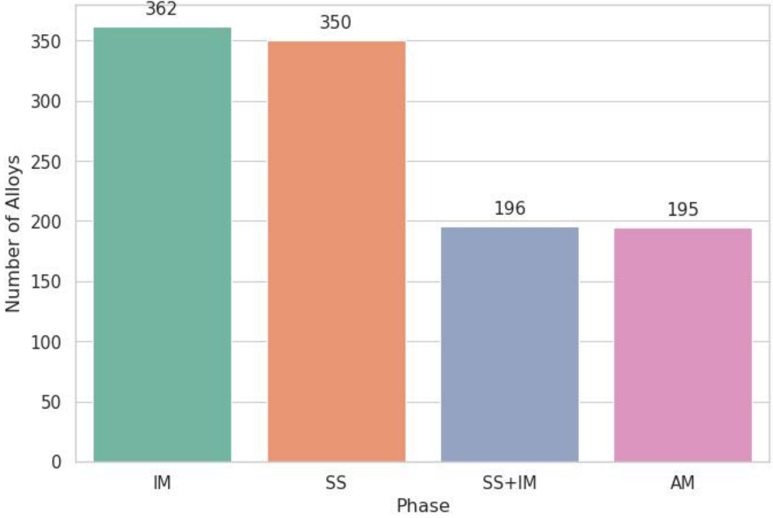

**FIGURE 1. PHASE DISTRIBUTION OF HIGH-ENTROPY ALLOYS**

### 3.2 PHASE-WISE COMPARISON OF ELEMENTAL, THERMODYNAMIC, AND ELECTRONIC PARAMETERS

The elemental complexity, atomic mismatch, thermodynamic stability, and electronic structure parameters of phases are extensively compared to determine controlling trends in phase formation.

Figure 2A shows that SS and SS+IM phases have the greatest elemental complexity, with mean values of 5.343 and 5.633, respectively, and IM phases have much less compositional diversity (3.506). AM phases are located in the middle (4.103), which means the alloy is moderately complex. Figure 2B demonstrates that the mismatch of the atomic size is greatest in the AM phases (0.112 ± 0.032), then the IM phases, and the SS phases have the lowest mismatch (0.049 ± 0.017). This trend suggests that larger atomic size mismatch encourages structural disorder that allows the formation of amorphous phases, and a smaller mismatch encourages the formation of solid solutions. Figure 2C displays the variation in mixing enthalpy with AM phases having the most negative values (−26.398 ± 11.966 kJ/mol), and then IM phases. SS phases have less negative values, which indicate weaker interactions between atoms. This implies that high negative enthalpy is conducive to the development of amorphous and intermetallic phases. Figure 2D shows that the ideal mixing entropy is the maximum when using SS+IM (1.645 ± 0.203) and SS (1.598 ± 0.231) phases, whereas AM and IM phases have lower values of the entropy. This justifies the contribution of configurational entropy in stabilizing solid solution structures. The trends in the electronic structures are shown in Figures 2E and 2F. Figure 2E indicates that SS and SS+IM phases have larger values of valence electron concentration than IM and AM phases, which is in accordance with known design criteria of HEA to have solid solution stability. Figure 2F shows that values of electronegativity are a little stronger in SS-type phases, but the difference between phases is not very large.

