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Data-driven study of the enthalpy of mixing in the liquid phase

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ABSTRACT

The enthalpy of mixing in the liquid phase is a thermodynamic property reflecting interactions between elements that is key to predict phase transformations. Widely used models exist to predict it, but they have never been systematically evaluated. To address this, we collect a large amount of enthalpy of mixing data in binary liquids from a review of about 1000 thermodynamic evaluations. This allows us to clarify the prediction accuracy of Miedema's model which is state-of-the-art. We show that more accurate predictions can be obtained from a machine learning model based on LightGBM, and we provide them in 2415 binary systems. The data we collect also allows us to evaluate another empirical model to predict the excess heat capacity that we apply to 2211 binary liquids. We then extend the data collection to ternary metallic liquids and find that, when mixing is exothermic, extrapolations from the binary systems by Muggianu's model systematically lead to slight overestimations of roughly 10 % close to the equimolar composition. Therefore, our LightGBM model can provide reasonable estimates for ternary alloys and, by extension, for multicomponent alloys. Our findings extracted from rich datasets can be used to feed thermodynamic, empirical and machine learning models for material development. Our data, predictions, and code to generate machine learning descriptors from thermodynamic properties are all made available.

1. Introduction

The enthalpy of mixing provides basic information on the nature, attractive or repulsive, of the interactions between elements in solutions. Therefore, it provides important information for understanding chemical-related issues in materials, such as the glass-forming ability of metallic glasses [1]. Moreover, it is an essential property for predicting phase transformations in materials. Generally, deep eutectics, solid solutions and compounds are found in systems where mixing in the liquid phase is exothermic, e.g., Au-Sn [2], whereas miscibility gaps form in those where mixing is endothermic, e.g., Ag-Ni [3]. The enthalpy of mixing in the liquid phase is used to determine the stability of liquids by thermodynamic calculations using the Calphad technique [4], which is

important for the processing and design of a large variety of alloys [5]. In addition, several empirical rules for alloy design are based on this property [6–8]. Besides, the thermodynamic properties of mixing in the liquid phase are important features for machine learning (ML) models to predict phase equilibria such as binary liquidus [5], ternary isothermal sections [9], or phase formation in high-entropy alloys [10–12].

At present, the most reliable way [13] to estimate the enthalpy of mixing in the liquid phase is to use the semi-empirical model established by Miedema *et al.* in 1980 [14]. It is remarkable that no better model has been developed since then. Miedema's model is widely used in ML models for predicting phase equilibria [5,10–12], and sometimes used in Calphad models in systems where experimental data is not available [15,16]. However, since it has never been systematically evaluated, the

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accuracy that can be expected from it is not well known, except for binary systems of magnesium [17].

In multicomponent liquids, data are scarce. Therefore, in ML [5, 10–12], empirical [6–8] and high-throughput [18,19] approaches, their enthalpy of mixing is extrapolated from the binary systems. This can be done by different geometric models [20], but the most widely used is the one proposed by Muggianu *et al.* [21] because of its simplicity. Again, the accuracy of this extrapolation has never been systematically studied.

In recent studies [18,19], the enthalpy of mixing in solid solutions was studied through high-throughput density functional theory calculations. It was approximated in binary systems from a single calculation performed at the equimolar composition. The underlying assumption is that the enthalpy of mixing is symmetrical with respect to composition and reaches its extremum at the equimolar composition. This introduces an error of unknown magnitude.

High-throughput *ab initio* approaches are currently not available to study the enthalpy of mixing of liquids. ML approaches represent an unexplored alternative. In a recent study, an ensemble of graph neural networks was developed to predict the zeroth-order parameter of the Redlich-Kister expansion used in Calphad models to describe the enthalpy of mixing in the liquid phase [22]. This study is based on a dataset of 524 Calphad models of different binary systems for which it was not checked whether the parameters are well constrained by experimental measurements. For solid solutions, a model was trained on data from density functional theory calculations to predict the enthalpy of mixing in the body-centered cubic phase for Fe-Cr-based alloys [23]. A neural network was developed to reproduce the enthalpy of mixing in binary and ternary face-centered cubic solutions obtained from a Calphad commercial database for high entropy alloys [24].

In this work, the enthalpy of mixing in the liquid phase is systematically studied using large datasets collected from a review of about 1000 thermodynamic Calphad assessments. First, we evaluate Miedema's model, and we develop a machine learning model that performs better. Second, we evaluate the performance of Witusiewicz and Sommer's empirical model [25] for predicting the temperature dependence of the enthalpy of mixing, i.e., the excess heat capacity. Third, we evaluate how accurately the enthalpy of mixing of ternary metallic liquids can be extrapolated from their binary subsystems by Muggianu's model. An overview of this work is presented in Fig. 1.

2. Methods

2.1. Datasets

About 1000 Calphad-type thermodynamic evaluations of binary systems were reviewed, and enthalpy of mixing data were collected in 375 binary systems from Refs. [2,3,26–335] in composition domains where the models are supported by experimental measurements with steps of 1 at%. 94 % of these data are supported by direct calorimetric measurements. The remaining 6 % are supported by activity or chemical potential data at different temperatures separated by at least 350 K (the contribution from the configurational entropy is then more than 2 kJ/mol), or data on both the liquidus and the thermodynamic properties of the solid phases involved. Calphad model parameters were retrieved from various sources: mainly NIMS CPDDB [336] and compilations by the authors, but also TDBDB [337], NUCLEA [132], and publications. When the liquid phase was described using a substitutional solution model, the enthalpy of mixing was calculated directly from the Redlich-Kister coefficients. For cases involving an associate or ionic model, the Pandat software [338] was used. When the enthalpy of mixing is temperature dependent, it is calculated at the composition-weighted average melting point of the elements.

Excess heat capacity data were obtained from measurements of the enthalpy of mixing at different temperatures that were digitized from figures found in publications. Data were collected in 43 binary systems for which it was found that a clear and consistent trend emerged from the experimental data. They were collected from Refs. [2,26–60, 339–344] at the composition where the enthalpy of mixing is at its maximum in absolute value, or at the closest composition where experimental data are available.

Data on ternary liquids were collected from Refs. [26–29,61–68, 345–383] in which a substitutional solution model is proposed based on experimental data covering a large part of a ternary system.

2.2. Miedema's model and descriptors

Miedema's theory is presented in detail elsewhere [14,384,385]. The equations of the model and the origin of the parameters used in this work are given in the appendix.

58 descriptors are obtained from composition-weighted mean and

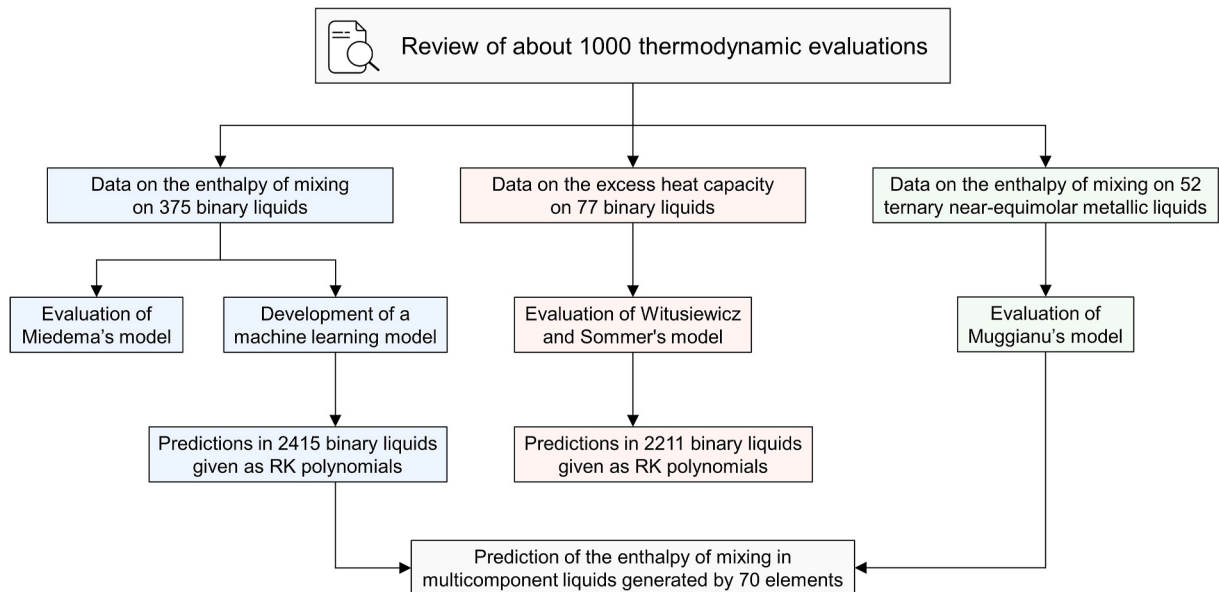


Fig. 1. Overview of this work on the prediction of the enthalpy of mixing in the liquid. RK stands for Redlich-Kister. Our datasets and predictions are made available as detailed in “Data availability.”

average deviation of the properties of the pure elements. They are listed in Table S1. The melting and thermodynamic properties of the pure elements are obtained from the SGTE unary database [386] in its 5.0 version, and other properties are calculated from magpie [387] using matminer [388].

2.3. Machine learning methods

Three algorithms are used: LightGBM [389], a gradient boosting decision tree, Gaussian process (GP) implemented using PHYSBO [390], and artificial neural network (ANN) with two to three hidden layers comprising 10 to 1200 nodes implemented using TensorFlow [391]. For LightGBM and ANN, the target variable is the error of Miedema's model from which the enthalpy of mixing is recalculated, and for GP it is the enthalpy of mixing directly and Miedema's model is used as a descriptor, since this leads to better results.

First, feature selection is performed based on a 5-fold group cross-validation (CV), with data for a binary system forming a group that cannot be split between the training and validation sets. For LightGBM and ANN, a preliminary hyperparameter tuning is performed using Optuna [392]. For LightGBM, recursive feature elimination is performed: starting from all 58 descriptors, the least important feature is dropped. This is repeated until only two features remain. For ANN and GP, sequential feature selection is performed: starting from a single-descriptor model, descriptors are tested one by one, and the one that leads to the model with the smaller RMSE is selected. This is repeated until a model based on all 58 or 59 descriptors is obtained for ANN or GP, respectively. This method requires a relatively high computation time, which is why feature selection was carried out as a first step on the whole dataset. The set of features that minimizes the RMSE is selected.

Second, a nested CV is performed as schematized in Fig. S3 of Ref. [5]. The advantage of this approach is that model performance is evaluated over the entire dataset. For LightGBM and ANN, a 5-fold group CV is performed in the inner loop to determine the best hyperparameters using Optuna [392]. A 12-fold group CV is performed in the outer loop to evaluate model performance.

2.4. Redlich-Kister substitutional solution model

For each binary system, the enthalpy of mixing is calculated at every at% from the value predicted by Miedema's model and the error on this value predicted by machine learning. Then, it is fitted by a Redlich-Kister polynomial:

$$H_{mix}^{liq} = x_A x_B \sum_v a_{A,B} (x_A - x_B)^v \quad (1)$$

with H_{mix}^{liq} the enthalpy of mixing in the A-B binary liquid phase, x_A and x_B the atomic fraction of A and B, and $a_{A,B}$ the parameter of order v . Starting from the order 0, additional parameters are iteratively added up to the order 3 if the RMSE between the predicted and the fitted enthalpy of mixing is higher than 0.5 kJ/mol. In systems where the maximum absolute value of the enthalpy of mixing is predicted to be less than 10 kJ/mol, no more than two parameters of order 0 and 1 are used to avoid overfitting.

In a multicomponent liquid composed of n elements, the binary contributions to the enthalpy of mixing can be calculated using Muggianu's model [21] by summing Eq. (1) over all binaries without weighting compositions:

$$H_{mix}^{bin, liq} = \sum_{i=1}^{n-1} \sum_{j=i+1}^n x_i x_j \sum_v a_{i,j}^v (x_i - x_j)^v \quad (2)$$

The excess heat capacity predicted by Witusiewicz and Sommer's model [25] using our LightGBM/RK model, melting points from the SGTE unary database [386], a temperature set to the

composition-weighted average melting point of the elements, and boiling points from magpie [387] as inputs is fitted and can be extrapolated using the same formalism as Eqs. (1) and (2).

3. Results

3.1. Prediction of the enthalpy of mixing in binary liquid phases

Reliable enthalpy of mixing data were collected in 375 binary liquids after a review of about 1000 systems. Data coverage is shown per binary system in Fig. 2, and per element in Fig. S1. In general, our dataset covers many binary systems of base alloy elements such as Al or Mg, low melting point metals such as Ga or Sn, and between elements of groups 10 to 14. In contrast, our dataset contains little information, if any, on binaries of refractory elements such as C or W, and of elements of groups 3 to 6 besides with elements of groups 8 to 14.

First, the performance of the Miedema model was evaluated on our dataset. The relation between the observed and predicted values is shown in Fig. 3, and a mean absolute error (MAE) of 4.2 kJ/mol is obtained. In systems where the enthalpy of mixing is exothermic, it generally gives values that are not sufficiently negative.

Next, we developed an ML model based on LightGBM to predict the enthalpy of mixing. It is based on 30 descriptors selected from the 58 descriptors considered in this work to obtain a better accuracy (Fig. S3). Its performance is evaluated on the entire dataset using a nested cross-validation approach, and the results are shown in Fig. 3. The values predicted by the LightGBM model are slightly noisy (Fig. S2) and fitting by a Redlich-Kister (RK) polynomial smooth them out without any significant impact on performance. The combination of the LightGBM and RK models is referred to as LightGBM/RK. The MAE of this model is of 3.0 kJ/mol in systems for which no data is included in the training set, which is better than that obtained with Miedema's model, while training data are reproduced closely with a training MAE of 0.4 kJ/mol for the final LightGBM/RK model. The mean absolute percentage error (MAPE) is an intuitive metric, but it is only meaningful for large values that are not close to zero. It is evaluated on data greater than 10 kJ/mol in absolute value from 199 binary systems. An error of 22 % is obtained with our LightGBM/RK model in systems where it has seen no data, compared with 34 % for Miedema's model. The LightGBM/RK model performs slightly better than the artificial neural network (ANN) and gaussian process (GP) models (Table 1). The MAE of the LightGBM/RK model is shown per element in Fig. S1. Predictions are relatively inaccurate for group 16 elements. However, the LightGBM/RK model still tends to outperform Miedema's model: its MAE over the 21 binaries of Te in the dataset is of 6.4 kJ/mol compared to 10.4 kJ/mol for Miedema's model. Excluding group 16 elements, the MAE of the LightGBM/RK model decreases to 2.6 kJ/mol.

There are 120 binary systems in our dataset for which the extremum in the enthalpy of mixing is well-defined in the sense that it is greater than 5 kJ/mol in absolute value and that experimental data are available over the whole compositional range. In these systems, the composition of the extremum differs from the equimolar composition by 8.6 at% in average, and by up to 30 at%. Miedema's model generally fails to account for an asymmetry with respect to composition (Fig. 4), with an MAE on the composition of the extremum of 7.4 at% on these 120 systems. While our ML model show some potential to correct this (Fig. 4), this MAE is only reduced to 6.7 at% on these systems when they are not included in the training set.

The enthalpy of mixing is then predicted in all the 2415 binary systems generated by 70 elements using our LightGBM/RK model. The extremum value obtained in each system is shown in Fig. 5. The enthalpy of mixing is predicted from the LightGBM/RK model to be most exothermic in binary systems between an element of groups 2 to 4 with an element of groups 9 to 16. For instance, extremum values of -150 kJ/mol are predicted in carbon - rare earths systems. It is most endothermic in binary systems between an alkali metal and an element of groups 3 to

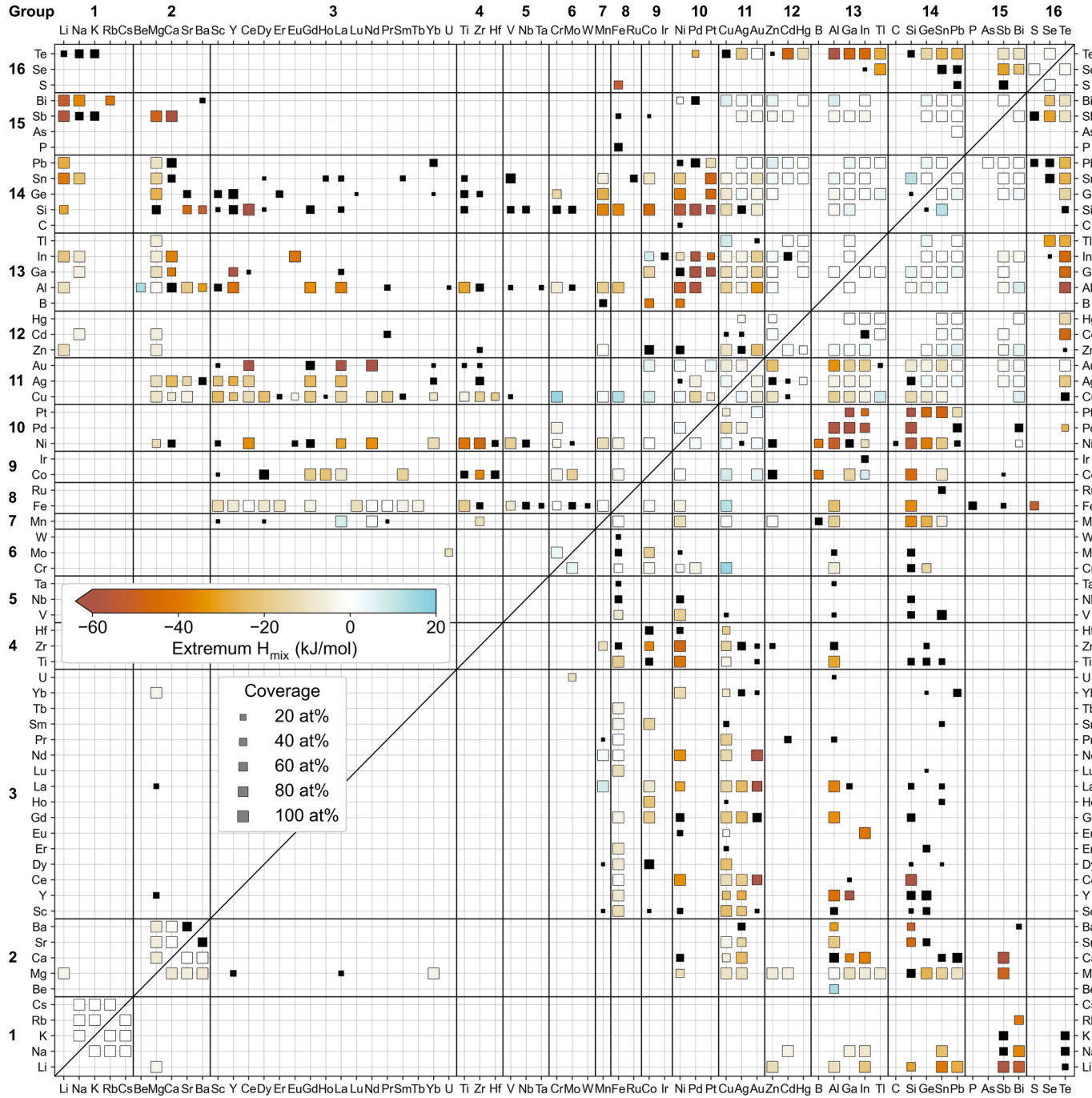


Fig. 2. Overview of our dataset on the enthalpy of mixing in binary liquid phases. For each of the 375 binary systems included, symbol size corresponds to the span of compositions over which reliable data have been found, and symbol color to the extremum value of the enthalpy of mixing. Symbols are black when the extremum is not well-defined.

