Table of Contents

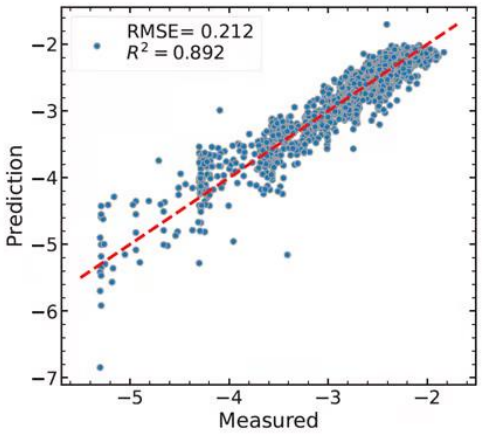
Research Article

1. Data-driven prediction of the glass-forming ability of modeled alloys by supervised machine learning

Full-Text PDF RIS

Cite this article: Hu YC, Tian J. Data-driven prediction of the glass-forming ability of modeled alloys by supervised machine learning. *J Mater Inf* 2023;3:1. http://dx.doi.org/10.20517/jmi.2022.28

Abstract



The ability of a matter to fall into a glassy state upon cooling differs greatly among metallic alloys. It is conventionally measured by the critical cooling rate Rc, below which crystallization inevitably happens. There are a lot of factors involved in determining Rc for an alloy, including both elemental features and alloy properties. However, the underlying physical mechanism is still far from being well understood. Therefore, the design of new metallic glasses is mainly by time- and labor-consuming trial-and-error experiments. This considerably slows down the development process of metallic glasses. Nowadays, large-scale computer simulations have been playing a significant role in understanding glass formation. Although the atomic-scale features can be well captured, the simulations themselves are constrained to a limited timescale. To overcome these issues, we propose to explore the glass-forming ability of the modeled alloys from computer simulations by supervised machine learning. We aim to gain insights into the key features determining Rc and found that the non-linear couplings of the geometrical and energetic factors are of great importance. An optimized machine learning model is then established to predict new glass formers with a timescale beyond the current simulation capability. This study will shed new light on both unveiling the glass formation mechanism and guiding new alloy design in practice.

Keywords

Metallic glasses, molecular dynamics simulations, glass-forming ability, machine learning, data mining

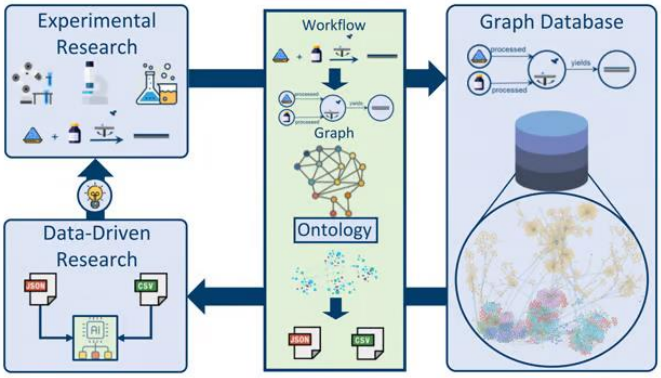
Research Article

2. Synergizing ontologies and graph databases for highly flexible materials-to-device workflow representations

Full-Text PDF RIS

Cite this article: Dreger M, Eslamibidgoli MJ, Eikerling MH, Malek K. Synergizing ontologies and graph databases for highly flexible materials-to-device workflow representations. *J Mater Inf* 2023;3:2. https://dx.doi.org/10.20517/jmi.2023.01

Abstract



The escalating adoption of high-throughput methods in applied materials science dramatically increases the amount of generated data and allows for the deployment and use of sophisticated data-driven methods. To exploit the full potential of these accelerated approaches, the generated data need to be managed, preserved and shared. The heterogeneity of such data calls for highly flexible models to represent the data from fabrication workflows, measurements and simulations. We propose the use of a native graph database to store the data instead of relying on rigid relational data models. To develop a flexible and extendable data model, we create an ontology that serves as the blueprint of the data model. The Python framework Django is used to enable seamless integration into the virtual materials intelligence platform VIMI. The Django framework relies on the Object Graph Mapper neomodel to create a mapping between database classes and Python objects. The model can store the whole bandwidth of the data from fabrication to simulation data.

Implementing the database into a platform will encourage researchers to share data while profiting from rich and highly curated data to accelerate their research.