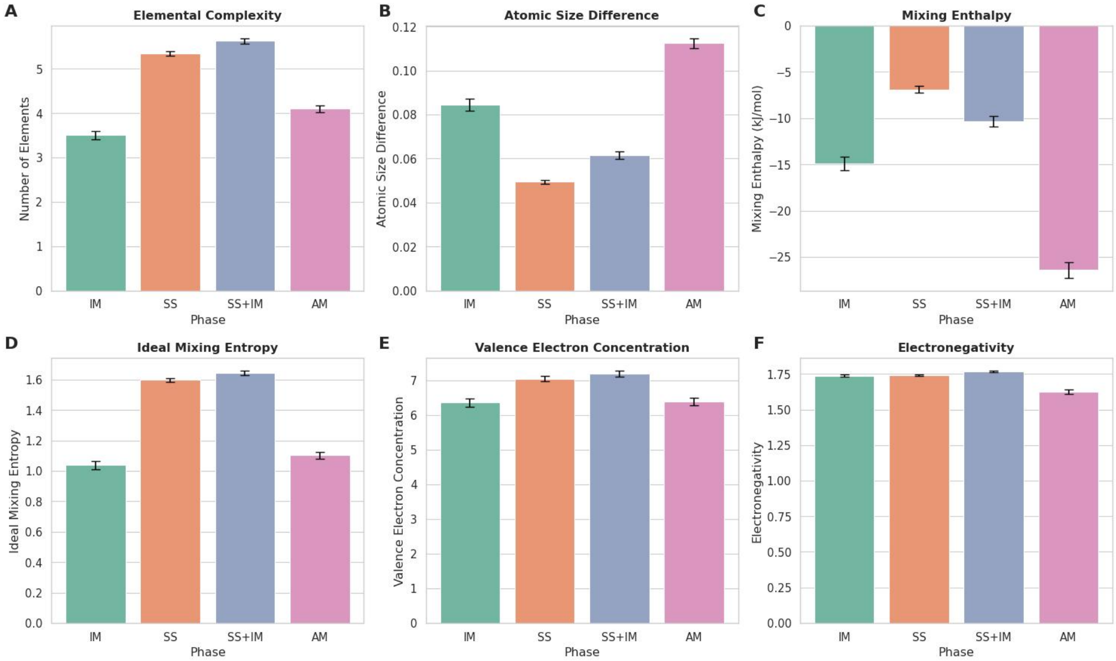

**FIGURE 2. PHASE-WISE COMPARISON OF KEY DESIGN PARAMETERS IN HIGH ENTROPY ALLOYS**

(A) Elemental Complexity; (B) Atomic Size Difference; (C) Mixing Enthalpy; (D) Ideal Mixing Entropy; (E) Valence Electron Concentration; (F) Electronegativity

The trends described in Table 2 support the idea that SS and SS+IM phases have a higher entropy and electron concentration, whereas AM phases are characterized by stronger enthalpic interactions and a b igger size mismatch of atoms.

**TABLE 2. DESCRIPTIVE STATISTICS OF KEY PARAMETERS BY PHASE (MEAN ± STANDARD DEVIATION)**

| Phase | Number of Elements | Atomic Size Difference | Mixing Enthalpy (kJ/mol) | Ideal Mixing Entropy | Valence Electron Concentration | Electronegativity |
|---|---|---|---|---|---|---|
| AM | 4.103 ± 1.070 | 0.112 ± 0.032 | -26.398 ± 11.966 | 1.102 ± 0.310 | 6.384 ± 1.590 | 1.625 ± 0.210 |
| IM | 3.506 ± 1.740 | 0.084 ± 0.053 | -14.907 ± 13.296 | 1.038 ± 0.482 | 6.350 ± 2.097 | 1.739 ± 0.197 |
| SS | 5.343 ± 1.036 | 0.049 ± 0.017 | -6.895 ± 6.382 | 1.598 ± 0.231 | 7.038 ± 1.420 | 1.743 ± 0.114 |
| SS+IM | 5.633 ± 0.852 | 0.062 ± 0.023 | -10.325 ± 7.850 | 1.645 ± 0.203 | 7.183 ± 1.277 | 1.767 ± 0.094 |

### 3.3 STATISTICAL SIGNIFICANCE OF PHASE-WISE DIFFERENCES

One-way ANOVA was conducted on each of the parameters to confirm that the differences among phases are statistically significant. There are statistically significant differences in all parameters between phases ($p < 0.001$). Among the above, ideal mixing entropy has the largest F-statistic, which implies the best discriminatory ability, followed by mixing enthalpy and atomic size difference (Table 3).

**TABLE 3. ONE-WAY ANOVA RESULTS FOR PHASE-WISE PARAMETER COMPARISON**

| Parameter | F-statistic | p-value |
|---|---|---|
| Atomic Size Difference | 145.268 | < 0.001 |
| Mixing Enthalpy (kJ/mol) | 156.670 | < 0.001 |
| Ideal Mixing Entropy | 242.671 | < 0.001 |
| Valence Electron Concentration | 17.603 | < 0.001 |
| Electronegativity | 31.560 | < 0.001 |

### 3.4 CORRELATION BETWEEN KEY DESIGN PARAMETERS

Correlation analysis was employed to evaluate a relationship between key design parameters with the view to determining potential relationships that impacted phase behavior. Figure 3 correlation matrix indicates that there is a moderate negative relationship between the difference in atomic size and mixing enthalpy (−0.54), whereby alloys with higher atomic mismatch are expected to have stronger enthalpic interactions. Also, there is a moderate positive relationship between valence electron concentration and electronegativity (0.58), indicating an association between electronic descriptors.