8. Mg and Be tend to behave more like Au and Zn, which are their neighbors in an ordering by Mendeleev number, than other alkaline-earth metals. In binary systems between two elements of the same group, the enthalpy of mixing tends to be small and no larger than 30 kJ/mol in absolute value.

3.2. Temperature dependence of the enthalpy of mixing in the liquid phase

The excess heat capacity is the temperature derivative of the enthalpy of mixing. It can be predicted from Witusiewicz and Sommer's empirical model [25] whose MAE on experimental data from 77 binary systems is of 3.7 J/K/mol (Fig. 6a). It takes the enthalpy of mixing as

input, and using our LightGBM/RK model predictions can be made with greater accuracy than using Miedema's model, especially in systems included in its training set (Fig. 6b). The results obtained this way in 2016 binary systems suggests that the excess heat capacity and the enthalpy of mixing are strongly correlated (Fig. 6c). As discussed in Ref. [393], they are in most cases of opposite signs, which means that temperature brings liquids closer to ideality. However, experimental evidence is lacking in systems where mixing is endothermic, such as Ag-Pb where measurements suggest an exception to this rule [28]. In 90 % of the binary systems, the extremum value of the enthalpy of mixing is predicted to decrease by 3.5–9.7 % in absolute value over 100 K (Fig. 6c).

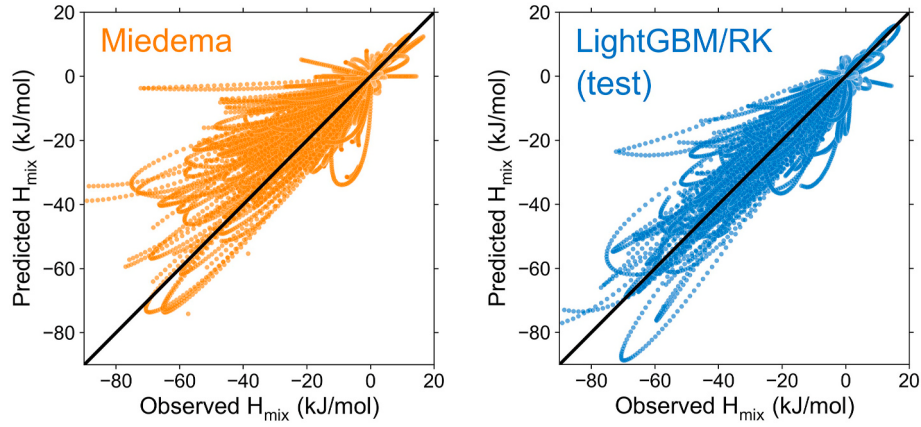


Fig. 3. Scatter plots showing the performance on data from 375 binaries of Miedema's model [14] and of our ML model (in test) after fitting by a Redlich-Kister substitutional solution model. The diagonal line represents perfect agreement.

Table 1

Performance metrics obtained on data from 375 binary systems for different models for predicting the enthalpy of mixing in binary liquids. RMSE stands for root mean squared error.

Model	MAE (kJ/mol)	RMSE (kJ/mol)
Miedema's model	4.2	7.5
LightGBM/RK (on test)	3.0	4.9
ANN (on test)	3.2	5.2
GP (on test)	3.3	5.1

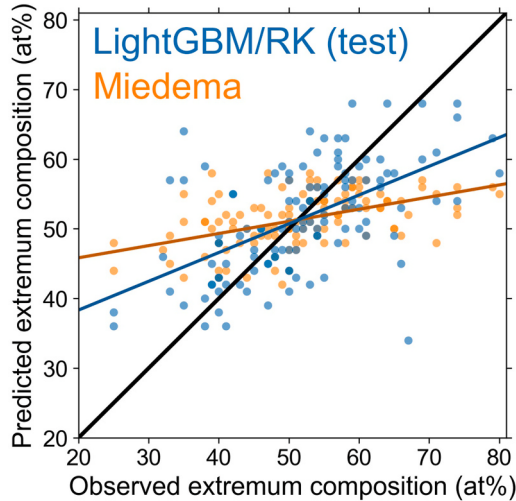


Fig. 4. Performance of Miedema's model and our ML model (on test) for predicting the composition of the extremum n data from 120 binaries for which the extremum is well-defined. Linear regression lines are plotted to guide the eye.

3.3. Extrapolation from the binary systems in ternary metallic liquids

In multicomponent liquids, the main contribution to the enthalpy of mixing comes from the binary contributions. The extent of higher-order contributions has never been studied systematically. To address this, we collected experimental data on 52 ternary metallic liquids close to the equimolar composition. We find that the enthalpy of mixing extrapolated from the binary systems by Muggianu's model [21] is reasonable, with an MAE of 1.6 kJ/mol. In liquids where mixing is exothermic, the extrapolations are systematically too negative (Fig. 7). The overestimation is of the order of 10 % (Fig. S5). In liquids where mixing is endothermic, more data is necessary to draw conclusions.

4. Discussion

We developed an ML model to predict the enthalpy of mixing in binary liquid phases. It is significantly more reliable than Miedema's model [14]. The prediction results obtained in all the 2415 binary systems generated by 70 elements are fitted by a substitutional solution model whose parameters are provided. From these parameters, the main contribution to the enthalpy of mixing can be easily calculated in multicomponent liquids using Eq. (2) or the open-access notebook linked in the Data availability section. In ML models for alloys, the enthalpy of mixing in the liquid phase is an important descriptor not only for predicting phase equilibria [5,9–12], but also properties of the alloys such as the Young's modulus [394] or the Vickers hardness [395]. Our ML model is used as an input to Witusiewicz and Sommer's model [25] to predict the excess heat capacity in 2016 binary liquids. Data on the excess heat capacity are scarce, so in thermodynamic evaluations it is common practice to set it to zero and to adjust the excess entropy to model the temperature dependence of the Gibbs energy. Instead, relying on the reasonable excess heat capacity estimates provided here should in most cases lead to a better description of the entropy and of the interactions at high temperature. Therefore, our predictions can be used as an input to thermodynamic, empirical and ML models for the development of a variety of materials.

We took a data-driven approach to evaluate different sources of error in estimation of the enthalpy of mixing in binary and multicomponent liquids: model error to predict its binary contributions, neglecting its temperature dependence, and neglecting its ternary contributions. The same type of approach should be applied to solid solutions, but similar deviations may be expected. The uncertainty from measurements or calculations is difficult to evaluate systematically and is not discussed. Our findings can be summarized as follows. First, the enthalpy of mixing predicted by Miedema's model in binary liquids where mixing is exothermic is in most cases not sufficiently negative. This is not the case with our LightGBM/RK model for which an MAE of 3.0 kJ/mol, or an MAPE of 22 %, can be expected in systems not included in its training set. However, its accuracy in predicting the composition of the extremum remains limited in systems for which no data is included in the training set, with an MAE of 6.7 at% obtained over 120 binaries. Second, neglecting the temperature dependence of the enthalpy of mixing can lead to an error of roughly 5 % per 100 K on the extremum value (Fig. 6c). Third, in metallic liquids where mixing is exothermic, close to ternary equimolar compositions, the enthalpy of mixing extrapolated from the binary systems by Muggianu's model is systematically overestimated, i.e., too negative, by roughly 10 %. The same is observed for the faced-centered cubic phase of the Co-Cr-Fe-Mn-Ni system [396], which strengthens this observation and suggests that it

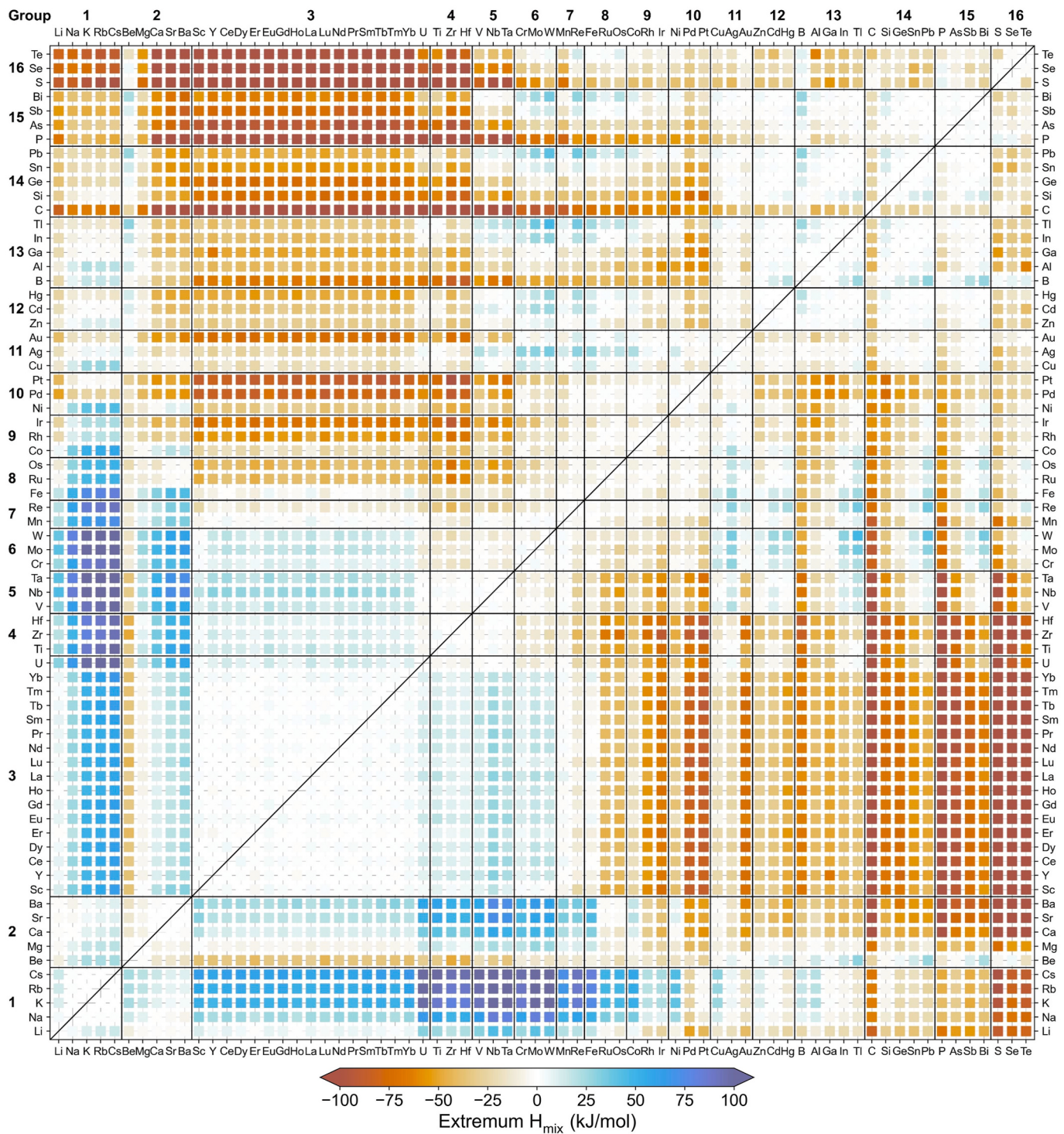


Fig. 5. Extremum value of the enthalpy of mixing in the liquid phase predicted using the LightGBM/RK model over all the 2415 binary systems generated by 70 elements.

may also holds for solid solutions. It is concluded that none of these errors is negligible, but when estimating the enthalpy of mixing of complex concentrated alloy, the prediction of its binary contributions remains the most important source of error.

The quality of our results depends on that of our datasets. They were obtained from Calphad assessments whose reliability was critically evaluated on a case-by-case basis. The advantages of this approach were discussed in Ref. [5]. It enabled us to collect an unprecedentedly large amount of data supported by direct and indirect measurements. Our

dataset on the enthalpy of mixing in binary liquids is centered on metals (Fig. 2). The LightGBM/RK model performs relatively poorly on group 16 elements. On test, this can be explained by the fact they tend to form complex liquids with strong short-range ordering that are underrepresented in the dataset. Their enthalpy of mixing has a characteristic V-shape, but an enthalpy with a U-shape is predicted as in metallic liquids (Fig. S2). On training, the problem comes from the use of a substitutional solution model (Eq. (1)) that is not well suited for these liquids. In immiscible systems where the enthalpy of mixing is

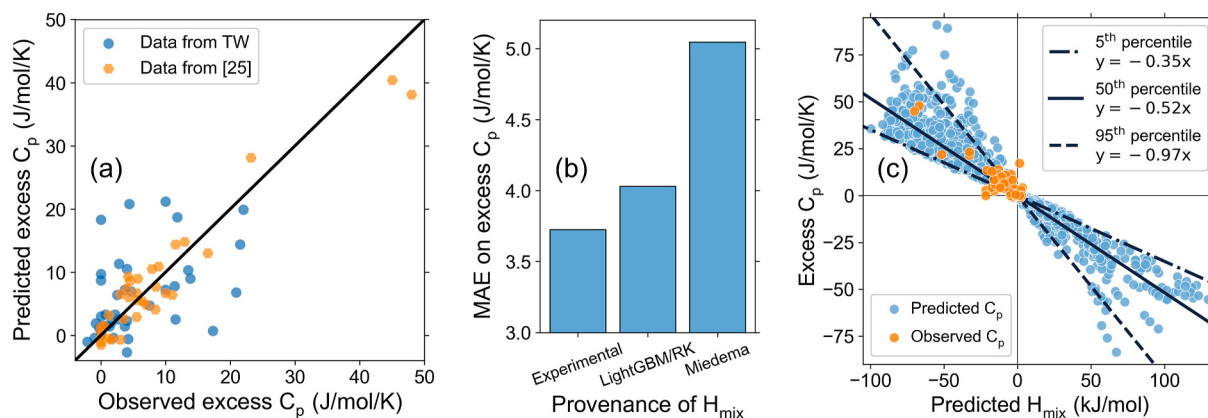


Fig. 6. Performances over data on 77 binary liquids of Witusiewicz and Sommer's model [25] using (a) experimental and (b) experimental or predicted values for the input enthalpy of mixing. (c) Relationship between the excess heat capacity and the enthalpy of mixing over 2016 binary liquids generated by 64 elements of groups 1 to 15 at the composition where the enthalpy of mixing reaches its extremum. Excess heat capacity predictions for As, C and P are abnormal due to their boiling points being lower than their melting points and are not plotted. Percentile regression lines are obtained from absolute values.

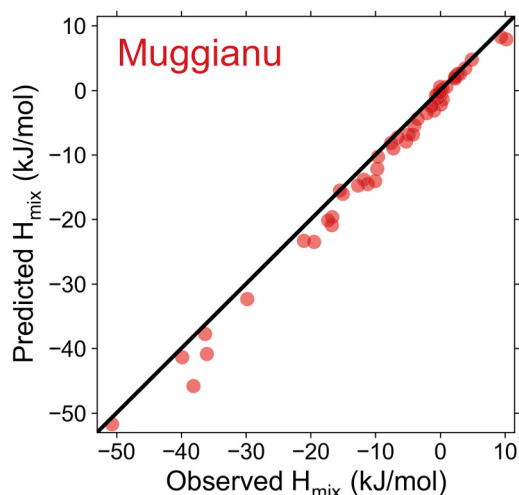


Fig. 7. Scatter plot showing the enthalpy of mixing extrapolated from the binary systems by Muggianu's model [21] against experimental data on 52 ternary near-equi-molar metallic liquids.

endothermic, measurements are difficult [3], and the model is only supported by a limited number of data all below 20 kJ/mol (Fig. 3). Our data on the enthalpy of mixing in binary liquids are within or close to experimental uncertainty. However, our data on the ternary contributions to the enthalpy of mixing are less reliable because they depend on the choice made regarding binary contributions. For example, in the Ag-Ga-Sn system, the maximum ternary contributions can vary from +4.8 to +2 kJ/mol on the basis of the same experimental data but a different description of the Ag-Ga binary [360,397]. Besides, data on the excess heat capacity are also less reliable since they are derived from two experimental data at different temperatures.

Model training time may be reduced without significantly decreasing performance by selecting a composition step higher than 1 at%. Model performance will be more sensitive to step size in systems where the enthalpy of mixing has a V-shape than a U-shape. Model training speed and interpretability can also be improved by using less features. Our LightGBM model is based on a set of 30 features to maximize accuracy, but comparable performance can be achieved with sets of 20–58 features (Fig. S3). A Pearson's correlation analysis between these 30 features and the error of Miedema's model as well as the enthalpy of mixing is shown in Fig. S4. There is a positive correlation between the enthalpy of mixing and the error of Miedema's model because it generally gives values that

not sufficiently negative (Fig. 3). Our features derived from the thermodynamic properties of the elements before and after melting are important for predicting the enthalpy of mixing in the liquid and to correct Miedema's model (Table S1), particularly for our LightGBM model for which they represent 7 of the 10 most important features (Fig. S4). In a future work, we plan to develop a more interpretable model with better performance based on an improved dataset.

Data availability

Our datasets on the excess heat capacity and on the enthalpy of mixing in ternary liquids are shared as supplementary materials. Our dataset on the enthalpy of mixing in binary liquids is shared in an open access data repository [398]. The parameters of our LightGBM/RK model obtained in the 2415 binary systems generated by 70 elements are shared as supplementary materials and in the same data repository. The binary contributions to the enthalpy of mixing in the liquid phase can be calculated in J/mol from these using Eqs. (1) and (2). The parameters to calculate the excess heat capacity in J/mol/K in 2211 binary liquids generated by 67 elements based on Witusiewicz and Sommer's model [25] are shared as supplementary materials. Descriptors for machine learning studies of alloys can be easily generated from our models and from the thermodynamic properties of pure elements using the open-access notebook at <https://colab.research.google.com/drive/1XRqgvP11JuU8pxHqlpkZQChAJ5tvLdVW>.

CRediT authorship contribution statement

Guillaume Deffrennes: Writing – original draft, Visualization, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. **Bengt Hallstedt:** Writing – review & editing, Methodology, Data curation, Resources. **Taichi Abe:** Writing – review & editing, Data curation, Resources. **Quentin Bizot:** Writing – review & editing, Formal analysis. **Evelyn Fischer:** Writing – review & editing, Data curation, Resources. **Jean-Marc Joubert:** Writing – review & editing, Visualization, Methodology. **Kei Terayama:** Writing – review & editing, Methodology. **Ryo Tamura:** Writing – original draft, Visualization, Methodology, Funding acquisition, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Our data, predictions, and code to generate machine learning descriptors from thermodynamic properties are all made available as detailed in “Data availability.”

[Dataset on the enthalpy of mixing in binary liquids \(Original data\) \(Mendeley Data\)](#)

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Appendix A. Supplementary data

Supplementary data to this article can be found online at <https://doi.org/10.1016/j.calphad.2024.102745>.