Keywords

FAIR, energy materials, fabrication workflow optimization, ontologies, graph databases

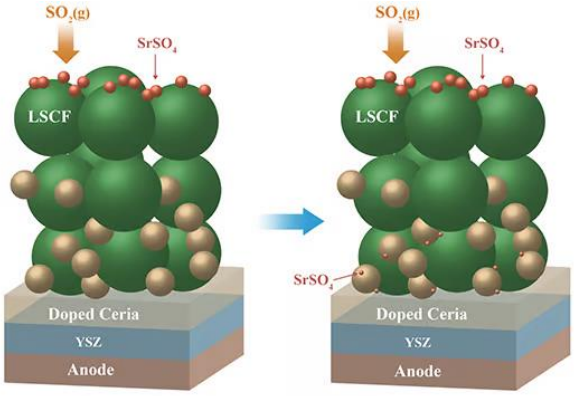
Research Article

3. Sulfur poisoning mechanism of LSCF cathode material in the presence of SO_2: a computational and experimental study

Full-Text **PDF** **RIS**

Cite this article: Wang R, Parent LR, Zhong Y. Sulfur poisoning mechanism of LSCF cathode material in the presence of SO_2: a computational and experimental study. *J Mater Inf* 2023;3:3. https://dx.doi.org/10.20517/jmi.2022.45

Abstract



Long-term degradation of LSCF in the presence of SO_2

Aiming at the comprehensive understanding of the single sulfur poisoning effect and, eventually, the multiple impurities poisoning phenomena on the SOFC (Solid Oxide Fuel Cell) cathode materials, the sulfur poisoning effect on the $(La_{0.6}Sr_{0.4})_{0.95}Co_{0.2}Fe_{0.8}O_3$ (LSCF-6428) has been investigated in the presence of 10 ppm SO_2 at 800, 900, and 1,000 °C, respectively, with a combined computational and experimental approach. The good agreement between the CALPHAD (Computer Coupling of Phase Diagrams and Thermochemistry) simulations and the XRD (X-Ray Diffraction), SEM (Scanning Electron Microscopy), and TEM (Transmission Electron Microscopy) characterization results support the reliability of the CALPHAD approach in the SOFC field. Furthermore, comprehensive simulations were made to understand the impact of temperature, $P(SO_2)$, $P(O_2)$, and

Sr concentration on the threshold of $SrSO_4$ stability. Results showed that the formation of $SrSO_4$ is thermodynamically favored at lower temperatures, higher $P(SO_2)$, higher $P(O_2)$, and higher Sr concentration. Finally, comparisons were also made between LSCF-6428 and LSM20 ($La_{0.8}Sr_{0.2}MnO_3$) using simulations, which confirmed that LSCF-6428 is a poor sulfur-tolerant cathode, in agreement with the literature.

Keywords

LSCF cathode, CALPHAD, sulfur poisoning, long-term degradation, accelerated testing

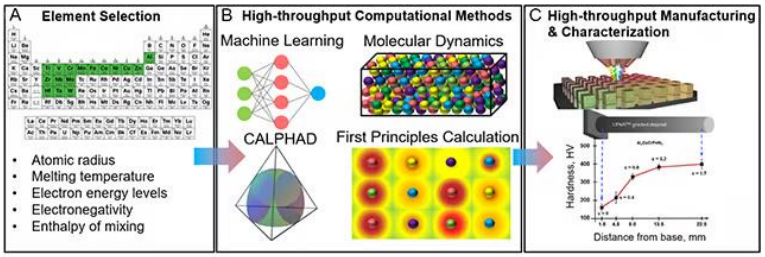
Review

4. A review on high-throughput development of high-entropy alloys by combinatorial methods

Full-Text **PDF** **RIS**

Cite this article: Mooraj S, Chen W. A review on high-throughput development of high-entropy alloys by combinatorial methods. *J Mater Inf* 2023;3:4. https://dx.doi.org/10.20517/jmi.2022.41

Abstract



High-entropy alloys (HEAs) are an emerging class of alloys with multi-principal elements that greatly expands the compositional space for advanced alloy design. Besides chemistry, processing history can also affect the phase and microstructure formation in HEAs. The number of possible alloy compositions and processing paths gives rise to enormous material design space, which makes it challenging to explore by traditional trial-and-error approaches. This review highlights the progress in combinatorial high-throughput studies towards rapid prediction, manufacturing, and

characterization of promising HEA compositions. This review begins with an introduction to HEAs and their unique properties. Then, this review describes high-throughput computational methods such as machine learning that can predict desired alloy compositions from hundreds or even thousands of candidates. The next section presents advances in combinatorial synthesis of material libraries by additive manufacturing for efficient development of high-performance HEAs at bulk scale. The final section discusses the high-throughput characterization techniques used to accelerate the material property measurements for systematic understanding of the composition-processing-structure-property relationships in combinatorial HEA libraries.