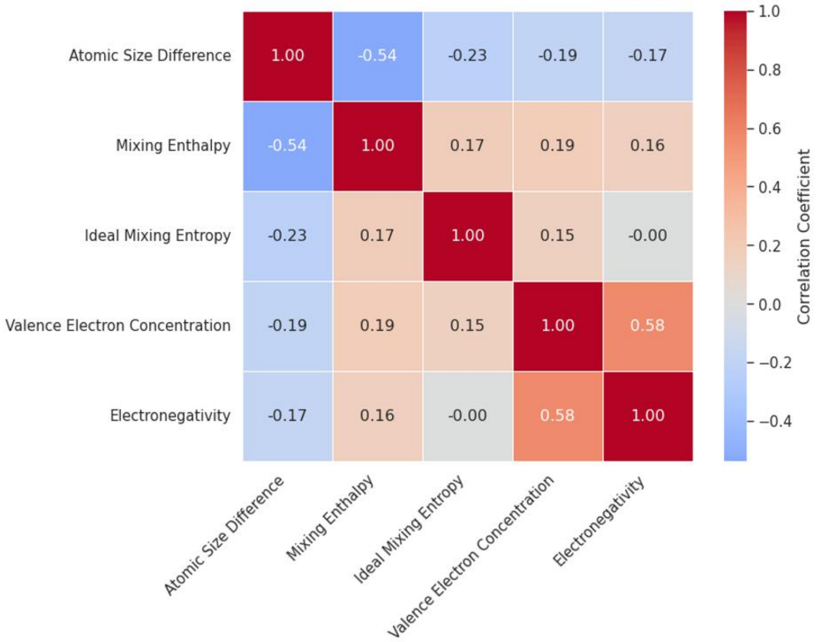

FIGURE 3. CORRELATION MATRIX OF KEY HEA DESIGN PARAMETERS

The other parameter relationships are weak, and this implies that the majority of the variables have independent contributions to the formation of the phases. This absence of sharp multicollinearity justifies the application of more than one descriptor to analyze and design a high entropy alloy.

## 4. DISCUSSION

The conclusions drawn from the study indicate that phase formation in HEAs is a consequence of the interaction between elements of complexity, thermal and electronic properties. A general pattern is found whereby the solid solution (SS) phases and mixed (SS+IM) phases are found to be more diversified in terms of elements than intermetallic (IM) phases. This indicates that the more the constituent elements, the more configurational disorder that stabilizes solid solution phases.

The difference in atomic size has a unique role in the distinction of phase behavior. Amorphous (AM) phases are characterized by the largest atomic mismatch, which means that the considerable lattice distortion breaks long-range order and facilitates amorphization. Conversely, there is a low level of size mismatch in SS phases, and this facilitates the development of stable crystalline structures. This difference is further supported by the difference in mixing enthalpy with the strongly negative values linked with AM and IM phases, and the stronger atomic interaction providing the favorable formation of compounds or disorder in the structure. The fact that negative values of SS phases are fewer negative shows that fewer interactions are present, which means that the disordered solid solutions can be stabilized. The effect of configurational entropy is quite strong. Increased entropy values of SS and SS+IM phases prove the stability of disordered structures, as they reduce the free energy of the system. Valence electron concentration and electronegativity are also electronic parameters that are involved in phase differentiation. The increased values of these parameters in the SS-type phases imply that electronic structure is supportive in stabilizing solid solutions. The general conclusion of the results is that the formation of phases is not a process that depends on one parameter but on a complex interaction of several thermodynamic and electronic descriptors.