Appendix. Prediction of the enthalpy of mixing in the liquid phase using Miedema’s model

The enthalpy of mixing in a binary A-B liquid is predicted by Miedema’s model by following steps S1 to S5:

$$c_B^s = \frac{x_B V_B^{2/3}}{x_A V_A^{2/3} + x_B V_B^{2/3}} \quad (S1)$$

with x_B , V_B and c_B^s the molar fraction, molar volume, and surface fraction of B.

$$\left(V_A^{2/3}\right)_{\text{alloy}} = V_A^{2/3} \left(1 + a_A c_B^s (\varphi_A - \varphi_B)\right) \quad (S2)$$

with a_A a parameter for A, φ_B the so-called work function of B, and $\left(V_A^{2/3}\right)_{\text{alloy}}$ the molar volume of A accounting for changes upon alloying.

$$\left(c_B^s\right)_{\text{alloy}} = \frac{x_B \left(V_B^{2/3}\right)_{\text{alloy}}}{x_A \left(V_A^{2/3}\right)_{\text{alloy}} + x_B \left(V_B^{2/3}\right)_{\text{alloy}}} \quad (S3)$$

with $\left(c_B^s\right)_{\text{alloy}}$ the surface fraction of B corrected as recommended in Ref. [399].

$$H_{\text{inter}}(\text{A in B}) = \frac{\left(V_A^{2/3}\right)_{\text{alloy}} \left(-P(\varphi_A - \varphi_B)^2 + Q\left(n_{\text{wsA}}^{1/3} - n_{\text{wsB}}^{1/3}\right)^2 + 0.73R_A R_B\right)}{\frac{1}{2} \left(\frac{1}{n_{\text{wsA}}^{1/3}} + \frac{1}{n_{\text{wsB}}^{1/3}}\right)} \quad (S4)$$

$H_{\text{inter}}(\text{A in B})$ is the interfacial enthalpy of solving 1 mol of A in B obtained for the liquid phase. P is a parameter equal to 14.2, 12.35 or 10.7 [385] for alloys of two transition metals, a transition metal with a non-transition metal, and two non-transition metals, respectively. Fig. 33 of Ref. [14] details which elements are considered transition metals and which are not. n_{wsA} is the averaged electron density at the boundary of the Wigner-Seitz cell of A. R is another parameter, and 0.73 is a reducing factor used for the liquid phase. The ratio of Q over P equals 9.4.

The enthalpy of mixing in the A-B liquid, H_{mix} , is finally obtained in step 5:

$$H_{\text{mix}} = c_A c_B^s H_{\text{inter}}(\text{A in B}) \quad (S5)$$

For elements of group 1 to 15, parameter values are taken from matminer [388] and checked against Refs. [14,384]. The R parameter for Ag is corrected from 0.3 to 0.15, and the a parameter for Eu and Yb are corrected from 0.1 to 0.07, which is the recommended value for trivalent metals [14]. For elements of group 16, parameter values are taken from Ref. [400]. The model is not straightforward to use. We have verified for a few systems that the values obtained in this work were the same as those obtained in Ref. [399]. Significantly different results can be obtained with other calculators proposed in the literature due to errors in parameters or possibly equations.

References

- [1] H.B. Yu, K. Samwer, W.H. Wang, H.Y. Bai, Chemical influence on β -relaxations and the formation of molecule-like metallic glasses, *Nat. Commun.* 4 (2013) 2204, <https://doi.org/10.1038/ncomms3204>.
- [2] V. Grolier, R. Schmid-Fetzer, Thermodynamic evaluation of the Au–Sn system, *JMR* 98 (2007) 797–806, <https://doi.org/10.3139/146.101544>.
- [3] X.J. Liu, F. Gao, C.P. Wang, K. Ishida, Thermodynamic assessments of the Ag–Ni binary and Ag–Cu–Ni ternary systems, *J. Electron. Mater.* 37 (2008) 210–217, <https://doi.org/10.1007/s11664-007-0315-1>.
- [4] H.L. Lukas, S.G. Fries, B. Sundman, *Computational Thermodynamics: the CALPHAD Method*, Cambridge University Press, Cambridge ; New York, 2007.
- [5] G. Deffrennes, K. Terayama, T. Abe, E. Ogamino, R. Tamura, A framework to predict binary liquidus by combining machine learning and CALPHAD

- assessments, *Mater. Des.* 232 (2023) 112111, <https://doi.org/10.1016/j.matdes.2023.112111>.
- [6] A. Takeuchi, A. Inoue, Classification of bulk metallic glasses by atomic size difference, heat of mixing and period of constituent elements and its application to characterization of the main alloying element, *Mater. Trans.* 46 (2005) 2817–2829, <https://doi.org/10.2320/matertrans.46.2817>.
 - [7] Y. Zhang, Y.J. Zhou, J.P. Lin, G.L. Chen, P.K. Liaw, Solid-solution phase formation rules for multi-component alloys, *Adv. Eng. Mater.* 10 (2008) 534–538, <https://doi.org/10.1002/adem.200700240>.
 - [8] Y. Lu, H. Jiang, S. Guo, T. Wang, Z. Cao, T. Li, A new strategy to design eutectic high-entropy alloys using mixing enthalpy, *Intermetallics* 91 (2017) 124–128, <https://doi.org/10.1016/j.intermet.2017.09.001>.
 - [9] G. Deffrennes, K. Terayama, T. Abe, R. Tamura, A machine learning-based classification approach for phase diagram prediction, *Mater. Des.* 215 (2022) 110497, <https://doi.org/10.1016/j.matdes.2022.110497>.
 - [10] Z. Zhou, Y. Zhou, Q. He, Z. Ding, F. Li, Y. Yang, Machine learning guided appraisal and exploration of phase design for high entropy alloys, *npj Comput. Mater.* 5 (2019) 128, <https://doi.org/10.1038/s41524-019-0265-1>.
 - [11] Y. Li, W. Guo, Machine-learning model for predicting phase formations of high-entropy alloys, *Phys. Rev. Mater.* 3 (2019) 095005, <https://doi.org/10.1103/PhysRevMaterials.3.095005>.
 - [12] G.L.W. Hart, T. Mueller, C. Toher, S. Curtarolo, Machine learning for alloys, *Nat. Rev. Mater.* 6 (2021) 730–755, <https://doi.org/10.1038/s41578-021-00340-w>.
 - [13] G. Arzpeyma, A.E. Gheribi, M. Medraj, On the prediction of Gibbs free energy of mixing of binary liquid alloys, *J. Chem. Thermodyn.* 57 (2013) 82–91, <https://doi.org/10.1016/j.jct.2012.07.020>.
 - [14] A.R. Miedema, P.F. De Châtel, F.R. De Boer, Cohesion in alloys — fundamentals of a semi-empirical model, *Phys. B+C* 100 (1980) 1–28, [https://doi.org/10.1016/0378-4363\(80\)90054-6](https://doi.org/10.1016/0378-4363(80)90054-6).
 - [15] S. Li, M.H. Rong, L. Xu, Q. Wei, J. Wang, G.H. Rao, H.Y. Zhou, Thermodynamic assessment of the RE-B (RE = Ce, Dy, Lu) binary systems, *Calphad* 68 (2020) 101740, <https://doi.org/10.1016/j.calphad.2020.101740>.
 - [16] M. Ait Boukideur, N. Selhaoui, F.Z. Chriifi Alaoui, D.O. Poletaev, H. Bouchta, K. Achgar, A. Aharoune, Thermodynamic assessment of the Ga–Lu system by the combination of ab-initio calculations and the CALPHAD approach, *Calphad* 79 (2022) 102464, <https://doi.org/10.1016/j.calphad.2022.102464>.
 - [17] R. Boom, F.R. De Boer, Enthalpy of formation of binary solid and liquid Mg alloys – comparison of Miedema-model calculations with data reported in literature, *Calphad* 68 (2020) 101647, <https://doi.org/10.1016/j.calphad.2019.101647>.
 - [18] W. Chen, A. Hilhorst, G. Bokas, S. Gorsse, P.J. Jacques, G. Hautier, A map of single-phase high-entropy alloys, *Nat. Commun.* 14 (2023) 2856, <https://doi.org/10.1038/s41467-023-38423-7>.
 - [19] Z. Zhang, M. Li, J. Cavin, C. Flores, R. Mishra, A fast and robust method for predicting the phase stability of refractory complex concentrated alloys using pairwise mixing enthalpy, *Acta Mater.* 241 (2022) 118389, <https://doi.org/10.1016/j.actamat.2022.118389>.
 - [20] P. Chartrand, A.D. Pelton, On the choice of “Geometric” thermodynamic models, *JPE* 21 (2000) 141–147, <https://doi.org/10.1361/105497100770340192>.
 - [21] Y.-M. Muggianu, M. Gambino, J.-P. Bros, Enthalpies de formation des alliages liquides bismuth-étain-gallium à 723 K. Choix d’une représentation analytique des grandeurs d’excès intégrales et partielles de mélange, *J. Chim. Phys.* 72 (1975) 83–88, <https://doi.org/10.1051/jcp/1975720083>.
 - [22] Q.-J. Hong, Deep learning for CALPHAD modeling: universal parameter learning solely based on chemical formula, *arXiv:2307.04283* (2023), <https://doi.org/10.48550/arXiv.2307.04283> [Cond-Mat.Mtrl-Sci].
 - [23] B.O. Mukhamedov, K.V. Karavaev, I.A. Abrikosov, Machine learning prediction of thermodynamic and mechanical properties of multicomponent Fe-Cr-based alloys, *Phys. Rev. Mater.* 5 (2021) 104407, <https://doi.org/10.1103/PhysRevMaterials.5.104407>.
 - [24] P. Laiu, Y. Yang, M. Lupo Pasini, J.Y. Choi, D. Shin, A neural network approach to predict Gibbs free energy of ternary solid solutions, *JPED* 43 (2022) 916–930, <https://doi.org/10.1007/s11669-022-01010-2>.
 - [25] V.T. Witusiewicz, F. Sommer, Estimation of the excess entropy of mixing and the excess heat capacity of liquid alloys, *J. Alloys Compd.* 312 (2000) 228–237, [https://doi.org/10.1016/S0925-8388\(00\)01158-0](https://doi.org/10.1016/S0925-8388(00)01158-0).
 - [26] W. Gierlotka, Y.-C. Tung, A new thermodynamic description of the Bi-Pb-Sn system, *J. Phase Equilib. Diffus.* 38 (2017) 814–828, <https://doi.org/10.1007/s11669-017-0572-5>.
 - [27] C.-S. Oh, J.-H. Shim, B.-J. Lee, Dong Nyung Lee, A thermodynamic study on the Ag-Sb-Sn system, *Journal of Alloys and Compounds* 238 (1996) 155–166, [https://doi.org/10.1016/0925-8388\(95\)02191-4](https://doi.org/10.1016/0925-8388(95)02191-4).
 - [28] S. Hassam, D. Boa, P. Benigni, J. Rogez, Critical assessment and optimization of the Ag-Au-Pb system, *Thermochim. Acta* 510 (2010) 37–45, <https://doi.org/10.1016/j.tca.2010.06.020>.
 - [29] A. Maitre, J.M. Fiorani, M. Vilasi, Thermodynamic study of phase equilibria in the Pb-Bi-Hg system, *JPE* 23 (2002) 329–338, <https://doi.org/10.1361/105497102770331578>.
 - [30] B.C. Rugg, T.G. Chart, A critical assessment of thermodynamic and phase diagram data for the gallium-indium system, *Calphad* 14 (1990) 115–123, [https://doi.org/10.1016/0364-5916\(90\)90013-P](https://doi.org/10.1016/0364-5916(90)90013-P).
 - [31] M. Jiang, J. Sato, I. Ohnuma, R. Kainuma, K. Ishida, A thermodynamic assessment of the Co-Sn system, *Calphad* 28 (2004) 213–220, <https://doi.org/10.1016/j.calphad.2004.08.001>.
 - [32] J.-B. Li, L.N. Ji, J.K. Liang, Y. Zhang, J. Luo, C.R. Li, G.H. Rao, A thermodynamic assessment of the copper-gallium system, *Calphad* 32 (2008) 447–453, <https://doi.org/10.1016/j.calphad.2008.03.006>.
 - [33] Z.H. Long, X.M. Tao, H.S. Liu, Z.P. Jin, First-Principle calculation assisted thermodynamic assessment of the Pt-Pb system, *J. Phase Equilib. Diffus.* 30 (2009) 318–322, <https://doi.org/10.1007/s11669-009-9530-1>.
 - [34] X. Zhou, F. Zhang, S. Liu, Y. Du, B. Jin, Phase equilibria and thermodynamic investigation of the In-Li system, *Calphad* 70 (2020) 101779, <https://doi.org/10.1016/j.calphad.2020.101779>.
 - [35] D. Li, P. Franke, S. Fürtauer, D. Cupid, H. Flandorfer, The Cu-Sn phase diagram part II: new thermodynamic assessment, *Intermetallics* 34 (2013) 148–158, <https://doi.org/10.1016/j.intermet.2012.10.010>.
 - [36] T.J. Anderson, I. Ansara, The Ga-Sn (gallium-tin) system, *JPE* 13 (1992) 181–189, <https://doi.org/10.1007/BF02667485>.
 - [37] F. Islam, M. Medraj, The phase equilibria in the Mg-Ni-Ca system, *Calphad* 29 (2005) 289–302, <https://doi.org/10.1016/j.calphad.2005.08.006>.
 - [38] O. Fikar, J. Vřešál, A. Kroupa, S. Chen, The study of the Pb-Se-Te phase diagram: Part 2 – the thermodynamic assessment of the Se-Te and Pb-Se-Te systems, *Calphad* 74 (2021) 102309, <https://doi.org/10.1016/j.calphad.2021.102309>.
 - [39] D. Li, S. Fürtauer, H. Flandorfer, D.M. Cupid, Thermodynamic assessment and experimental investigation of the Li-Sn system, *Calphad* 47 (2014) 181–195, <https://doi.org/10.1016/j.calphad.2014.09.002>.
 - [40] L. Dreval, M. Zschornak, W. Münchgesang, O. Fabricnaya, D. Rafaja, M. L. Martine, L. Giebler, M. Motylenko, Thermodynamic assessment and first principle calculations of the Na Sb Sn system, *Journal of Alloys and Compounds* 695 (2017) 1725–1742, <https://doi.org/10.1016/j.jallcom.2016.11.003>.
 - [41] I. Ansara, N. Dupin, H.L. Lukas, B. Sundman, Thermodynamic assessment of the Al-Ni system, *Journal of Alloys and Compounds* 247 (1997) 20–30, [https://doi.org/10.1016/S0925-8388\(96\)02652-7](https://doi.org/10.1016/S0925-8388(96)02652-7).
 - [42] J. Wang, H.S. Liu, Z.P. Jin, Thermodynamic assessment of the Au-Pb system, *Calphad* 28 (2004) 91–95, <https://doi.org/10.1016/j.calphad.2004.05.003>.
 - [43] A. Qin, R. Wang, Y. Wang, J. Wang, S. Liu, K. Cheng, Y. Du, B. Sundman, Thermodynamic assessment of the Cd-X (X=Sn, Mn, Fe) systems, *Calphad* 47 (2014) 83–91, <https://doi.org/10.1016/j.calphad.2014.06.006>.
 - [44] H.S. Liu, Y. Cui, K. Ishida, X.J. Liu, C.P. Wang, I. Ohnuma, R. Kainuma, Z.P. Jin, Thermodynamic assessment of the Cu-In binary system, *JPE* 23 (2002) 409–415, <https://doi.org/10.1361/105497102770331352>.
 - [45] W. Gierlotka, J. Sopousek, K. Fitzner, Thermodynamic assessment of the Hg-Tl system, *Calphad* 30 (2006) 425–430, <https://doi.org/10.1016/j.calphad.2006.07.006>.
 - [46] F. Zhang, Y. Tang, B. Hu, S. Liu, Y. Du, Y. Zhang, Thermodynamic assessment of the Mg-Pb and Mg-Bi systems using substitutional solution and associate models for the liquid phase, *J. Min Metall B Metall* 50 (2014) 115–126, <https://doi.org/10.2298/JMMB130824017Z>.
 - [47] C.-S. Oh, D.N. Lee, Thermodynamic assessments of the In-Te and Al-Te systems, *Calphad* 17 (1993) 175–187, [https://doi.org/10.1016/0364-5916\(93\)90018-7](https://doi.org/10.1016/0364-5916(93)90018-7).
 - [48] W. Gierlotka, D. Jendrzeczyk-Handzik, Thermodynamic description of the binary Ag-Ga system, *Journal of Alloys and Compounds* 509 (2011) 38–42, <https://doi.org/10.1016/j.jallcom.2010.08.136>.
 - [49] A. Berche, E. Ruiz-Théron, J.-C. Tedenac, R.-M. Ayrat, F. Rouessac, P. Jund, Thermodynamic description of the Mn-Si system: an experimental and theoretical work, *Journal of Alloys and Compounds* 615 (2014) 693–702, <https://doi.org/10.1016/j.jallcom.2014.06.202>.
 - [50] A. Schlieper, Y. Feutelaïs, S.G. Fries, B. Legendre, R. Blachnik, Thermodynamic evaluation of the germanium — tellurium system, *Calphad* 23 (1999) 1–18, [https://doi.org/10.1016/S0364-5916\(99\)00012-7](https://doi.org/10.1016/S0364-5916(99)00012-7).
 - [51] J. Wang, C. Leinenbach, M. Roth, Thermodynamic modeling of the Au-Ge-Sn ternary system, *Journal of Alloys and Compounds* 481 (2009) 830–836, <https://doi.org/10.1016/j.jallcom.2009.03.114>.
 - [52] D. Liu, H. Yan, X. Yuan, Y. Chung, Y. Du, H. Xu, L. Liu, P. Nash, Thermodynamic modeling of the Ge-Ti system supported by key experiment, *Thermochimica Acta* 521 (2011) 148–154, <https://doi.org/10.1016/j.tca.2011.04.017>.
 - [53] F.G. Meng, J. Wang, L.B. Liu, Z.P. Jin, Thermodynamic modeling of the Mg-Sn-Zn ternary system, *Journal of Alloys and Compounds* 508 (2010) 570–581, <https://doi.org/10.1016/j.jallcom.2010.08.124>.
 - [54] G. Ghosh, Thermodynamic modeling of the palladium-lead-tin system, *Metall Mater Trans A* 30 (1999) 5–18, <https://doi.org/10.1007/s11661-999-0191-9>.
 - [55] S.G. Fries, I. Ansara, H.L. Lukas, Thermodynamic optimisation of the Pb-Tl binary system, *Journal of Alloys and Compounds* 320 (2001) 228–233, [https://doi.org/10.1016/S0925-8388\(00\)01492-4](https://doi.org/10.1016/S0925-8388(00)01492-4).
 - [56] J. Liu, C. Guo, C. Li, Z. Du, Thermodynamic re-assessment of the Ni – Sn system, *International Journal of Materials Research* 104 (2013) 51–59, <https://doi.org/10.3139/146.110827>.
 - [57] J. Wang, X. Lu, B. Sundman, X. Su, Thermodynamic reassessment of the Au-Te system, *Journal of Alloys and Compounds* 407 (2006) 106–111, <https://doi.org/10.1016/j.jallcom.2005.05.038>.
 - [58] A. Chari, A. Garay, R. Arróyave, Thermodynamic remodeling of the Co-Ga system, *Calphad* 34 (2010) 189–195, <https://doi.org/10.1016/j.calphad.2010.02.004>.
 - [59] S. Jin, C. Leinenbach, J. Wang, L.I. Duarte, S. Delsante, G. Borzone, A. Scott, A. Watson, Thermodynamic study and re-assessment of the Ge-Ni system, *Calphad* 38 (2012) 23–34, <https://doi.org/10.1016/j.calphad.2012.03.003>.
 - [60] H. Ohtani, M. Miyashita, K. Ishida, Thermodynamic study of phase equilibria in the Sn-Ag-Zn system, *J. Japan Inst. Metals* 63 (1999) 685–694, <https://doi.org/10.2320/jinstmet1952.63.6.685>.
 - [61] J. Liao, H. Wang, T.-Y. Chen, Experimental investigation and thermodynamic calculation of Ni-Al-La ternary system in nickel-rich region: a new intermetallic compound Ni₂AlLa, *Materials* 11 (2018) 2396, <https://doi.org/10.3390/ma11122396>.