Keywords

High-entropy alloys, machine learning, combinatorial studies, high throughput, additive manufacturing, alloy design

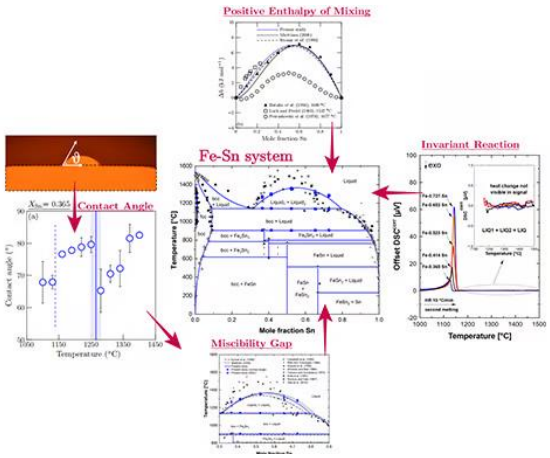
Research Article

5. Thermodynamic modeling of the Fe-Sn system including an experimental re-assessment of the liquid miscibility gap

Full-Text PDF RIS

Cite this article: Park WB, Bernhard M, Presoly P, Kang YB. Thermodynamic modeling of the Fe-Sn system including an experimental re-assessment of the liquid miscibility gap. *J Mater Inf* 2023;3:5. https://dx.doi.org/10.20517/jmi.2022.37

Abstract



The usage of low-grade ferrous scrap has increased over decades to decrease CO_2 emissions and to produce steel products at a low cost. A serious problem in melting post-consumer scrap material is the accumulation of tramp elements, e.g., Cu and

Sn, in the liquid steel. These tramp elements are difficult to remove during conventional steelmaking processes. Sn is considered as one of the most harmful tramp elements because, together with Cu, it sometimes induces the liquid metal embrittlement in high-temperature ferrous processing, e.g., continuous casting and hot rolling. Furthermore, the chemical interaction between Fe and Sn plays an important role in the Sn smelting process. The raw material used in the Sn smelting process is SnO_2 (cassiterite), in which Fe_3O_4 is a gangue in the Sn ore. In the process, the reduction of Fe_3O_4 is unavoidable, which results in forming a Fe-Sn alloy (hardhead). The recirculation of the hardhead decreases the furnace capacity and increases the energy consumption in the smelting. The need to efficiently recover Sn from secondary resources is therefore inevitable. The CALculation of PHAse Diagrams (CALPHAD) approach helps to predict the equilibrium state of the multicomponent system. Previously reported studies of the Fe-Sn system show inconsistencies in the calculations and the experimental results. Mainly the miscibility gap in the liquid phase was under debate, as experimental data of the phase boundary are scattered. Experimental study and re-optimization of model parameters were carried out with emphasis on the correct shape of the miscibility gap. Three different experimental techniques were employed: differential scanning calorimetry, electromagnetic levitation, and contact angle measurement. The present thermodynamic model has higher accuracy in predicting the solubility of Sn in the body-centered cubic (bcc), compared to previous assessments. This is achieved by re-evaluating the Gibbs energies of the FeSn and $FeSn_2$ compounds and the peritectic reaction related to $Fe5Sn_3$. Also, the inconsistencies related to the miscibility gap around XSn = 0.31-0.81 were resolved. The database developed in the present study can contribute to the development of a large CALPHAD database containing tramp elements.