The trends observed can be related to the known results about the role of thermodynamic and compositional descriptors in phase formation. The prevalence of configurational entropy in stabilizing the solid solution phases is consistent with previous literature highlighting the role of entropy in phase stability of complex alloy systems (Zhang et al., 2020). Likewise, the effects of mixing enthalpy and atomic size disparity in the separation of ordered and disordered phases align with strategies of thermodynamic design that are documented in the literature (Odetola et al., 2024). Other recent research in the area of machine learning enabled the identification of such key descriptors as valence electron concentration and electronegativity as important predictors of the phase behavior and demonstrated the trends in the current analysis (Syarif et al., 2023). Multi-descriptor methods have shown better ability to capture trends in phase formation, and it is important to note that combined parameters analysis is better than the application of single parameters (Shuai et al., 2025).

This high statistical significance of entropy and enthalpy is consistent with the model prediction of descriptors in predicting phase stability, where both the parameters are repeatedly found to be the most significant predictors of phase stability (Gong et al., 2024). Moreover, recent trends in the design of alloys with the use of data focus on the necessity to include not only thermodynamic but also electronic descriptors to predict the phases correctly (Zheng et al., 2025). The effectiveness of the method of descriptors in the description of the phase behavior of different alloy systems is further supported by experimental and computational validation studies (Khoa et al., 2025). Moreover, new machine learning-based classification methods have proven the ability to describe high entropy alloys with complex phase combinations, which enhances the significance of multi-descriptor frameworks in predicting phases reliably (Thampiriyanon & Khumkoa, 2025).

The results offer some useful information on designing and developing high entropy alloys. The determination of important parameters like the configurational entropy, mixing enthalpy and valence electron concentration makes it possible to screen alloy compositions more intelligently before experimental synthesis. This can greatly decrease the use of trial-and-error methods and efficiency in the development of materials. The findings also show that phase formation trends can be effectively modeled using interpretable statistical techniques without the complexity of modeling frameworks. This is very handy in material design at an early stage, where a clear picture of the influence of parameters is required. These types of applications, for which the phase structure plays an important role in their performance, can benefit from such kinds of knowledge.

Some of the limitations of this study include the use of secondary data, which can limit the scope of the study due to factors like data inconsistency, quality, and lack of representation. Another limitation is the use of only a few design parameters that were chosen for the analysis, whereas some others may also be important but have not been considered in this study. Furthermore, the fact that there was no experimental validation for the predictions means that the applicability of these findings in reality is limited to those specific materials used in this study. Future research could be extended to larger and more diverse data sets and experimental validation of the results obtained from this study. More descriptors, along with a combination of machine learning algorithms, could be helpful for understanding phase formation.

## 5. CONCLUSION

The synergistic role of elemental variety, thermodynamic stability, and electronic factors in the formation of phases in HEAs is described. According to our results, SS and SS + IM phases are associated with greater elemental variety, higher ideal mixing entropy, and valence electron density, while AM phases are characterized by greater atomic size disparity and more negative mixing enthalpy. Different choices of features were obtained for each phase class, justifying the validity of these parameters for predicting the behavior of phases in alloys. Moreover, based on the correlation matrix of selected descriptors, we can conclude that there is a relative independence among them, hence the need for simultaneous consideration rather than separate ones. These results provide a statistically valid basis for preliminary identification of HEA and alloy design. However, due to the secondary use of data and the selection of features, generalizing the findings from this experiment is not possible. Future research should include larger datasets, additional material features, and experimental confirmation.

## REFERENCES

1. Balaji, V., & Xavior, A. (2024). Development of high entropy alloys (HEAs): Current trends. *Heliyon*, *10*(7).
2. Ding, Z., Li, Y., Jiang, H., Zhou, Y., Wan, H., Qiu, J., ... & Pan, F. (2025). The integral role of high-entropy alloys in advancing solid-state hydrogen storage. *Interdisciplinary Materials*, *4*(1), 75-108.
3. Fracchia, M., Coduri, M., Ghigna, P., & Anselmi-Tamburini, U. (2024). Phase stability of high entropy oxides: A critical review. *Journal of the European Ceramic Society*, *44*(2), 585-594.
4. George, E. P., Raabe, D., & Ritchie, R. O. (2019). High-entropy alloys. *Nature reviews materials*, *4*(8), 515-534.
5. Gong, H., Chen, Z. Q., Shang, Y. H., Wang, H., Hu, S. J., & Yang, Y. (2024). Thermodynamic Descriptors for Rapid Search of Compositional Complex Spinodal Alloys with Artificial Neural Network. *High Entropy Alloys & Materials*, *2*(2), 374-386.
6. Guo, Q., Xu, X., Pei, X., Duan, Z., Liaw, P. K., Hou, H., & Zhao, Y. (2023). Predict the phase formation of high-entropy alloys by compositions. *Journal of Materials Research and Technology*, *22*, 3331-3339.
7. Khoa, N. L., Khanh, N. D., Quyen, H. T. N., Oanh, N. T. H., Thang, L. H., Khiem, N. H., & Viet, N. H. (2025). Thermodynamic and Electronic Descriptor-Driven Machine Learning for Phase Prediction in High-Entropy Alloys: Experimental Validation. *Journal of Powder Materials*, *32*(3), 191-201.
8. Li, M., Henein, H., Zhou, C., & Liu, J. (2024). Towards high-entropy alloys with high-temperature corrosion resistance and structural stability. *Journal of Materials Science & Technology*, *174*, 133-144.