- [62] V.T. Witusiewicz, U. Hecht, S.G. Fries, S. Rex, The Ag–Al–Cu system, *Journal of Alloys and Compounds* 387 (2005) 217–227, <https://doi.org/10.1016/j.jallcom.2004.06.078>.
- [63] H. Ohtani, I. Satoh, M. Miyashita, K. Ishida, Thermodynamic analysis of the Sn–Ag–Bi ternary phase diagram, *Mater. Trans.* 42 (2001) 722–731, <https://doi.org/10.2320/matertrans.42.722>.
- [64] H.Q. Dong, V. Vuorinen, X.M. Tao, T. Laurila, M. Paulasto-Kröckel, Thermodynamic reassessment of Au–Cu–Sn ternary system, *Journal of Alloys and Compounds* 588 (2014) 449–460, <https://doi.org/10.1016/j.jallcom.2013.11.041>.
- [65] J. Vizdal, M.H. Braga, A. Kroupa, K.W. Richter, D. Soares, L.F. Malheiros, J. Ferreira, Thermodynamic assessment of the Bi–Sn–Zn system, *Calphad* 31 (2007) 438–448, <https://doi.org/10.1016/j.calphad.2007.05.002>.
- [66] Y. Cui, S. Ishihara, X. Liu, I. Ohnuma, R. Kainuma, H. Ohtani, K. Ishida, Thermodynamic calculation of phase diagram in the Bi–in–Sb ternary system, *Mater. Trans.* 43 (2002) 1879–1886, <https://doi.org/10.2320/matertrans.43.1879>.
- [67] J. Miettinen, Thermodynamic description of the Cu–Ni–Zn system above 600°C, *Calphad* 27 (2003) 263–274, <https://doi.org/10.1016/j.calphad.2003.09.002>.
- [68] H. Ohtani, K. Okuda, K. Ishida, Thermodynamic study of phase equilibria in the Pb–Sn–Sb system, *JPE* 16 (1995) 416–429, <https://doi.org/10.1007/BF02645349>.
- [69] J. Cui, Y. Zhang, X. Hao, X. Liu, Y. Shen, Thermodynamic calculation of S–Sb system and Cu–S–Sb system, *Calphad* 75 (2021) 102362, <https://doi.org/10.1016/j.calphad.2021.102362>.
- [70] I. Ansara, C. Chatillon, H.L. Lukas, T. Nishizawa, H. Ohtani, K. Ishida, M. Hillert, B. Sundman, B.B. Argent, A. Watson, T.G. Chart, T. Anderson, A binary database for III–V compound semiconductor systems, *Calphad* 18 (1994) 177–222, [https://doi.org/10.1016/0364-5916\(94\)90027-2](https://doi.org/10.1016/0364-5916(94)90027-2).
- [71] F. Islam, A.K. Thykadavil, M. Medraj, A computational thermodynamic model of the Mg–Al–Ge system, *Journal of Alloys and Compounds* 425 (2006) 129–139, <https://doi.org/10.1016/j.jallcom.2006.01.050>.
- [72] X. Yuan, L. Zhang, Y. Du, W. Xiong, Y. Tang, A. Wang, S. Liu, A new approach to establish both stable and metastable phase equilibria for fcc ordered/disordered phase transition: application to the Al–Ni and Ni–Si systems, *Materials Chemistry and Physics* 135 (2012) 94–105, <https://doi.org/10.1016/j.matchemphys.2012.04.028>.
- [73] N. Saunders, A review and thermodynamic assessment of the Al–Mg and Mg–Li systems, *Calphad* 14 (1990) 61–70, [https://doi.org/10.1016/0364-5916\(90\)90040-7](https://doi.org/10.1016/0364-5916(90)90040-7).
- [74] B. Sundman, S.G. Fries, W.A. Oates, A thermodynamic assessment of the Au–Cu system, *Calphad* 22 (1998) 335–354, [https://doi.org/10.1016/S0364-5916\(98\)00034-0](https://doi.org/10.1016/S0364-5916(98)00034-0).
- [75] X. Ren, C. Li, C. Guo, Z. Du, A thermodynamic assessment of the Cd–Mg system, *Thermochimica Acta* 534 (2012) 1–8, <https://doi.org/10.1016/j.tca.2012.01.016>.
- [76] X. Wang, X. Su, J.C. Tedenac, F. Yin, J. Wang, A thermodynamic assessment of the Dy–Sn system, *Journal of Alloys and Compounds* 396 (2005) 169–174, <https://doi.org/10.1016/j.jallcom.2004.12.033>.
- [77] J.-B. Li, M.-C. Record, J.-C. Tedenac, A thermodynamic assessment of the In–Se system, *International Journal of Materials Research* 94 (2022) 381–389, <https://doi.org/10.1515/ijmr-2003-0069>.
- [78] B. Pei, B. Björkman, B. Sundman, B. Jansson, A thermodynamic assessment of the iron – antimony system, *Calphad* 19 (1995) 1–15, [https://doi.org/10.1016/0364-5916\(95\)00001-U](https://doi.org/10.1016/0364-5916(95)00001-U).
- [79] M. Huang, X. Su, F. Yin, P. Zhang, Z. Li, C. Chen, A thermodynamic assessment of the La–Sn system, *Journal of Alloys and Compounds* 309 (2000) 147–153, [https://doi.org/10.1016/S0925-8388\(00\)01077-X](https://doi.org/10.1016/S0925-8388(00)01077-X).
- [80] I. Kainulainen, P. Taskinen, J. Gisby, A thermodynamic assessment of the nickel–lead system, *Calphad* 34 (2010) 441–445, <https://doi.org/10.1016/j.calphad.2010.08.001>.
- [81] F. Yin, X. Su, Z. Li, P. Zhang, A thermodynamic assessment of the Pr–Al system, *International Journal of Materials Research* 92 (2001) 447–450.
- [82] Z. Pan, Y. Du, B.Y. Huang, Y. Liu, R.C. Wang, A thermodynamic description of the Al–Be system: modeling and experiment, *Calphad* 28 (2004) 371–378.
- [83] Y. Du, J.C. Schuster, Y. Austin Chang, Z. Jin, B. Huang, A thermodynamic description of the B–Co system: modeling and experiment, *International Journal of Materials Research* 93 (2022) 1157–1163, <https://doi.org/10.1515/ijmr-2002-0198>.
- [84] C. Guo, Z. Du, C. Li, A thermodynamic description of the Gd–Mg–Y system, *Calphad* 31 (2007) 75–88, <https://doi.org/10.1016/j.calphad.2006.10.004>.
- [85] Y. Du, L. Li, J. Wang, J. Wang, Z. Jin, A thermodynamic description of the Ge–Sr system acquired via a hybrid approach of CALPHAD and first-principles calculations, *Calphad* 33 (2009) 719–722, <https://doi.org/10.1016/j.calphad.2009.09.004>.
- [86] Z. Du, C. Guo, X. Yang, T. Liu, A thermodynamic description of the Pd–Si–C system, *Intermetallics* 14 (2006) 560–569, <https://doi.org/10.1016/j.intermet.2005.09.008>.
- [87] P.-Y. Chevalier, A thermodynamic evaluation of the Au–Sb and Au–Ti systems, *Thermochimica Acta* 155 (1989) 211–225, [https://doi.org/10.1016/0040-6031\(89\)87147-3](https://doi.org/10.1016/0040-6031(89)87147-3).
- [88] P.-Y. Chevalier, A thermodynamic evaluation of the Cu–Ti system, *Thermochimica Acta* 156 (1989) 383–392, [https://doi.org/10.1016/0040-6031\(89\)87205-3](https://doi.org/10.1016/0040-6031(89)87205-3).
- [89] P.-Y. Chevalier, A thermodynamic evaluation of the Ge–In, Ge–Pb, Ge–Sb, Ge–Ti and Ge–Zn systems, *Thermochimica Acta* 155 (1989) 227–240, [https://doi.org/10.1016/0040-6031\(89\)87148-5](https://doi.org/10.1016/0040-6031(89)87148-5).
- [90] Y. Feutelais, A. Haloui, B. Legendre, A thermodynamic evaluation of the Te–Zn system, *JPE* 18 (1997) 48–61, <https://doi.org/10.1007/BF02646758>.
- [91] M. Li, Z. Du, C. Guo, C. Li, A thermodynamic modeling of the Cu–Pd system, *Calphad* 32 (2008) 439–446, <https://doi.org/10.1016/j.calphad.2008.04.004>.
- [92] B. Lindahl, X.L. Liu, Z.-K. Liu, M. Selleby, A thermodynamic re-assessment of Al–V toward an assessment of the ternary Al–Ti–V system, *Calphad* 51 (2015) 75–88, <https://doi.org/10.1016/j.calphad.2015.07.002>.
- [93] M. Idbenali, C. Servant, N. Selhaoui, L. Bouriden, A thermodynamic reassessment of the Ca–Pb system, *Calphad* 32 (2008) 64–73, <https://doi.org/10.1016/j.calphad.2007.10.004>.
- [94] K.C. Hari Kumar, V. Raghavan, A thermodynamic reassessment of the Fe–V system, *Calphad* 15 (1991) 307–314, [https://doi.org/10.1016/0364-5916\(91\)90008-8](https://doi.org/10.1016/0364-5916(91)90008-8).
- [95] H. Ohtani, K. Ishida, A thermodynamic study of the phase equilibria in the Bi–Sn–Sb system, *JEM* 23 (1994) 747–755, <https://doi.org/10.1007/BF02651369>.
- [96] A. Berche, J.C. Tedenac, P. Jund, Ab-initio calculations and CALPHAD description of Cr–Ge–Mn and Cr–Ge–Si, *Calphad* 49 (2015) 50–57, <https://doi.org/10.1016/j.calphad.2015.02.004>.
- [97] K. Frisk, P. Gustafson, An assessment of the Cr–Mo–W system, *Calphad* 12 (1988) 247–254, [https://doi.org/10.1016/0364-5916\(88\)90004-1](https://doi.org/10.1016/0364-5916(88)90004-1).
- [98] P. Franke, An assessment of the ordered phases in Mn–Ni using two- and four-sublattice models, *International Journal of Materials Research* 98 (2007) 954–960, <https://doi.org/10.3139/146.101558>.
- [99] O. Teppo, J. Niemelä, P. Taskinen, An assessment of the thermodynamic properties and phase diagram of the system Bi–Cu, *Thermochimica Acta* 173 (1990) 137–150, [https://doi.org/10.1016/0040-6031\(90\)80598-S](https://doi.org/10.1016/0040-6031(90)80598-S).
- [100] H. Rannikko, S. Sundström, P. Taskinen, An optimised equilibrium phase diagram and solution thermodynamics of arsenic–lead alloys, *Thermochimica Acta* 216 (1993) 1–14, [https://doi.org/10.1016/0040-6031\(93\)80375-K](https://doi.org/10.1016/0040-6031(93)80375-K).
- [101] E. Fischer, C. Colinet, An updated thermodynamic modeling of the Al–Zr system, *J. Phase Equilib. Diffus.* 36 (2015) 404–413, <https://doi.org/10.1007/s11669-015-0398-y>.
- [102] H. Ye, M. Rong, Q. Chen, Q. Yao, J. Wang, G. Rao, H. Zhou, Assessment of phase equilibria and thermodynamic properties in the Fe–RE (RE = rare earth metals) binary systems, *J. Mater. Inf.* 3 (2023), <https://doi.org/10.20517/jmi.2023.08>.
- [103] J. Vreštal, J. Pinkas, A. Watson, A. Scott, J. Houserová, A. Kroupa, Assessment of the thermodynamic properties and phase diagram of the Bi–Pd system, *Calphad* 30 (2006) 14–17, <https://doi.org/10.1016/j.calphad.2005.12.001>.
- [104] A. Fernández Guillermet, Assessment of the thermodynamic properties of the Ni–Co system, *International Journal of Materials Research* 78 (1987) 639–647, <https://doi.org/10.1515/ijmr-1987-780905>.
- [105] Y. Zhong, M. Yang, Z.-K. Liu, Contribution of first-principles energetics to Al–Mg thermodynamic modeling, *Calphad* 29 (2005) 303–311, <https://doi.org/10.1016/j.calphad.2005.08.004>.
- [106] L. Duriška, I. Černíková, R. Číčka, J. Janovec, Contribution to thermodynamic description of Al–Pd system, *J. Phys.: Conf. Ser.* 809 (2017) 012008, <https://doi.org/10.1088/1742-6596/809/1/012008>.
- [107] A.V. Davydov, U.R. Kattner, D. Josell, R.M. Waterstrat, W.J. Boettinger, J. E. Blendell, A.J. Shapiro, Determination of the CoTi congruent melting point and thermodynamic reassessment of the Co–Ti system, *Metall. Mater. Trans. A* 32 (2001) 2175–2186, <https://doi.org/10.1007/s11661-001-0193-8>.
- [108] K. Oikawa, G.-W. Qin, T. Ikeshoji, R. Kainuma, K. Ishida, Direct evidence of magnetically induced phase separation in the fcc phase and thermodynamic calculations of phase equilibria of the Co–Cr system, *Acta Materialia* 50 (2002) 2223–2232, [https://doi.org/10.1016/S1359-6454\(01\)00433-5](https://doi.org/10.1016/S1359-6454(01)00433-5).
- [109] T.L. Reichmann, K.W. Richter, S. Delsante, G. Borzone, H. Ipser, Enthalpies of formation of Cd–Pr intermetallic compounds and thermodynamic assessment of the Cd–Pr system, *Calphad* 47 (2014) 56–62, <https://doi.org/10.1016/j.calphad.2014.06.005>.
- [110] S. Hassam, M. Gambino, M. Gaune-escard, J.P. Bros, J. Ågren, Experimental and calculated Ag + Au + Ge phase diagram, *Metall. Trans. A* 19 (1988) 409–416, <https://doi.org/10.1007/BF02649254>.
- [111] Y. Zhong, A. Saengdeejing, L. Kecses, B. Klotz, Z.-K. Liu, Experimental and computational studies of the Cu–Hf binary system, *Acta Materialia* 61 (2013) 660–669, <https://doi.org/10.1016/j.actamat.2012.10.014>.
- [112] J. Sopoušek, A. Zemanová, J. Vreštal, P. Brož, Experimental determination of phase equilibria and reassessment of Ag–Pd system, *Journal of Alloys and Compounds* 504 (2010) 431–434, <https://doi.org/10.1016/j.jallcom.2010.05.141>.
- [113] J. Wang, C. Liu, C. Leinenbach, U.E. Klotz, P.J. Uggowitzer, J.F. Löffler, Experimental investigation and thermodynamic assessment of the Cu–Sn–Ti ternary system, *Calphad* 35 (2011) 82–94, <https://doi.org/10.1016/j.calphad.2010.12.006>.
- [114] T.L. Chen, J. Wang, M.H. Rong, G.H. Rao, H.Y. Zhou, Experimental investigation and thermodynamic assessment of the Fe–Pr and Fe–Nd binary systems, *Calphad* 55 (2016) 270–280, <https://doi.org/10.1016/j.calphad.2016.10.004>.
- [115] X. Si, S. Liu, X. Li, C. Shi, Y. Liu, Y. Du, Z. Zhang, Experimental investigation and thermodynamic assessment of the Mn–Zr system, *Calphad* 72 (2021) 102243, <https://doi.org/10.1016/j.calphad.2020.102243>.
- [116] L. Zhang, Y. Du, H. Xu, Z. Pan, Experimental investigation and thermodynamic description of the Co–Si system, *Calphad* 30 (2006) 470–481, <https://doi.org/10.1016/j.calphad.2006.06.001>.
- [117] D. Huang, S. Liu, Y. Tang, Y. Du, P. Nash, B. Sundman, Experimental investigation and thermodynamic modeling of the Ce–Si system, *Thermochimica Acta* 646 (2016) 49–58, <https://doi.org/10.1016/j.tca.2016.11.003>.

- [118] M. Huang, D.L. Schlager, F.A. Schmidt, T.A. Lograsso, Experimental investigation and thermodynamic modeling of the Gd–Si system, *Journal of Alloys and Compounds* 441 (2007) 94–100, <https://doi.org/10.1016/j.jallcom.2006.09.068>.
- [119] F. Zhang, S. Liu, Y. Du, Experimental investigation and thermodynamic modeling of the La–Mg system, *Journal of Alloys and Compounds* 663 (2016) 279–288, <https://doi.org/10.1016/j.jallcom.2015.12.105>.
- [120] S.G. Fries, H.L. Lukas, R. Konetzki, R. Schmid-Fetzer, Experimental investigation and thermodynamic optimization of the Y–Cu binary system, *JPE* 15 (1994) 606–614, <https://doi.org/10.1007/BF02647621>.
- [121] M. Rong, L. Wang, J. Wang, C. Zhu, T. Chen, G. Rao, H. Zhou, Experimental investigation and thermodynamic re-assessment of the Mn–Nd binary system, *J Therm Anal Calorim* 126 (2016) 1437–1445, <https://doi.org/10.1007/s10973-016-5636-y>.
- [122] C. Mao, M. Tan, L. Zhang, D. Wu, W. Bai, L. Liu, Experimental reinvestigation and thermodynamic description of Bi–Te binary system, *Calphad* 60 (2018) 81–89, <https://doi.org/10.1016/j.calphad.2017.11.007>.
- [123] T. Wang, Z. Jin, J.-C. Zhao, Experimental study and reassessment of the Ni–Hf binary system, *International Journal of Materials Research* 92 (2001) 441–446.
- [124] A. Fisch, R. Schmid-Fetzer, Experimental study and thermodynamic assessment of phase equilibria in the Mn–Sc system, *International Journal of Materials Research* 98 (1998) 700–703.
- [125] V.T. Witusiewicz, A.A. Bondar, U. Hecht, J. Zollinger, V.M. Petyukh, O. S. Fomichov, V.M. Voblikov, S. Rex, Experimental study and thermodynamic re-assessment of the binary Al–Ta system, *Intermetallics* 18 (2010) 92–106.
- [126] N. Wang, C. Li, Z. Du, F. Wang, Experimental study and thermodynamic re-assessment of the Ni–Zr system, *Calphad* 31 (2007) 413–421, <https://doi.org/10.1016/j.calphad.2007.07.001>.
- [127] V. Grolrier, R. Schmid-Fetzer, Experimental study of Au–Pt–Sn phase equilibria and thermodynamic assessment of the Au–Pt and Au–Pt–Sn systems, *Journal of Elec Materi* 37 (2008) 264–278, <https://doi.org/10.1007/s11664-007-0352-9>.
- [128] P.-W. Guan, S.-L. Shang, G. Lindwall, T. Anderson, Z.-K. Liu, First-principles calculations and thermodynamic modeling of the S–Se system and implications for chalcogenide alloys, *Journal of Alloys and Compounds* 694 (2017) 510–521, <https://doi.org/10.1016/j.jallcom.2016.10.037>.
- [129] J.S. Wang, S. Jin, W.J. Zhu, H.Q. Dong, X.M. Tao, H.S. Liu, Z.P. Jin, First-principles calculations assisted thermodynamic assessment of the Pt–Ga–Ge ternary system, *Calphad* 33 (2009) 561–569, <https://doi.org/10.1016/j.calphad.2009.05.002>.
- [130] V.B. Rajkumar, K.C. Hari Kumar, Gibbs energy modeling of Fe–Ta system by Calphad method assisted by experiments and ab initio calculations, *Calphad* 48 (2015) 157–165, <https://doi.org/10.1016/j.calphad.2014.12.006>.
- [131] A. Qin, D. Liu, C. Chen, S. Liu, Y. Du, M. Wang, P. Nash, Heat contents of Sc₅Si₃ and ScSi intermetallics and thermodynamic modeling of the Sc–Si system, *J Therm Anal Calorim* 119 (2015) 1315–1321, <https://doi.org/10.1007/s10973-014-4216-2>.
- [132] S. Bakardjeva, M. Barrachin, S. Bechta, D. Bottomley, L. Brissoneau, B. Cheynet, E. Fischer, C. Journeau, M. Kiselova, L. Mezentseva, P. Piluso, T. Wiss, Improvement of the European thermodynamic database NUCLEA, *Prog. Nucl.* 52 (2010) 84–96, <https://doi.org/10.1016/j.pnucene.2009.09.014>.
- [133] D. Mirković, J. Gröbner, I. Kaban, W. Hoyer, R. Schmid-Fetzer, Integrated approach to thermodynamics, phase relations, liquid densities and solidification microstructures in the Al–Bi–Cu system, *International Journal of Materials Research* 100 (2009) 176–188, <https://doi.org/10.3139/146.110009>.
- [134] S.-M. Liang, M. Engstler, V. Groten, J. Barriero, F. Mücklich, A. Bührig-Polaczek, R. Schmid-Fetzer, Key experiments and thermodynamic revision of the binary Al–Sr system, *Journal of Alloys and Compounds* 610 (2014) 443–450, <https://doi.org/10.1016/j.jallcom.2014.05.018>.
- [135] M.H. Braga, A. Dębski, W. Gasiör, Li–Si phase diagram: enthalpy of mixing, thermodynamic stability, and coherent assessment, *Journal of Alloys and Compounds* 616 (2014) 581–593, <https://doi.org/10.1016/j.jallcom.2014.06.212>.
- [136] K. Ozturk, Y. Zhong, L.-Q. Chen, Z.-K. Liu, J.O. Sofo, C. Wolverton, Linking first-principles energetics to CALPHAD: an application to thermodynamic modeling of the Al–Ca binary system, *Metall Mater Trans A* 36 (2005) 5–13, <https://doi.org/10.1007/s11661-005-0133-0>.
- [137] A. Jacob, C. Schmetterer, A. Khvan, A. Kondratiev, D. Ivanov, B. Hallstedt, Liquidus projection and thermodynamic modeling of the Cr–Fe–Nb ternary system, *Calphad* 54 (2016) 1–15, <https://doi.org/10.1016/j.calphad.2016.04.013>.
- [138] A. Jacob, C. Schmetterer, L. Singheiser, A. Gray-Weale, B. Hallstedt, A. Watson, Modeling of Fe–W phase diagram using first principles and phonons calculations, *Calphad* 50 (2015) 92–104, <https://doi.org/10.1016/j.calphad.2015.04.010>.
- [139] I. Saenko, O. Fabrichnaya, A. Udovsky, New thermodynamic assessment of the Fe–Y system, *J. Phase Equilib. Diffus.* 38 (2017) 684–699, <https://doi.org/10.1007/s11669-017-0574-3>.
- [140] W. Gierlotka, J. Lee, V. Lim, W. Gasiör, A. Dębski, On the Bi–Ni system. Ab initio calculations and thermodynamic remodeling, *Calphad* 69 (2020) 101750, <https://doi.org/10.1016/j.calphad.2020.101750>.
- [141] W. Gierlotka, On the binary Sb–Sn system: ab initio calculation and thermodynamic remodeling, *J Mater Sci* 55 (2020) 347–357, <https://doi.org/10.1007/s10853-019-03934-6>.
- [142] H. Chen, Y. Du, J.C. Schuster, On the melting of Cr₅Si₃ and update of the thermodynamic description of Cr–Si, *Calphad* 33 (2009) 211–214, <https://doi.org/10.1016/j.calphad.2008.05.005>.
- [143] B.-J. Lee, On the stability of Cr carbides, *Calphad* 16 (1992) 121–149, [https://doi.org/10.1016/0364-5916\(92\)90002-F](https://doi.org/10.1016/0364-5916(92)90002-F).
- [144] Z. Li, X. Su, F. Yin, C. Chen, On the thermodynamic assessment of the Ag–La system, *Journal of Alloys and Compounds* 299 (2000) 195–198, [https://doi.org/10.1016/S0925-8388\(99\)00686-6](https://doi.org/10.1016/S0925-8388(99)00686-6).
- [145] M. Helena Braga, A. Dębski, W. Gasiör, Optimization and assessment of the Ag–Ca phase diagram, *Journal of Alloys and Compounds* 612 (2014) 280–286, <https://doi.org/10.1016/j.jallcom.2014.05.141>.
- [146] M.H.G. Jacobs, R. Schmid-Fetzer, Phase behavior and thermodynamic properties in the system Fe–Al, *Calphad* 33 (2009) 170–178, <https://doi.org/10.1016/j.calphad.2008.07.010>.
- [147] L. Soldi, A. Laplace, M. Roskosz, S. Gossé, Phase diagram and thermodynamic model for the Cu–Si and the Cu–Fe–Si systems, *Journal of Alloys and Compounds* 803 (2019) 61–70, <https://doi.org/10.1016/j.jallcom.2019.06.236>.
- [148] F. Römermann, Y. Feutelais, S.G. Fries, R. Blachnik, Phase diagram experimental investigation and thermodynamic assessment of the thallium–selenium system, *Intermetallics* 8 (2000) 53–65, [https://doi.org/10.1016/S0966-9795\(99\)00068-0](https://doi.org/10.1016/S0966-9795(99)00068-0).
- [149] Y. Feutelais, M. Majid, B. Legendre, S.G. Fries, Phase diagram investigation and proposition of a thermodynamic evaluation of the Tin–Selenium system, *JPE* 17 (1996) 40–49, <https://doi.org/10.1007/BF02648368>.
- [150] Y. Chen, Y. Liu, M. Chu, L. Wang, Phase diagrams and thermodynamic descriptions for Na–Te and K–Te binary systems, *Journal of Alloys and Compounds* 588 (2014) 605–610, <https://doi.org/10.1016/j.jallcom.2013.11.094>.
- [151] Y. Chen, Y. Liu, M. Chu, L. Wang, Phase diagrams and thermodynamic descriptions for the Bi–Se and Zn–Se binary systems, *Journal of Alloys and Compounds* 617 (2014) 423–428, <https://doi.org/10.1016/j.jallcom.2014.08.001>.
- [152] Y. Liu, Z. Kang, G. Sheng, L. Zhang, J. Wang, Z. Long, Phase equilibria and thermodynamic basis for the Cd–Se and Pb–Se binary systems, *Journal of Elec Materi* 41 (2012) 1915–1923, <https://doi.org/10.1007/s11664-012-2016-7>.
- [153] V.B. Rajkumar, S.-W. Chen, Phase equilibria and thermodynamic descriptions of Ag–Ge and Ag–Ge–Ni systems, *Journal of Elec Materi* 47 (2018) 3666–3677, <https://doi.org/10.1007/s11664-018-6216-7>.
- [154] Y. Liu, G. Wang, J. Wang, Y. Chen, Z. Long, Phase equilibria and thermodynamic functions for Ag–Hg and Cu–Hg binary systems, *Thermochimica Acta* 547 (2012) 83–88, <https://doi.org/10.1016/j.tca.2012.08.004>.
- [155] C. Sha, L. Zhou, S. Liu, Y. Du, T. Gang, H. Xu, Phase equilibria and thermodynamic modeling in the Ge–Zr binary system, *J Mater Sci* 46 (2011) 1405–1413, <https://doi.org/10.1007/s10853-010-4934-1>.
- [156] H. Ye, M. Rong, Q. Yao, Q. Chen, J. Wang, G. Rao, H. Zhou, Phase equilibria and thermodynamic properties in the RE–Ni (RE = rare earth metals) binary systems, *J Mater Sci* 58 (2023) 1260–1292, <https://doi.org/10.1007/s10853-022-08039-1>.
- [157] M.A. Turchanin, Phase equilibria and thermodynamics of binary copper systems with 3d-metals. III. Copper–chromium system, *Powder Metall Met Ceram* 45 (2006) 457–467, <https://doi.org/10.1007/s11106-006-0106-x>.
- [158] D. Kevorkov, R. Schmid-Fetzer, F. Zhang, Phase equilibria and thermodynamics of the Mg–Si–Li system and remodeling of the Mg–Si system, *Journal of Phase Equilibria & Diffusion* 25 (2004) 140–151, <https://doi.org/10.1361/15477030418569>.
- [159] L.A. Zabdyr, Phase equilibria in ternary Cd–Sb–Zn system, *Calphad* 21 (1997) 349–358, [https://doi.org/10.1016/S0364-5916\(97\)00036-9](https://doi.org/10.1016/S0364-5916(97)00036-9).
- [160] I. Ohnuma, H. Enoki, O. Ikeda, R. Kainuma, H. Ohtani, B. Sundman, K. Ishida, Phase equilibria in the Fe–Co binary system, *Acta Materialia* 50 (2002) 379–393, [https://doi.org/10.1016/S1359-6454\(01\)00337-8](https://doi.org/10.1016/S1359-6454(01)00337-8).
- [161] A. Kozlov, M. Ohno, R. Arroyave, Z.K. Liu, R. Schmid-Fetzer, Phase equilibria, thermodynamics and solidification microstructures of Mg–Sn–Ca alloys, Part 1: experimental investigation and thermodynamic modeling of the ternary Mg–Sn–Ca system, *Intermetallics* 16 (2008) 299–315, <https://doi.org/10.1016/j.intermet.2007.10.010>.
- [162] D. Su, K.C. Yang, M.H. Rong, P.P. Liu, Q.R. Yao, J. Wang, Q. Chen, G.H. Rao, H. Y. Zhou, Phase transition, microstructure and solidification of Ce–La–Fe and Ce–Nd–Fe alloys: experimental investigation and thermodynamic calculation, *Calphad* 80 (2023) 102506, <https://doi.org/10.1016/j.calphad.2022.102506>.
- [163] S.-M. Liang, R. Schmid-Fetzer, Phosphorus in Al–Si cast alloys: thermodynamic prediction of the AlP and eutectic (Si) solidification sequence validated by microstructure and nucleation undercooling data, *Acta Materialia* 72 (2014) 41–56, <https://doi.org/10.1016/j.actamat.2014.02.042>.
- [164] A. Watson, Re-assessment of phase diagram and thermodynamic properties of the Al–Ga system, *Calphad* 16 (1992) 207–217, [https://doi.org/10.1016/0364-5916\(92\)90009-M](https://doi.org/10.1016/0364-5916(92)90009-M).
- [165] W. Gierlotka, I. Lin, S. Chen, W. Gasiör, A. Dębski, Re-optimization of the binary Sb – Se system aided by ab-initio calculations, *Calphad* 73 (2021) 102257, <https://doi.org/10.1016/j.calphad.2021.102257>.
- [166] Y. Du, J. Wang, J. Zhao, J.C. Schuster, F. Weitzer, R. Schmid-Fetzer, M. Ohno, H. Xu, Z. Liu, S. Shang, W. Zhang, Reassessment of the Al–Mn system and a thermodynamic description of the Al–Mg–Mn system, *International Journal of Materials Research* 98 (2007) 855–871, <https://doi.org/10.3139/146.101547>.
- [167] W. Xiong, Y. Du, X. Lu, J.C. Schuster, H. Chen, Reassessment of the Ce–Ni binary system supported by key experiments and ab initio calculations, *Intermetallics* 15 (2007) 1401–1408, <https://doi.org/10.1016/j.intermet.2007.04.004>.
- [168] W.-H. Sun, Y. Du, Y. Kong, H.-H. Xu, W. Xiong, S.-H. Liu, Reassessment of the Ni–B system supported by key experiments and first-principles calculation, *International Journal of Materials Research* 100 (2009) 59–67, <https://doi.org/10.3139/146.101786>.