9. Liang, J., Wang, W., Cao, Z., Guo, J., Sun, Z., & Hai, Y. (2024). Corrosion resistance and mechanism of high-entropy alloys: A review. *Materials and Corrosion*, *75*(4), 424-432.
10. Lin, S., Yao, Y., Yao, Z., Liu, Y., Liu, Y., Zhang, P., ... & Wu, X. (2023). Construction of FeCrVTiMoX high-entropy alloys with enhanced mechanical properties based on electronegativity difference regulation strategy. *Journal of Alloys and Compounds*, *957*, 170431.
11. Luan, H. W., Shao, Y., Li, J. F., Mao, W. L., Han, Z. D., Shao, C., & Yao, K. F. (2020). Phase stabilities of high entropy alloys. *Scripta Materialia*, *179*, 40-44.
12. Odetola, P. I., Babalola, B. J., Afolabi, A. E., Anamu, U. S., Olorundaisi, E., Umba, M. C., ... & Olubambi, P. A. (2024). Exploring high entropy alloys: A review on thermodynamic design and computational modeling strategies for advanced materials applications. *Heliyon*, *10*(22).
13. Precker, C. E., Gregores Coto, A., & Muíños Landín, S. (2021). Materials for Design Open Repository. High Entropy Alloys (Version 0) [Data set]. Zenodo. https://doi.org/10.5281/zenodo.5155150
14. Ren, J. T., Chen, L., Wang, H. Y., & Yuan, Z. Y. (2023). High-entropy alloys in electrocatalysis: from fundamentals to applications. *Chemical Society Reviews*, *52*(23), 8319-8373.
15. Shuai, L. I., Jia, Y. A. N. G., Shu, L. I., & Dong-rong, L. I. U. (2025). Phase classification of high entropy alloys with composition, common physical, elemental-property descriptors and periodic table representation. *Transactions of Nonferrous Metals Society of China*, *35*(6), 1855-1874.
16. Syarif, J., Elbeltagy, M. B., & Nassif, A. B. (2023). A machine learning framework for discovering high entropy alloys phase formation drivers. *Heliyon*, *9*(1).
17. Thampiriyanon, J., & Khumkoa, S. (2025). Machine learning–based prediction of complex combination phases in high-entropy alloys. *Metals*, *15*(3), 227.
18. Ye, Z., Li, C., & Gu, J. (2022). Phase Stability in High-Entropy Alloys: The Role of Configurational Entropy: Ye, Li, and Gu. *Jom*, *74*(11), 4154-4161.
19. Zhang, W. T., Wang, X. Q., Zhang, F. Q., Cui, X. Y., Fan, B. B., Guo, J. M., ... & Lan, S. (2024). Frontiers in high entropy alloys and high entropy functional materials. *Rare Metals*, *43*(10), 4639-4776.
20. Zhang, Y., Wen, C., Wang, C., Antonov, S., Xue, D., Bai, Y., & Su, Y. (2020). Phase prediction in high entropy alloys with a rational selection of materials descriptors and machine learning models. *Acta Materialia*, *185*, 528-539.
21. Zheng, Y., Qiu, X., Li, H., Qu, K., Yan, H., & Li, R. (2025). Machine-Learning-Driven Prediction of Formation Energy and Compositional Design for IrRuRhMoW High-Entropy Alloys. *Langmuir*, *41*(32), 21846-21858.