- [169] Y. Pan, Y. Du, J. Lv, T. Liang, F. Luo, Reassessment of the Ni–V system and a new thermodynamic modeling of the Mo–Ni–V system, *Thermochimica Acta* 661 (2018) 137–146, <https://doi.org/10.1016/j.tca.2018.01.020>.
- [170] S.A. Mey, Reevaluation of the Al–Zn system, *International Journal of Materials Research* 84 (1993) 451–455, <https://doi.org/10.1515/ijmr-1993-840704>.
- [171] V.T. Witusiewicz, F. Sommer, E.J. Mittermeijer, Reevaluation of the Fe–Mn phase diagram, *Journal of Phase Equilibria & Diffusion* 25 (2004) 346–354, <https://doi.org/10.1361/15477030420115>.
- [172] H. Chen, Y. Du, Refinement of the thermodynamic modeling of the Nb–Ni system, *Calphad* 30 (2006) 308–315, <https://doi.org/10.1016/j.calphad.2006.02.005>.
- [173] A.V. Davydov, U.R. Kattner, Revised thermodynamic description for the Co–Mo system, *JPE* 24 (2003) 209–211, <https://doi.org/10.1361/105497103770330505>.
- [174] A. Jacob, E. Povoden-Karadeniz, E. Kozeschni, Revised thermodynamic description of the Fe–Cr system based on an improved sublattice model of the σ phase, *Calphad* 60 (2018) 16–28, <https://doi.org/10.1016/j.calphad.2017.10.002>.
- [175] Y.-Y. Chuang, J.-S. Paik, C. Zhang, J.H. Perepezko, Y.A. Chang, Stable and metastable equilibria in the Pb–Cd system, *Metall Mater Trans A* 44 (2013) 3004–3013, <https://doi.org/10.1007/s11661-013-1652-8>.
- [176] V.T. Witusiewicz, A.A. Bondar, U. Hecht, S. Rex, T.Ya Velikanova, The Al–B–Nb–Ti system, *Journal of Alloys and Compounds* 465 (2008) 64–77, <https://doi.org/10.1016/j.jallcom.2007.10.061>.
- [177] G. Cacciamani, A. Dinsdale, M. Palumbo, A. Pasturel, The Fe–Ni system: thermodynamic modelling assisted by atomistic calculations, *Intermetallics* 18 (2010) 1148–1162, <https://doi.org/10.1016/j.intermet.2010.02.026>.
- [178] I. Ansara, F. Ajersch, The Ga–Pb (Gallium–Lead) system, *JPE* 12 (1991) 73–77, <https://doi.org/10.1007/BF02663678>.
- [179] J. Klingbeil, R. Schmid-Fetzer, The Ga–Tl (gallium–thallium) system, *JPE* 12 (1991) 652–660, <https://doi.org/10.1007/BF02645165>.
- [180] J. Dutkiewicz, Z. Moser, L. Zabdyr, D.D. Gohil, T.G. Chart, I. Ansara, C. Girard, The Ga–Zn (Gallium–Zinc) system, *Bulletin of Alloy Phase Diagrams* 11 (1990) 77–82, <https://doi.org/10.1007/BF02841587>.
- [181] D. Li, A. Beutl, H. Flandorfer, D.M. Cupid, The Li–Sb phase diagram part II: calorimetry and thermodynamic assessment, *Journal of Alloys and Compounds* 701 (2017) 186–199, <https://doi.org/10.1016/j.jallcom.2016.12.399>.
- [182] Y. Yuan, F. Pan, D. Li, A. Watson, The re-assessment of the Mg–Zn and Fe–Si systems and their incorporation in thermodynamic descriptions of the Al–Mg–Zn and Fe–Si–Zn systems, *Calphad* 44 (2014) 54–61, <https://doi.org/10.1016/j.calphad.2013.07.007>.
- [183] Y. Zhang, C. Li, Z. Du, T. Geng, The thermodynamic assessment of the Co–Sb system, *Calphad* 32 (2008) 56–63, <https://doi.org/10.1016/j.calphad.2007.11.001>.
- [184] H. Bo, L.B. Liu, Z.P. Jin, Thermodynamic analysis of Al–Sc, Cu–Sc and Al–Cu–Sc system, *Journal of Alloys and Compounds* 490 (2010) 318–325, <https://doi.org/10.1016/j.jallcom.2009.10.003>.
- [185] H. Ohtani, N. Hanaya, M. Hasebe, S. Teraoka, M. Abe, Thermodynamic analysis of the Fe–Ti–P ternary system by incorporating first-principles calculations into the CALPHAD approach, *Calphad* 30 (2006) 147–158, <https://doi.org/10.1016/j.calphad.2005.09.006>.
- [186] T. Tokunaga, K. Hashima, H. Ohtani, M. Hasebe, Thermodynamic analysis of the Ni–Si–Ti system using thermochemical properties determined from ab initio calculations, *Mater. Trans.* 45 (2004) 1507–1514, <https://doi.org/10.2320/matertrans.45.1507>.
- [187] V. Grolrier, R. Schmid-Fetzer, Thermodynamic analysis of the Pt–Sn system, *Journal of Alloys and Compounds* 450 (2008) 264–271, <https://doi.org/10.1016/j.jallcom.2006.11.027>.
- [188] M. Palumbo, S. Curiotto, L. Battezzati, Thermodynamic analysis of the stable and metastable Co–Cu and Co–Cu–Fe phase diagrams, *Calphad* 30 (2006) 171–178, <https://doi.org/10.1016/j.calphad.2005.10.007>.
- [189] Y. Jianrong, N.J. Silk, A. Watson, A.W. Bryant, B.B. Argent, Thermodynamic and phase diagram assessment of the Cd–Te and Hg–Te systems, *Calphad* 19 (1995) 399–414, [https://doi.org/10.1016/0364-5916\(95\)00038-G](https://doi.org/10.1016/0364-5916(95)00038-G).
- [190] H.Q. Dong, X.M. Tao, H.S. Liu, T. Laurila, M. Paulastro-Kröckel, Thermodynamic assessment of Au–La and Au–Er binary systems, *Journal of Alloys and Compounds* 509 (2011) 4439–4444, <https://doi.org/10.1016/j.jallcom.2011.01.072>.
- [191] S.C. Hansen, Thermodynamic assessment of binary Zn–Hg, Cd–Hg, AND In–Hg amalgams, *Calphad* 22 (1998) 359–373, [https://doi.org/10.1016/S0364-5916\(98\)00036-4](https://doi.org/10.1016/S0364-5916(98)00036-4).
- [192] X. Chen, L. Liu, L. Zhang, H. Bo, Z. Jin, Thermodynamic assessment of Cu–Cd system, *Transactions of Nonferrous Metals Society of China* 20 (2010) 649–654, [https://doi.org/10.1016/S1003-6326\(09\)60193-X](https://doi.org/10.1016/S1003-6326(09)60193-X).
- [193] L.G. Zhang, L.B. Liu, H.S. Liu, Z.P. Jin, Thermodynamic assessment of Cu–Eu and Cu–Yb system, *Calphad* 31 (2007) 264–268, <https://doi.org/10.1016/j.calphad.2006.11.003>.
- [194] S. Zhou, L. Liu, X. Yuan, F. Zheng, Z. Jin, Thermodynamic assessment of La–Si and Mg–La–Si systems, *Journal of Alloys and Compounds* 490 (2010) 253–259, <https://doi.org/10.1016/j.jallcom.2009.09.171>.
- [195] D. Zhu, C. Li, C. Guo, Z. Du, J. Li, Thermodynamic assessment of Ni–Yb binary system, *Transactions of Nonferrous Metals Society of China* 26 (2016) 1055–1062, [https://doi.org/10.1016/S1003-6326\(16\)64202-4](https://doi.org/10.1016/S1003-6326(16)64202-4).
- [196] T. Gómez-Acebo, Thermodynamic assessment of the Ag–Zn system, *Calphad* 22 (1998) 203–220, [https://doi.org/10.1016/S0364-5916\(98\)00024-8](https://doi.org/10.1016/S0364-5916(98)00024-8).
- [197] H.-M. Hsiao, S.-M. Liang, R. Schmid-Fetzer, Y. Yen, Thermodynamic assessment of the Ag–Zr and Cu–Zr binary systems, *Calphad* 55 (2016) 77–87, <https://doi.org/10.1016/j.calphad.2016.08.001>.
- [198] F. Yin, M. Huang, X. Su, P. Zhang, Z. Li, Y. Shi, Thermodynamic assessment of the Ag–Ce (silver–cerium) system, *Journal of Alloys and Compounds* 334 (2002) 154–158, [https://doi.org/10.1016/S0925-8388\(01\)01757-1](https://doi.org/10.1016/S0925-8388(01)01757-1).
- [199] H. Wang, L.G. Zhang, W.J. Zhu, H.S. Liu, Z.P. Jin, Thermodynamic assessment of the Ag–Gd binary system, *Journal of Alloys and Compounds* 466 (2008) 165–168, <https://doi.org/10.1016/j.jallcom.2007.11.049>.
- [200] M. Lim, J.E. Tibballs, P.L. Rossiter, Thermodynamic assessment of the Ag–Mg binary system, *International Journal of Materials Research* 88 (1997) 162–169.
- [201] L.G. Zhang, F.G. Meng, H.S. Liu, L.B. Liu, Z.P. Jin, Thermodynamic assessment of the Ag–Yb system, *Journal of Alloys and Compounds* 452 (2008) 304–306.
- [202] X. Bao, L. Liu, Y. Jiang, Y. Jiang, C. Mao, X. Li, L. Zhang, Thermodynamic assessment of the Al–Ba system, *J. Phase Equilib. Diffus.* 37 (2016) 345–349, <https://doi.org/10.1007/s11669-016-0466-y>.
- [203] M. Li, C. Li, F. Wang, D. Luo, W. Zhang, Thermodynamic assessment of the Al–Au system, *Journal of Alloys and Compounds* 385 (2004) 199–206, <https://doi.org/10.1016/j.jallcom.2004.05.007>.
- [204] L.G. Zhang, L.B. Liu, G.X. Huang, H.Y. Qi, B.R. Jia, Z.P. Jin, Thermodynamic assessment of the Al–Cu–Er system, *Calphad* 32 (2008) 527–534, <https://doi.org/10.1016/j.calphad.2008.05.002>.
- [205] L.G. Zhang, H.Q. Dong, G.X. Huang, J. Shan, L.B. Liu, Z.P. Jin, Thermodynamic assessment of the Al–Cu–Gd system, *Calphad* 33 (2009) 664–672, <https://doi.org/10.1016/j.calphad.2009.08.003>.
- [206] S.-M. Liang, H.-M. Hsiao, R. Schmid-Fetzer, Thermodynamic assessment of the Al–Cu–Zn system, part I: Cu–Zn binary system, *Calphad* 51 (2015) 224–232, <https://doi.org/10.1016/j.calphad.2015.09.010>.
- [207] B. Hallstedt, O. Kim, Thermodynamic assessment of the Al–Li system, *International Journal of Materials Research* 98 (2007) 961–969, <https://doi.org/10.3139/146.101553>.
- [208] W. Luo, Z. Jin, H. Liu, T. Wang, Thermodynamic assessment of the Au–Ti system, *Calphad* 25 (2001) 19–26, [https://doi.org/10.1016/S0364-5916\(01\)00026-8](https://doi.org/10.1016/S0364-5916(01)00026-8).
- [209] J. Wang, X.-G. Lu, B. Sundman, X. Su, Thermodynamic assessment of the Au–Ni system, *Calphad* 29 (2005) 263–268, <https://doi.org/10.1016/j.calphad.2005.09.004>.
- [210] H.S. Liu, K. Ishida, Z.P. Jin, Y. Du, Thermodynamic assessment of the Au–Zn binary system, *Intermetallics* 11 (2003) 987–994, [https://doi.org/10.1016/S0966-9795\(03\)00115-8](https://doi.org/10.1016/S0966-9795(03)00115-8).
- [211] M. Liu, C. Li, Z. Du, C. Guo, C. Niu, Thermodynamic assessment of the Bi–Rb binary system, *Thermochimica Acta* 551 (2013) 27–32, <https://doi.org/10.1016/j.tca.2012.10.012>.
- [212] P. Agraval, L. Dreval, M. Turchanin, T. Velikanova, Thermodynamic assessment of the Co–Zr system, *J. Phase Equilib. Diffus.* 41 (2020) 491–499, <https://doi.org/10.1007/s11669-020-00805-5>.
- [213] S. Jin, J. Wang, L.G. Zhang, H.S. Liu, L.B. Liu, F. Zheng, Z.P. Jin, Thermodynamic assessment of the Co–Ho binary system, *Journal of Alloys and Compounds* 477 (2009) 233–238, <https://doi.org/10.1016/j.jallcom.2008.10.062>.
- [214] C.P. Wang, J. Wang, X.J. Liu, I. Ohnuma, R. Kainuma, K. Ishida, Thermodynamic assessment of the Co–La and Mo–La systems, *Journal of Alloys and Compounds* 453 (2008) 174–179, <https://doi.org/10.1016/j.jallcom.2006.11.155>.
- [215] L.G. Zhang, G.X. Huang, H.Y. Qi, B.R. Jia, L.B. Liu, Z.P. Jin, Thermodynamic assessment of the Cu–Dy binary system, *Journal of Alloys and Compounds* 470 (2009) 214–217, <https://doi.org/10.1016/j.jallcom.2008.03.007>.
- [216] J. Wang, S. Jin, C. Leinenbach, A. Jacot, Thermodynamic assessment of the Cu–Ge binary system, *Journal of Alloys and Compounds* 504 (2010) 159–165, <https://doi.org/10.1016/j.jallcom.2010.05.077>.
- [217] Z. Du, Y. Xu, W. Zhang, Thermodynamic assessment of the Cu–La system, *Journal of Alloys and Compounds* 289 (1999) 88–95, [https://doi.org/10.1016/S0925-8388\(99\)00080-8](https://doi.org/10.1016/S0925-8388(99)00080-8).
- [218] T. Abe, B. Sundman, H. Onodera, Thermodynamic assessment of the Cu–Pt system, *JPE* 27 (2006) 5–13, <https://doi.org/10.1361/105497196X92736>.
- [219] X. Li, K. Cheng, X. Yuan, D. Zhao, J. Xin, W. Wang, C. Zhang, Y. Du, Thermodynamic assessment of the Ga–X (X=B, Ca, Sr, Ba) systems supported by first-principles calculations, *Calphad* 43 (2013) 52–60, <https://doi.org/10.1016/j.calphad.2013.09.002>.
- [220] Y.-W. Yen, J. Gröbner, R. Schmid-Fetzer, Y.-W. Yen, S.C. Hansen, Thermodynamic assessment of the Hg–Sn system, *JPE* 24 (2003) 151–167, <https://doi.org/10.1361/105497103770330776>.
- [221] C. Servant, M. Idbenali, Thermodynamic assessment of the In–Ir system in the rich part, *Thermochimica Acta* 517 (2011) 1–8, <https://doi.org/10.1016/j.tca.2010.12.019>.
- [222] W. Sun, Y. Du, S. Liu, B. Huang, C. Jiang, Thermodynamic assessment of the Mn–B system, *J. Phase Equilib. Diffus.* 31 (2010) 357–364, <https://doi.org/10.1007/s11669-010-9740-6>.
- [223] T. Geng, C. Li, X. Zhao, H. Xu, Z. Du, C. Guo, Thermodynamic assessment of the Nb–Si–Mo system, *Calphad* 34 (2010) 363–376, <https://doi.org/10.1016/j.calphad.2010.07.003>.
- [224] T. Geng, C. Li, J. Bao, X. Zhao, Z. Du, C. Guo, Thermodynamic assessment of the Nb–Si–Ti system, *Intermetallics* 17 (2009) 343–357, <https://doi.org/10.1016/j.intermet.2008.11.011>.
- [225] D. Zhu, C. Li, C. Guo, Z. Du, J. Li, Thermodynamic assessment of the Ni–Sc binary system, *Calphad* 48 (2015) 106–112, <https://doi.org/10.1016/j.calphad.2014.11.005>.
- [226] S. Gossé, C. Guéneau, Thermodynamic assessment of the palladium–tellurium (Pd–Te) system, *Intermetallics* 19 (2011) 621–629, <https://doi.org/10.1016/j.intermet.2010.12.014>.
- [227] N. David, J. Hertz, J.-M. Fiorani, Thermodynamic assessment of the Pb–Zn system, *International Journal of Materials Research* 94 (2003) 8–11.

- [228] L.L. Xu, J. Wang, H.S. Liu, Z.P. Jin, Thermodynamic assessment of the Pt-Si binary system, *Calphad* 32 (2008) 101–105.
- [229] X.J. Liu, M.H. Chen, Y. Lu, Y.X. Huang, D. Wang, Q. He, D.L. Zhao, C.P. Wang, Thermodynamic assessment of the Sb-Sm and Sm-Sn systems, *Calphad* 47 (2014) 129–135, <https://doi.org/10.1016/j.calphad.2014.07.002>.
- [230] H. Yuan, J. Wang, B. Hu, R. Zhao, Y. Du, S.-Y. Zhang, Thermodynamic assessment of the Te-X (X = As, Si, Co) systems, *Calphad* 68 (2020) 101743, <https://doi.org/10.1016/j.calphad.2020.101743>.
- [231] D. Boa, I. Ansara, Thermodynamic assessment of the ternary system Bi-In-Pb, *Thermochimica Acta* 314 (1998) 79–86, [https://doi.org/10.1016/S0040-6031\(98\)00237-8](https://doi.org/10.1016/S0040-6031(98)00237-8).
- [232] X. Zhang, Y.F. Cui, G.L. Xu, W.J. Zhu, H.S. Liu, B.Y. Yin, Z.P. Jin, Thermodynamic assessment of the U-Mo-Al system, *Journal of Nuclear Materials* 402 (2010) 15–24, <https://doi.org/10.1016/j.jnucmat.2010.04.018>.
- [233] K. Achgar, S. Kardellass, N. Selhaoui, Thermodynamic assessment of the Ytterbium-Germanium binary system, *J Therm Anal Calorim* 131 (2018) 443–453, <https://doi.org/10.1007/s10973-017-6203-x>.
- [234] M. Peters, Thermodynamic assessments of Bi-Te Bi-Se Sb-Te. <http://hdl.handle.net/11256/974>, 2018.
- [235] X. Ren, C. Li, Z. Du, C. Guo, Thermodynamic assessments of six binary systems of alkali metals, *Calphad* 35 (2011) 446–454, <https://doi.org/10.1016/j.calphad.2011.06.005>.
- [236] S.L. Wang, C.P. Wang, X.J. Liu, K. Ishida, Thermodynamic assessments of the Ag-Y and Sc-Y systems, *Journal of Alloys and Compounds* 476 (2009) 187–192, <https://doi.org/10.1016/j.jallcom.2008.09.053>.
- [237] S.L. Wang, L.J. Zhou, Z.F. Lan, J.L. Li, Y.H. Lin, C.P. Wang, X.J. Liu, Thermodynamic assessments of the Au-Nd and Au-Dy systems, *J. Phase Equilib. Diffus.* 36 (2015) 241–247, <https://doi.org/10.1007/s11669-015-0378-2>.
- [238] S.L. Wang, L.J. Zhou, X. Qin, Y.H. Li, J.L. Li, Y. Pan, Y.H. Lin, C.P. Wang, X.J. Liu, Thermodynamic assessments of the Au-Gd and Au-Yb systems, *Calphad* 53 (2016) 90–96, <https://doi.org/10.1016/j.calphad.2016.02.002>.
- [239] C.P. Wang, Z. Lin, X.J. Liu, Thermodynamic assessments of the Dy-Mn and Mn-Pr systems, *Journal of Alloys and Compounds* 469 (2009) 123–128, <https://doi.org/10.1016/j.jallcom.2008.01.092>.
- [240] C.P. Wang, S.H. Guo, X.J. Liu, A.T. Tang, F.S. Pan, Thermodynamic assessments of the Ho-X (X: Cu, Mo, V) systems, *Journal of Alloys and Compounds* 487 (2009) 173–178, <https://doi.org/10.1016/j.jallcom.2009.08.042>.
- [241] F. Gao, S.L. Wang, C.P. Wang, X.J. Liu, Thermodynamic assessments of the In-Eu and In-Yb systems, *Calphad* 35 (2011) 1–5, <https://doi.org/10.1016/j.calphad.2010.10.003>.
- [242] X.J. Liu, S.L. Wang, C.P. Wang, Thermodynamic assessments of the Sc-M (M: Ag, B and Th) systems, *Journal of Alloys and Compounds* 469 (2009) 186–192, <https://doi.org/10.1016/j.jallcom.2008.02.018>.
- [243] B.-J. Lee, Thermodynamic assessments of the Sn-Zn and In-Zn binary systems, *Calphad* 20 (1996) 471–480, [https://doi.org/10.1016/S0364-5916\(97\)00009-6](https://doi.org/10.1016/S0364-5916(97)00009-6).
- [244] Y. Liu, Z. Kang, J. Wang, Thermodynamic basis and related phase equilibria for Bi-Li and Bi-Na binary systems, *Thermochimica Acta* 558 (2013) 53–60, <https://doi.org/10.1016/j.tca.2013.01.029>.
- [245] L. Wang, Y. Liu, J. Liu, Thermodynamic basis and related phase equilibria for in-Na and in-Ca binary systems, *J. Phase Equilib. Diffus.* 34 (2013) 447–452, <https://doi.org/10.1007/s11669-013-0258-6>.
- [246] J. Gröbner, R. Wenzel, G.G. Fischer, R. Schmid-Fetzer, Thermodynamic calculation of the binary systems M-Ga and investigation of ternary M-Ga-N phase equilibria (M=Ni, Co, Pd, Cr), *JPE* 20 (1999) 615–625, <https://doi.org/10.1361/105497199770340608>.
- [247] K. Xu, S. Liu, F. Zhang, Y. Du, Z. Jin, Thermodynamic calculations of the Au-Sc and Fe-Sc systems, *Calphad* 54 (2016) 158–164, <https://doi.org/10.1016/j.calphad.2016.07.002>.
- [248] B.-J. Lee, B. Sundman, S.I. Kim, K.-G. Chin, Thermodynamic calculations on the stability of Cu₂S in low carbon steels, *ISIJ Int* 47 (2007) 163–171, <https://doi.org/10.2355/isijinternational.47.163>.
- [249] W. Gierlotka, J. Łapsa, K. Fitzner, Thermodynamic description of the Ag-Pb-Te ternary system, *J. Phase Equilib. Diffus.* 31 (2010) 509–517, <https://doi.org/10.1007/s11669-010-9791-8>.
- [250] Z. Du, C. Guo, C. Li, W. Zhang, Thermodynamic description of the Al-Mo and Al-Fe-Mo systems, *J. Phase Equilib. Diffus.* 30 (2009) 487–501, <https://doi.org/10.1007/s11669-009-9564-4>.
- [251] F.G. Meng, H.S. Liu, L.B. Liu, Z.P. Jin, Thermodynamic description of the Au-Si-Sn system, *Journal of Alloys and Compounds* 431 (2007) 292–297, <https://doi.org/10.1016/j.jallcom.2006.05.066>.
- [252] M. Idbenali, C. Servant, M. Feddaoui, Thermodynamic description of the Ce-Ga binary system, *J. Phase Equilib. Diffus.* 34 (2013) 467–473, <https://doi.org/10.1007/s11669-013-0261-y>.
- [253] J. Miettinen, Thermodynamic description of the Cu-Mn-Zn system in the copper-rich corner, *Calphad* 28 (2004) 313–320, <https://doi.org/10.1016/j.calphad.2004.09.003>.
- [254] K. Xu, L. Chen, K. Chang, P. Wan, M. Li, Z. Deng, F. Huang, Q. Huang, Thermodynamic description of the Dy-Si-C system in silicon carbide ceramics, *Calphad* 68 (2020) 101738, <https://doi.org/10.1016/j.calphad.2020.101738>.
- [255] M. Idbenali, C. Servant, Thermodynamic description of the Gallium-Lanthanum binary system, in: XXXVII JEEP – 37th Conference on Phase Equilibria, EDP Sciences, Saint-Avoid, France, 2011 00008, <https://doi.org/10.1051/jeep/201100008>.
- [256] S. Kardellass, C. Servant, N. Selhaoui, Thermodynamic description of the Ni-Yb and Ni-Eu binary systems, *J Therm Anal Calorim* 125 (2016) 255–269, <https://doi.org/10.1007/s10973-016-5380-3>.
- [257] M. Idbenali, C. Servant, N. Selhaoui, L. Bouriden, Thermodynamic description of the Pb-Yb binary system, *Calphad* 33 (2009) 570–575, <https://doi.org/10.1016/j.calphad.2009.05.001>.
- [258] Z. Long, F. Yin, Y. Liu, J. Wang, H. Liu, Z. Jin, Thermodynamic description of the Ru-(Si,Ge)-Sn ternary systems, *J. Phase Equilib. Diffus.* 33 (2012) 97–105, <https://doi.org/10.1007/s11669-012-0002-7>.
- [259] K. Xu, H. Zou, K. Chang, Z. Deng, X. Zhou, Y. Huang, L. Chen, F. Huang, Q. Huang, Thermodynamic description of the sintering aid system in silicon carbide ceramics with the addition of yttrium, *Journal of the European Ceramic Society* 39 (2019) 4510–4519, <https://doi.org/10.1016/j.jeurceramsoc.2019.07.012>.
- [260] W. Gierlotka, Thermodynamic description of the Te-Tl binary system using the associate solution model, *Journal of Elec Materi* 39 (2010) 1319–1325, <https://doi.org/10.1007/s11664-010-1248-7>.
- [261] S. Huang, Y. Liu, Y. Chen, Z. Kang, Thermodynamic descriptions and phase diagrams for Pb-S and Bi-S binary systems, *Journal of Elec Materi* 43 (2014) 1237–1243, <https://doi.org/10.1007/s11664-014-3004-x>.
- [262] Y. Liu, J. Xu, Z. Kang, J. Wang, Thermodynamic descriptions and phase diagrams for Sb-Na and Sb-K binary systems, *Thermochimica Acta* 569 (2013) 119–126, <https://doi.org/10.1016/j.tca.2013.07.009>.
- [263] Y. Liu, L. Zhang, D. Yu, Thermodynamic descriptions for the Cd-Te, Pb-Te, Cd-Pb and Cd-Pb-Te systems, *Journal of Elec Materi* 38 (2009) 2033–2045, <https://doi.org/10.1007/s11664-009-0875-3>.
- [264] Y. Liu, D. Liang, L. Zhang, Thermodynamic descriptions for the Sn-Te and Pb-Sn-Te systems, *Journal of Elec Materi* 39 (2010) 246–257, <https://doi.org/10.1007/s11664-009-0985-y>.
- [265] W. Yi, J. Gao, Y. Tang, L. Zhang, Thermodynamic descriptions of ternary Al-Si-Sr system supported by key experiments, *Calphad* 68 (2020) 101732, <https://doi.org/10.1016/j.calphad.2019.101732>.
- [266] P.-Y. Chevalier, Thermodynamic evaluation of the Bi-Ge system, *Thermochimica Acta* 132 (1988) 111–116, [https://doi.org/10.1016/0040-6031\(88\)87100-4](https://doi.org/10.1016/0040-6031(88)87100-4).
- [267] D. Boa, B.K. Dongui, I. Ansara, Thermodynamic evaluation of the Co-In system, *Calphad* 25 (2001) 645–650, [https://doi.org/10.1016/S0364-5916\(02\)00014-7](https://doi.org/10.1016/S0364-5916(02)00014-7).
- [268] X.J. Liu, P. Yu, C.P. Wang, K. Ishida, Thermodynamic evaluation of the Co-Sc and Fe-Sc systems, *Journal of Alloys and Compounds* 466 (2008) 169–175, <https://doi.org/10.1016/j.jallcom.2007.11.069>.
- [269] W. Zhuang, Z.-Y. Qiao, S. Wei, J. Shen, Thermodynamic evaluation of the Cu-R (R: Ce, Pr, Nd, Sm) binary systems, *JPE* 17 (1996) 508–521, <https://doi.org/10.1007/BF02665998>.
- [270] M. Idbenali, C. Servant, Thermodynamic evaluation of the Ga-Y system, *J Therm Anal Calorim* 112 (2013) 245–253, <https://doi.org/10.1007/s10973-012-2861-x>.
- [271] K. Achgar, N. Selhaoui, A. Iddoudi, R. Tamim, H. Azza, L. Bouriden, Thermodynamic evaluation of the germanium-lutetium and dysprosium-germanium binary systems, *Calphad* 62 (2018) 18–29, <https://doi.org/10.1016/j.calphad.2018.05.001>.
- [272] Y. Feutalais, B. Legendre, S.G. Fries, Thermodynamic evaluation of the system germanium – tin, *Calphad* 20 (1996) 109–123, [https://doi.org/10.1016/0364-5916\(96\)00018-1](https://doi.org/10.1016/0364-5916(96)00018-1).
- [273] P.-Y. Chevalier, Thermodynamic evaluation of the Ag-Si system, *Thermochimica Acta* 130 (1988) 33–41, [https://doi.org/10.1016/0040-6031\(88\)87048-5](https://doi.org/10.1016/0040-6031(88)87048-5).
- [274] C. Bergman, R. Chastel, R. Castanet, Thermodynamic investigation on the si-ge binary system by calorimetry and knudsen cell mass spectrometry, *JPE* 13 (1992) 113–118, <https://doi.org/10.1007/BF02667471>.
- [275] H.Q. Dong, X.M. Tao, T. Laurila, V. Vuorinen, M. Paulasto-Kröckel, Thermodynamic modeling of Au-Ce-Sn ternary system, *Calphad* 42 (2013) 38–50, <https://doi.org/10.1016/j.calphad.2013.07.013>.
- [276] Y. Liu, D. Liang, Thermodynamic modeling of the Ag-Sr system, *Journal of Alloys and Compounds* 407 (2006) 74–77, <https://doi.org/10.1016/j.jallcom.2005.06.019>.
- [277] J. Wang, Y.J. Liu, L.B. Liu, H.Y. Zhou, Z.P. Jin, Thermodynamic modeling of the Au-Sb-Si ternary system, *Journal of Alloys and Compounds* 509 (2011) 3057–3064, <https://doi.org/10.1016/j.jallcom.2010.11.199>.
- [278] X. Ren, C. Li, Z. Du, C. Guo, S. Chen, Thermodynamic modeling of the Ba-Mg binary system, *International Journal of Materials Research* 104 (2013) 358–363, <https://doi.org/10.3139/146.110870>.
- [279] Y. Zhong, K. Ozturk, Z.-K. Liu, Thermodynamic modeling of the Ca-Sr-Zn ternary system, *JPE* 24 (2003) 340–346, <https://doi.org/10.1361/105497103770330325>.
- [280] S. Qin, S. Liu, C. Zhang, J. Xin, Y. Wang, Y. Du, Thermodynamic modeling of the Ca-In and Ca-Sb systems supported with first-principles calculations, *Calphad* 48 (2015) 35–42, <https://doi.org/10.1016/j.calphad.2014.10.008>.
- [281] M. Ohno, A. Kozlov, R. Arroyave, Z. Liu, R. Schmidfetzner, Thermodynamic modeling of the Ca-Sn system based on finite temperature quantities from first-principles and experiment, *Acta Materialia* 54 (2006) 4939–4951, <https://doi.org/10.1016/j.actamat.2006.06.017>.
- [282] Y. Liu, J.-C. Tedenac, Thermodynamic modeling of the Cd-Sb-Zn ternary system, *Calphad* 33 (2009) 684–694, <https://doi.org/10.1016/j.calphad.2009.08.006>.
- [283] X. Su, W. Zhang, Z. Du, Thermodynamic modeling of the Co-Dy system, *International Journal of Materials Research* 89 (1998) 522–526.
- [284] X. Lu, S. Liu, K. Cheng, Y. Tang, P. Ou, P. Nash, B. Sundman, Y. Du, F. Zheng, Thermodynamic modeling of the Co-Hf system supported by key experiments and first-principles calculations, *Thermochimica Acta* 608 (2015) 49–58.
- [285] Y. Yuan, J. Yi, G. Borzone, A. Watson, Thermodynamic modeling of the Co-Sm system, *Calphad* 35 (2011) 416–420, <https://doi.org/10.1016/j.calphad.2011.06.001>.
- [286] G. Ghosh, G.B. Olson, Thermodynamic modeling of the Cr-Pd and Mo-Pd systems, *JPE* 21 (2000) 32–39, <https://doi.org/10.1361/105497100770340390>.

- [287] C. He, Y. Du, H.-L. Chen, S. Liu, H. Xu, Y. Ouyang, Z.-K. Liu, Thermodynamic modeling of the Cu–Mn system supported by key experiments, *Journal of Alloys and Compounds* 457 (2008) 233–238, <https://doi.org/10.1016/j.jallcom.2007.03.041>.
- [288] V.B. Rajkumar, K.C. Hari Kumar, Thermodynamic modeling of the Fe–Mo system coupled with experiments and ab initio calculations, *Journal of Alloys and Compounds* 611 (2014) 303–312, <https://doi.org/10.1016/j.jallcom.2014.05.030>.
- [289] J. Wang, W. Yuan, M. Li, Thermodynamic modeling of the Ga–N–Na system, *Journal of Crystal Growth* 307 (2007) 59–65, <https://doi.org/10.1016/j.jcrysgro.2007.05.044>.
- [290] K. Cheng, B. Hu, Y. Du, H. Xu, Q. Gao, Thermodynamic modeling of the Ge–Sc system supported by key experiments and first-principles calculation, *Calphad* 37 (2012) 18–24, <https://doi.org/10.1016/j.calphad.2011.12.010>.
- [291] A. Berche, J.C. Tedenac, P. Jund, Thermodynamic modeling of the germanium–manganese system, *Intermetallics* 47 (2014) 23–30, <https://doi.org/10.1016/j.intermet.2013.12.009>.
- [292] Y. Liang, C. Guo, C. Li, Z. Du, Thermodynamic modeling of the In–Pt system, *Journal of Alloys and Compounds* 475 (2009) 220–226, <https://doi.org/10.1016/j.jallcom.2008.07.086>.
- [293] C. Jiang, Z.-K. Liu, Thermodynamic modeling of the indium–palladium system, *Metall Mater Trans A* 33 (2002) 3597–3603, <https://doi.org/10.1007/s11661-002-0235-x>.
- [294] Y. Liang, Z. Du, C. Guo, C. Li, Thermodynamic modeling of the Li–Zn system, *Journal of Alloys and Compounds* 455 (2008) 236–242, <https://doi.org/10.1016/j.jallcom.2007.01.154>.
- [295] T. Balakumar, M. Medraj, Thermodynamic modeling of the Mg–Al–Sb system, *Calphad* 29 (2005) 24–36, <https://doi.org/10.1016/j.calphad.2005.03.001>.
- [296] K. Yaqoob, J.-C. Crivello, J.-M. Joubert, Thermodynamic modeling of the Mo–Ni system, *Calphad* 62 (2018) 215–222, <https://doi.org/10.1016/j.calphad.2018.07.002>.
- [297] Z. Sun, X. Guo, C. Zhang, Thermodynamic modeling of the Nb-rich corner in the Nb–Si–Sn system, *Calphad* 36 (2012) 82–88, <https://doi.org/10.1016/j.calphad.2011.12.002>.
- [298] G. Ghosh, C. Kantner, G.B. Olson, Thermodynamic modeling of the Pd–X (X=Ag, Co, Fe, Ni) systems, *JPE* 20 (1999) 295–308, <https://doi.org/10.1361/10549719970335811>.
- [299] Q. Yue, Y.-Q. Liu, M.-Y. Chu, J.-Y. Shen, Thermodynamic modeling of the Sn–V binary system, *Calphad* 33 (2009) 539–544, <https://doi.org/10.1016/j.calphad.2009.03.003>.
- [300] R. Arroyave, Z.-K. Liu, Thermodynamic modelling of the Zn–Zr system, *Calphad* 30 (2006) 1–13, <https://doi.org/10.1016/j.calphad.2005.12.006>.
- [301] K.C.H. Kumar, I. Ansara, P. Wollants, L. Delaey, Thermodynamic optimisation of the Cu–Ti system, *International Journal of Materials Research* 87 (1996) 666–672, <https://doi.org/10.1515/ijmr-1996-870811>.
- [302] D. Risold, B. Hallstedt, L.J. Gauckler, H.L. Lukas, S.G. Fries, Thermodynamic optimization of the Ca–Cu and Sr–Cu systems, *Calphad* 20 (1996) 151–160, [https://doi.org/10.1016/S0364-5916\(96\)00022-3](https://doi.org/10.1016/S0364-5916(96)00022-3).
- [303] Y. Liu, D. Yu, Y. Ge, Thermodynamic optimization of the Cd–Na and Cd–Ti binary systems, *Journal of Alloys and Compounds* 473 (2009) 60–64, <https://doi.org/10.1016/j.jallcom.2008.05.106>.
- [304] G.P. Vassilev, M. Jiang, Thermodynamic optimization of the Co–Zn system, *Journal of Phase Equilibria & Diffusion* 25 (2004) 259–268, <https://doi.org/10.1361/1547730419522>.
- [305] P. Wang, L. Zhou, Y. Du, H. Xu, S. Liu, L. Chen, Y. Ouyang, Thermodynamic optimization of the Cu–Nd system, *Journal of Alloys and Compounds* 509 (2011) 2679–2683, <https://doi.org/10.1016/j.jallcom.2010.11.160>.
- [306] K. Achgar, S. Kardellass, N. Selhaoui, L. Bouriden, Thermodynamic optimization of the Erbium–Germanium binary system, *Journal of Alloys and Compounds* 724 (2017) 1157–1166, <https://doi.org/10.1016/j.jallcom.2017.07.129>.
- [307] M. Idbenali, C. Servant, Thermodynamic optimization of the germanium–yttrium system, *J Therm Anal Calorim* 111 (2013) 911–916, <https://doi.org/10.1007/s10973-012-2271-0>.
- [308] A. Iddoudi, N. Selhaoui, S. Kardellass, M. Ait Amar, K. Mahdoui, H. Najih, L. Bouriden, Thermodynamic optimization of the Ho–Sn system, *J Therm Anal Calorim* 115 (2014) 941–945, <https://doi.org/10.1007/s10973-013-3352-4>.
- [309] C. Zhou, C. Guo, C. Li, Z. Du, Thermodynamic optimization of the Li–Pb system aided by first-principles calculations, *Journal of Nuclear Materials* 477 (2016) 95–101, <https://doi.org/10.1016/j.jnucmat.2016.04.061>.
- [310] C. Guo, Z. Du, Thermodynamic optimization of the Mg–Tb and Mg–Yb systems, *Journal of Alloys and Compounds* 422 (2006) 102–108, <https://doi.org/10.1016/j.jallcom.2005.11.060>.
- [311] H. Jürgen Seifert, H.L. Lukas, G. Petzow, Thermodynamic Optimization of the Ti–Si System/Thermodynamische Optimierung des Systems Ti–Si: Dedicated to Professor Dr. rer. nat. Dr. h.c. Hein Peter Stüwe on the occasion of his 65th birthday, *International Journal of Materials Research* 87 (1996) 2–13, <https://doi.org/10.1515/ijmr-1996-870102>.
- [312] J. Liu, P.-W. Guan, C.N. Marker, N.D. Smith, N. Orabona, S.-L. Shang, H. Kim, Z.-K. Liu, Thermodynamic properties and phase stability of the Ba–Bi system: a combined computational and experimental study, *Journal of Alloys and Compounds* 771 (2019) 281–289, <https://doi.org/10.1016/j.jallcom.2018.08.324>.
- [313] H. Bo, J. Wang, L. Duarte, C. Leinenbach, L. Liu, H. Liu, Z. Jin, Thermodynamic re-assessment of Fe–Ti binary system, *Transactions of Nonferrous Metals Society of China* 22 (2012) 2204–2211, [https://doi.org/10.1016/S1003-6326\(11\)61450-7](https://doi.org/10.1016/S1003-6326(11)61450-7).
- [314] H. Bo, L.B. Liu, J.L. Hu, X.D. Zhang, Z.P. Jin, Thermodynamic re-assessment of the Al–Gd and Gd–Zr systems, *Thermochimica Acta* 591 (2014) 51–56, <https://doi.org/10.1016/j.tca.2014.07.014>.
- [315] X.L. Chen, J. Wang, T.L. Chen, X.D. Lin, M.H. Rong, G.H. Rao, H.Y. Zhou, Thermodynamic re-assessment of the Fe–Gd and Fe–Sm binary systems, *Calphad* 58 (2017) 151–159, <https://doi.org/10.1016/j.calphad.2017.07.005>.
- [316] S. An Mey, Thermodynamic re-evaluation of the Cu–Ni system, *Calphad* 16 (1992) 255–260, [https://doi.org/10.1016/0364-5916\(92\)90022-P](https://doi.org/10.1016/0364-5916(92)90022-P).
- [317] W. Wang, C. Guo, C. Li, Z. Du, Thermodynamic re-modeling of the Co–Gd system: paper presented at the 2nd sino-German symposium on computational thermodynamics and kinetics and their applications to solidification, *International Journal of Materials Research* 101 (2010) 1339–1346, <https://doi.org/10.3139/146.110415>.
- [318] V.T. Witusiewicz, A.A. Bondar, U. Hecht, T.Ya Velikanova, Thermodynamic re-modelling of the ternary Al–Cr–Ti system with refined Al–Cr description, *Journal of Alloys and Compounds* 644 (2015) 939–958, <https://doi.org/10.1016/j.jallcom.2015.04.231>.
- [319] Y. Feng, R. Wang, C. Peng, H. Liu, Thermodynamic reassessment of Ga–Hg and Mg–Hg systems, *J. Cent. South Univ. Technol.* 16 (2009) 32–37, <https://doi.org/10.1007/s11771-009-0005-7>.
- [320] Z. Rahou, K. Mahdoui, Thermodynamic reassessment of Gd–Ni system, *Journal of Alloys and Compounds* 648 (2015) 346–352, <https://doi.org/10.1016/j.jallcom.2015.06.201>.
- [321] H.S. Liu, Y. Cui, K. Ishida, Z.P. Jin, Thermodynamic reassessment of the Au–In binary system, *Calphad* 27 (2003) 27–37, [https://doi.org/10.1016/S0364-5916\(03\)00028-2](https://doi.org/10.1016/S0364-5916(03)00028-2).
- [322] C. Servant, E. Zoro, B. Legendre, Thermodynamic reassessment of the Au–Bi system, *Calphad* 30 (2006) 443–448, <https://doi.org/10.1016/j.calphad.2006.07.002>.
- [323] J. Zhao, Y. Du, L. Zhang, H. Xu, Thermodynamic reassessment of the Cu–V system supported by key experiments, *Calphad* 32 (2008) 252–255, <https://doi.org/10.1016/j.calphad.2007.07.009>.
- [324] Y. Wang, B. Hu, S. Liu, Y. Du, Thermodynamic reassessment of the La–Mn system, *J Min Metall B Metall* 48 (2012) 391–394, <https://doi.org/10.2298/JMMB120717049W>.
- [325] L. Liu, Z. Jin, Thermodynamic reassessment of the La–Ni system, *International Journal of Materials Research* 91 (2000) 739–743, <https://doi.org/10.1515/ijmr-2000-910906>.
- [326] Y. Feng, R. Wang, H. Liu, Z. Jin, Thermodynamic reassessment of the magnesium–gallium system, *Journal of Alloys and Compounds* 486 (2009) 581–585, <https://doi.org/10.1016/j.jallcom.2009.07.010>.
- [327] T.T. Dorini, L.T.F. Eleno, Thermodynamic reassessment of the Ni–In system using ab-initio data for end-member compound energies, *Calphad* 62 (2018) 42–48, <https://doi.org/10.1016/j.calphad.2018.05.004>.
- [328] Y. Liu, D. Liang, Thermodynamic reevaluation of the Mg–Ti system, *Journal of Alloys and Compounds* 459 (2008) 286–290, <https://doi.org/10.1016/j.jallcom.2007.04.031>.
- [329] J. Miettinen, Thermodynamic solution phase data for binary Mn-based systems, *Calphad* 25 (2001) 43–58, [https://doi.org/10.1016/S0364-5916\(01\)00029-3](https://doi.org/10.1016/S0364-5916(01)00029-3).
- [330] D. Jendrzyszczak-Handzlik, Thermodynamic study and Re-optimization of the Au–Ga binary system, *J. Phase Equilib. Diffus.* 38 (2017) 305–318, <https://doi.org/10.1007/s11669-017-0543-x>.
- [331] J.L. Hu, H. Bo, L.B. Liu, Z.P. Jin, Thermodynamic study of the Al–Sc–Y system, *Thermochimica Acta* 661 (2018) 147–159, <https://doi.org/10.1016/j.tca.2018.01.018>.
- [332] Y. Zhong, J.O. Sofo, A.A. Luo, Z.-K. Liu, Thermodynamics modeling of the Mg–Sr and Ca–Mg–Sr systems, *Journal of Alloys and Compounds* 421 (2006) 172–178, <https://doi.org/10.1016/j.jallcom.2005.09.076>.
- [333] M.A. Turchanin, P.G. Agraval, I.V. Nikolaenko, Thermodynamics of alloys and phase equilibria in the copper–iron system, *JPE* 24 (2003) 307–319, <https://doi.org/10.1361/105497103770330280>.
- [334] T. Cheng, Y. Tang, L. Zhang, Update of thermodynamic descriptions of the binary Al–Sn and ternary Mg–Al–Sn systems, *Calphad* 64 (2019) 354–363, <https://doi.org/10.1016/j.calphad.2019.01.005>.
- [335] F. Tang, B. Hallstedt, Using the PARROT module of Thermo-Calc with the Cr–Ni system as example, *Calphad* 55 (2016) 260–269, <https://doi.org/10.1016/j.calphad.2016.10.003>.
- [336] T. Abe, K. Hashimoto, Y. Goto, Y. Sawada, K. Hirose, CPDDB (2007), <https://doi.org/10.48505/NIMS.3060>.
- [337] A. Van De Walle, C. Nataraj, Z.-K. Liu, The thermodynamic database database, *Calphad* 61 (2018) 173–178, <https://doi.org/10.1016/j.calphad.2018.04.003>.
- [338] W. Cao, S.-L. Chen, F. Zhang, K. Wu, Y. Yang, Y.A. Chang, R. Schmid-Fetzer, W. A. Oates, PANDAT software with PanEngine, PanOptimizer and PanPrecipitation for multi-component phase diagram calculation and materials property simulation, *Calphad* 33 (2009) 328–342, <https://doi.org/10.1016/j.calphad.2008.08.004>.
- [339] Y. Zhong, C. Wolverton, Y. Austin Chang, Z.-K. Liu, A combined CALPHAD/first-principles remodeling of the thermodynamics of Al–Sr: unsuspected ground state energies by “rounding up the (un)usual suspects,” *Acta Materialia* 52 (2004) 2739–2754, <https://doi.org/10.1016/j.actamat.2004.02.022>.
- [340] L.A. Zabdyr, Equilibrium diagram and thermodynamic properties of cadmium – antimony binary alloys, *Critical assessment*, *Calphad* 17 (1993) 125–132, [https://doi.org/10.1016/0364-5916\(93\)90012-Z](https://doi.org/10.1016/0364-5916(93)90012-Z).
- [341] U.R. Kattner, W.J. Boettinger, On the Sn–Bi–Ag ternary phase diagram, *J. Electron. Mater.* 23 (1994) 603–610, <https://doi.org/10.1007/BF02653345>.

- [342] R.C. Sharma, T.L. Ngai, Y.A. Chang, The In-Sb (Indium-Antimony) system, *Bulletin of Alloy Phase Diagrams* 10 (1989) 657–664, <https://doi.org/10.1007/BF02877639>.
- [343] H.Q. Dong, S. Jin, L.G. Zhang, J.S. Wang, X.M. Tao, H.S. Liu, Z.P. Jin, Thermodynamic assessment of the Au-Co-Sn ternary system, *Journal of Elec Materi* 38 (2009) 2158–2169, <https://doi.org/10.1007/s11664-009-0874-4>.
- [344] N. David, K. El Aissaoui, J.M. Fiorani, J. Hertz, M. Vilasi, Thermodynamic optimization of the In-Pb-Sn system based on new evaluations of the binary borders In-Pb and In-Sn, *Thermochimica Acta* 413 (2004) 127–137, <https://doi.org/10.1016/j.tca.2003.10.020>.
- [345] S. Kulawik, W. Gierlotka, A. Dębski, W. Gąsior, A. Zajczkowski, Calorimetric and phase diagram studies of the Ga-In-Zn system, *Journal of Molecular Liquids* 325 (2021) 115114, <https://doi.org/10.1016/j.molliq.2020.115114>.
- [346] A. Dębski, W. Gąsior, W. Gierlotka, M. Polański, Calorimetric studies and thermodynamic modelling of liquid Mg-Pb-Pd alloys, *J. Mol. Liq.* 371 (2023) 121123, <https://doi.org/10.1016/j.molliq.2022.121123>.
- [347] A. Dębski, S. Terlicka, W. Gąsior, M. Saterus, A. Fornalczyk, Calorimetric studies and thermodynamic properties of Li-Pb-Pd liquid alloys, *Journal of Molecular Liquids* 339 (2021) 116791, <https://doi.org/10.1016/j.molliq.2021.116791>.
- [348] J. Fels, P. Berger, T.L. Reichmann, H.J. Seifert, H. Flandorfer, Calorimetric studies of mixing enthalpy in the liquid system Ga-Li, and Ga-Li-Sn, *Journal of Molecular Liquids* 295 (2019) 111578, <https://doi.org/10.1016/j.molliq.2019.111578>.
- [349] M. Zabrocki, W. Gąsior, A. Dębski, Calorimetric study and thermodynamic description of Ga-Ge-Li liquid alloys, *Calphad* 71 (2020) 102204, <https://doi.org/10.1016/j.calphad.2020.102204>.
- [350] V.T. Witusiewicz, S.G. Fries, U. Hecht, A. Drevermann, S. Rex, Enthalpies of formation measurements and thermodynamic description of the Ag-Cu-Zn system, *International Journal of Materials Research* 97 (2006) 556–568, <https://doi.org/10.3139/146.101272>.
- [351] N. Usenko, M. Ivanov, N. Kotova, Enthalpies of mixing in binary Cu-Eu and ternary Al-Cu-Eu liquid alloys, *International Journal of Materials Research* 111 (2020) 273–282, <https://doi.org/10.3139/146.111895>.
- [352] M. Ivanov, N. Usenko, N. Kotova, Enthalpies of mixing in binary Mn-In and ternary Mn-In-Gd liquid alloys, *International Journal of Materials Research* 109 (2018) 291–300, <https://doi.org/10.3139/146.111611>.
- [353] C. Luef, H. Flandorfer, H. Ipser, Enthalpies of mixing of liquid alloys in the In-Pd-Sn system and the limiting binary systems, *Thermochimica Acta* 417 (2004) 47–57, <https://doi.org/10.1016/j.tca.2004.01.019>.
- [354] M. Rechchach, A. Sabbar, H. Flandorfer, H. Ipser, Enthalpies of mixing of liquid In-Sn and In-Sn-Zn alloys, *Thermochimica Acta* 502 (2010) 66–72, <https://doi.org/10.1016/j.tca.2010.02.008>.
- [355] H. Flandorfer, M. Rechchach, A. Elmahfoudi, L. Bencze, A. Popović, H. Ipser, Enthalpies of mixing of liquid systems for lead free soldering: Al-Cu-Sn system, *The Journal of Chemical Thermodynamics* 43 (2011) 1612–1622, <https://doi.org/10.1016/j.jct.2011.05.021>.
- [356] P. Benigni, S. Hassam, A. Decretion, G. Mikaelian, K. Gajavalli, M. Barrachin, E. Fischer, J. Rogez, Enthalpy of mixing in the Ag-Cd-In ternary liquid phase, *The Journal of Chemical Thermodynamics* 107 (2017) 207–215, <https://doi.org/10.1016/j.jct.2016.12.005>.
- [357] P. Fima, H. Flandorfer, Enthalpy of mixing of liquid Ag-Bi-Cu alloys at 1073K, *Thermochimica Acta* 575 (2014) 336–342, <https://doi.org/10.1016/j.tca.2013.11.018>.
- [358] P. Berger, H. Flandorfer, Enthalpy of mixing of liquid Li-Sb-Sn alloys, *Journal of Molecular Liquids* 298 (2020) 112036, <https://doi.org/10.1016/j.molliq.2019.112036>.
- [359] A. Elmahfoudi, S. Fürtauer, A. Sabbar, H. Flandorfer, Enthalpy of mixing of liquid systems for lead free soldering: Ni-Sb-Sn system, *Thermochimica Acta* 534 (2012) 33–40, <https://doi.org/10.1016/j.tca.2012.01.024>.
- [360] M. Premović, Y. Du, D. Minić, B. Sundman, C. Zhang, A. Watson, D. Manasijević, A. Djordjević, Experimental investigation and thermodynamic calculations of the Ag-Ga-Sn phase diagram, *Calphad* 56 (2017) 215–223, <https://doi.org/10.1016/j.calphad.2017.01.010>.
- [361] C.-Y. He, Y. Du, H.-L. Chen, H. Xu, Experimental investigation and thermodynamic modeling of the Al-Cu-Si system, *Calphad* 33 (2009) 200–210, <https://doi.org/10.1016/j.calphad.2008.07.015>.
- [362] S. Terlicka, A. Dębski, W. Gąsior, A. Fornalczyk, M. Saterus, Experimental results of the Li-Pb-Pt system obtained by the high temperature drop calorimetry, *Journal of Molecular Liquids* 332 (2021) 115824, <https://doi.org/10.1016/j.molliq.2021.115824>.
- [363] E. Fischer, K. Gajavalli, G. Mikaelian, P. Benigni, J. Rogez, A. Decretion, M. Barrachin, Experimental study and thermodynamic modelling of the Ag-Cd-In system, *Calphad* 64 (2019) 292–305, <https://doi.org/10.1016/j.calphad.2019.01.001>.
- [364] D. Jendrzeczyk-Handzlik, P. Handzlik, Heat of mixing of the liquid silver-indium and silver-gallium-indium alloys, *Metall Mater Trans A* 54 (2023) 4744–4756, <https://doi.org/10.1007/s11661-023-07196-5>.
- [365] C. Luef, H. Flandoreer, H. Ipser, Lead-free solder materials: experimental enthalpies of mixing of liquid Ag-In-Pd-Sn alloys, *Metall Mater Trans A* 36 (2005) 1273–1277, <https://doi.org/10.1007/s11661-005-0219-8>.
- [366] V. Singh, D. Pathote, D. Jaiswal, M.R. Kumar, K.K. Singh, C.K. Behera, Measurement of mixing enthalpies for Sn-Bi-Sb lead-free solder system, *J. Electron. Mater.* 52 (2023) 6316–6334, <https://doi.org/10.1007/s11664-023-10579-4>.
- [367] A. Dębski, W. Gąsior, W. Gierlotka, M. Polański, Mixing enthalpies of liquid Ag-Mg-Pb alloys: experiment vs. Thermodynamic modeling, *Materials* 15 (2022) 7360, <https://doi.org/10.3390/ma15207360>.
- [368] M.A. Turchanin, L.A. Dreval, A.R. Abdulov, P.G. Agraval, Mixing enthalpies of liquid alloys and thermodynamic assessment of the Cu-Fe-Co system, *Powder Metall Met Ceram* 50 (2011) 98–116, <https://doi.org/10.1007/s11106-011-9307-z>.
- [369] M.A. Turchanin, T.Ya Velikanova, L.A. Dreval, A.R. Abdulov, P.G. Agraval, Mixing enthalpies of liquid alloys and thermodynamic assessment of the Cu-Fe-Ni system, *Powder Metall Met Ceram* 48 (2009) 672–692, <https://doi.org/10.1007/s11106-010-9186-8>.
- [370] D. Jendrzeczyk-Handzlik, P. Handzlik, Mixing enthalpies of liquid Au-Ga-In alloys, *J. Mol. Liq.* 301 (2020) 112439, <https://doi.org/10.1016/j.molliq.2019.112439>.
- [371] M.A. Turchanin, A.A. Bondar, L.A. Dreval, A.R. Abdulov, P.G. Agraval, Mixing enthalpies of melts and thermodynamic assessment of the Cu-Fe-Cr system, *Powder Metall Met Ceram* 53 (2014) 70–90, <https://doi.org/10.1007/s11106-014-9589-z>.
- [372] W. Gierlotka, D. Jendrzeczyk-Handzlik, K. Fitzner, P. Handzlik, On the ternary Ag – Cu – Ga system: electromotive force measurement and thermodynamic modeling, *Journal of Alloys and Compounds* 646 (2015) 1023–1031, <https://doi.org/10.1016/j.jallcom.2015.06.163>.
- [373] C. Zhou, H. Jin, H. Yang, J. Liu, H. Wang, B. Yang, Phase diagram, thermodynamic modeling and predictions of glass-forming range and ability in the Co-Cu-Zr system, *Journal of Non-Crystalline Solids* 588 (2022) 121615, <https://doi.org/10.1016/j.jnoncrysol.2022.121615>.
- [374] E. Zoro, C. Servant, B. Legendre, Thermodynamic assessment of the Ag-Au-Bi system, *Calphad* 31 (2007) 89–94, <https://doi.org/10.1016/j.calphad.2006.10.003>.
- [375] J. Wang, Y.J. Liu, C.Y. Tang, L.B. Liu, H.Y. Zhou, Z.P. Jin, Thermodynamic description of the Au-Ag-Ge ternary system, *Thermochimica Acta* 512 (2011) 240–246, <https://doi.org/10.1016/j.tca.2010.11.003>.
- [376] W. Gąsior, A. Dębski, M. Zabrocki, Thermodynamic description of the Ge-In-Li liquid alloys, *Journal of Molecular Liquids* 260 (2018) 415–422, <https://doi.org/10.1016/j.molliq.2018.03.118>.
- [377] G. Vassilev, V. Gandova, N. Milcheva, G. Wnuk, Thermodynamic description of the system Ag-Sn-Zn, *Calphad* 43 (2013) 133–138, <https://doi.org/10.1016/j.calphad.2013.03.003>.
- [378] M. Zabrocki, W. Gąsior, A. Dębski, Thermodynamic properties of Ga-In-Li alloys - a potential material for liquid metal batteries, *Journal of Molecular Liquids* 332 (2021) 115765, <https://doi.org/10.1016/j.molliq.2021.115765>.
- [379] D. Jendrzeczyk-Handzlik, K. Fitzner, Thermodynamic properties of liquid (antimony + tin) and (gold + antimony + tin) alloys determined from e.m.f. measurements, *The Journal of Chemical Thermodynamics* 85 (2015) 86–93, <https://doi.org/10.1016/j.jct.2015.01.010>.
- [380] D. Jendrzeczyk-Handzlik, W. Gierlotka, K. Fitzner, Thermodynamic properties of liquid copper-antimony-tin alloys determined from e.m.f. measurements, *International Journal of Materials Research* 103 (2012) 1007–1014, <https://doi.org/10.3139/146.110746>.
- [381] D. Jendrzeczyk-Handzlik, W. Gierlotka, K. Fitzner, Thermodynamic properties of liquid copper-indium-tin alloys determined from e.m.f. measurements, *The Journal of Chemical Thermodynamics* 41 (2009) 250–256, <https://doi.org/10.1016/j.jct.2008.09.007>.
- [382] D. Jendrzeczyk-Handzlik, Thermodynamic properties of liquid silver-gold-gallium alloys determined from EMF measurements with solid YSZ electrolyte, *Thermochimica Acta* 662 (2018) 126–134, <https://doi.org/10.1016/j.tca.2018.02.012>.
- [383] S. Kulawik, A. Zajczkowski, A. Dębski, W. Gąsior, W. Gierlotka, Thermodynamics of liquid Ga-Sn-Zn alloys determined by vapor pressure method, *Journal of Molecular Liquids* 300 (2020) 112310, <https://doi.org/10.1016/j.molliq.2019.112310>.
- [384] H. Bakker, Enthalpies in Alloys, *Trans Tech Publications*, 1998. <https://doi.org/10.4028/www.scientific.net/MSFo.1>.
- [385] F.R. de Boer, W.C.M. Mattens, R. Boom, A.R. Miedema, A.K. Niessen, Cohesion in metals, *Amsterdam*, <https://api.semanticscholar.org/CorpusID:136637986>, 1988.
- [386] A.T. Dinsdale, SGTE data for pure elements, *Calphad* 15 (1991) 317–425, [https://doi.org/10.1016/0364-5916\(91\)90030-N](https://doi.org/10.1016/0364-5916(91)90030-N).
- [387] L. Ward, A. Agrawal, A. Choudhary, C. Wolverton, A general-purpose machine learning framework for predicting properties of inorganic materials, *Npj Comput. Mater.* 2 (2016) 16028, <https://doi.org/10.1038/npjcompumats.2016.28>.
- [388] L. Ward, A. Dunn, A. Faghaninia, N.E.R. Zimmermann, S. Bajaj, Q. Wang, J. Montoya, J. Chen, K. Bystrom, M. Dylla, K. Chard, M. Asta, K.A. Persson, G. J. Snyder, I. Foster, A. Jain, Matminer: an open source toolkit for materials data mining, *Comput. Mater. Sci.* 152 (2018) 60–69, <https://doi.org/10.1016/j.commatsci.2018.05.018>.
- [389] G. Ke, Q. Meng, T. Finley, T. Wang, W. Chen, W. Ma, Q. Ye, T.-Y. Liu, LightGBM: a highly efficient gradient boosting decision tree, in: I. Guyon, U.V. Luxburg, S. Bengio, H. Wallach, R. Fergus, S. Vishwanathan, R. Garnett (Eds.), *Advances in Neural Information Processing Systems*, Curran Associates, Inc., 2017, in: <https://proceedings.neurips.cc/paper/2017/file/6449f44a102fde84869b9dd9eb6b76fa-Paper.pdf>.
- [390] Y. Motoyama, R. Tamura, K. Yoshimi, K. Terayama, T. Ueno, K. Tsuda, Bayesian optimization package: PHYSBO, *Comput. Phys. Commun.* 278 (2022) 108405, <https://doi.org/10.1016/j.cpc.2022.108405>.
- [391] M. Abadi, P. Barham, J. Chen, Z. Chen, A. Davis, J. Dean, M. Devin, S. Ghemawat, G. Irving, M. Isard, M. Kudlur, J. Levenberg, R. Monga, S. Moore, D.G. Murray, B. Steiner, P. Tucker, V. Vasudevan, P. Warden, M. Wicke, Y. Yu, X. Zheng, TensorFlow: a system for large-scale machine learning, *OSDI'16: Proceedings of*

- the 12th USENIX Conference on Operating Systems Design and Implementation, 2016.
- [392] T. Akiba, S. Sano, T. Yanase, T. Ohta, M. Koyama, Optuna: a next-generation hyperparameter optimization framework, in: Proceedings of the 25th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining, ACM, Anchorage AK, USA, 2019, pp. 2623–2631, <https://doi.org/10.1145/3292500.3330701>.
- [393] G. Kaptay, On the tendency of solutions to tend toward ideal solutions at high temperatures, *Metall. Mater. Trans. A* 43 (2012) 531–543, <https://doi.org/10.1007/s11661-011-0902-x>.
- [394] A. Roy, T. Babuska, B. Krick, G. Balasubramanian, Machine learned feature identification for predicting phase and Young's modulus of low-, medium- and high-entropy alloys, *Scr. Mater.* 185 (2020) 152–158, <https://doi.org/10.1016/j.scriptamat.2020.04.016>.
- [395] J.M. Rickman, H.M. Chan, M.P. Harmer, J.A. Smeltzer, C.J. Marvel, A. Roy, G. Balasubramanian, Materials informatics for the screening of multi-principal elements and high-entropy alloys, *Nat. Commun.* 10 (2019) 2618, <https://doi.org/10.1038/s41467-019-10533-1>.
- [396] G. Bracq, J.-C. Crivello, M. Laurent-Brocq, J.-M. Joubert, I. Guillot, What is the enthalpy contribution to the stabilization of the Co–Cr–Fe–Mn–Ni faced-centered cubic solid solution? *JPED* 42 (2021) 561–570, <https://doi.org/10.1007/s11669-021-00922-9>.
- [397] D. Li, S. Delsante, W. Gong, G. Borzone, Partial and integral enthalpies of mixing of Ag–Ga–Sn liquid alloys, *Thermochim. Acta* 523 (2011) 51–62, <https://doi.org/10.1016/j.tca.2011.04.032>.
- [398] G. Deffrennes, B. Hallstedt, T. Abe, Q. Bizot, E. Fischer, J.-M. Joubert, K. Terayama, R. Tamura, Dataset on the enthalpy of mixing in binary liquids, *Mendeley Data* (2024), <https://doi.org/10.17632/6wt6t9kswt>.
- [399] A. Takeuchi, A. Inoue, Mixing enthalpy of liquid phase calculated by miedema's scheme and approximated with sub-regular solution model for assessing forming ability of amorphous and glassy alloys, *Intermetallics* 18 (2010) 1779–1789, <https://doi.org/10.1016/j.intermet.2010.06.003>.
- [400] J. Neuhausen, B. Eichler, Extension of mediema's macroscopic atom model to the elements of group 16 (O, S, Se, Te ,Po), Switzerland, http://inis.iaea.org/search/search.aspx?orig_q=RN:34081384, 2003.