Keywords
Fe-Sn, thermodynamics, CALPHAD, miscibility gap, contact angle measurement, DSC

Research Article

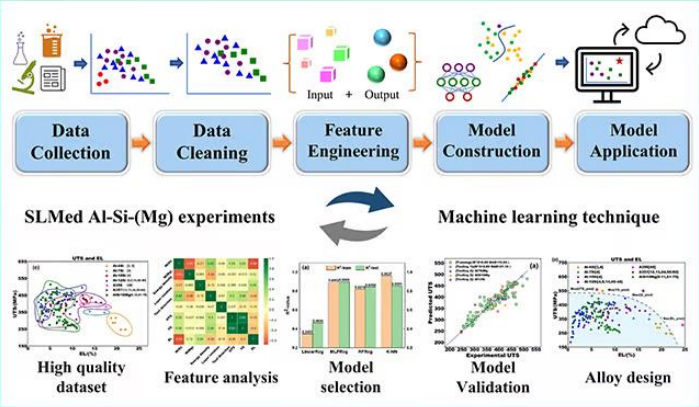
6. **Development of an accurate "composition-process-properties" dataset for SLMed Al-Si-(Mg) alloys and its application in alloy design**

Full-Text PDF RIS

Cite this article: Gao T, Gao J, Zhang J, Song B, Zhang L. Development of an accurate "composition-process-properties" dataset for SLMed Al-Si-(Mg) alloys

and its application in alloy design. *J Mater Inf* 2023;3:6. https://dx.doi.org/10.20517/jmi.2023.03

Abstract



Al-Si-Mg series alloys are the most common alloys available for additive manufacturing forming with low cracking tendency. However, there is no systematic study on the computational design of SLMed Al-Si-(Mg) alloys due to the huge parameter space of composition and processes. In this paper, a high-quality dataset of SLMed Al-Si-(Mg) alloys containing 176 pieces of data from 50 publications was first established, which recorded the information, including alloy compositions, process parameters, test conditions, and mechanical properties. A threshold value of 35 J/mm3 for energy density (Ed) was then proposed as a criterion to clean the data points with lower ultimate tensile strength (UTS) and elongation (EL). The cleaned dataset consists of a first training/testing dataset with 142 data for model construction and a second testing dataset with 9 data for model verification. After that, four machine learning models were applied to establish the quantitative relation of "composition-processes-properties" in SLMed Al-Si-(Mg) alloys. The MLPReg model was chosen as the optimal one considering its best performance and subsequently utilized to design novel compositions and process parameters for SLMed Al-Si-(Mg) alloys. The UTS and EL of the designed alloy with a maximum comprehensive mechanical property are 549 MPa and 16%, both of which are higher than all the available experimental data. It is anticipated that the present design strategy based on the machine learning method should generally be applicable to other SLMed alloy systems.

Keywords

Selective laser melting, Al-Si-Mg alloy, machine learning, alloy design, mechanical properties

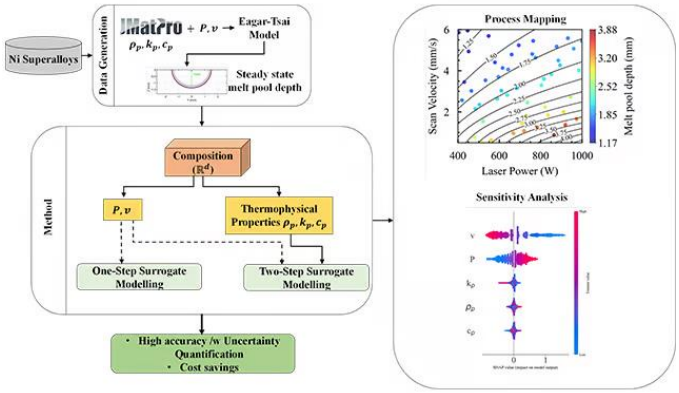
Research Article

7. Linking processing parameters with melt pool properties of multiple nickel-based superalloys via high-dimensional Gaussian process regression

Full-Text PDF RIS

Cite this article: Menon N, Mondal S, Basak A. Linking processing parameters with melt pool properties of multiple nickel-based superalloys via high-dimensional Gaussian process regression. *J Mater Inf* 2023;3:7. https://dx.doi.org/10.20517/jmi.2022.38

Abstract



A physics-based model is used to predict the melt pool properties in the laser-directed energy deposition of several nickel-based superalloys for different process parameters. The input space is high-dimensional, consisting of a common 19-dimensional composition space for each alloy and the process parameters (laser power and scan velocity). Gaussian Process-based regression frameworks are developed by training surrogates on data generated by a validated analytical model. These surrogates are thereafter used to predict and define relationships between the composition, resultant thermophysical properties, process parameters, and the subsequent melt pool property. The probabilistic predictions are augmented by uncertainty quantification and sensitivity analysis to substantiate the findings further.

Keywords

Laser directed energy deposition, Gaussian process, nickel-based superallloys, melt pool properties, uncertainty quantification, sensitivity analysis

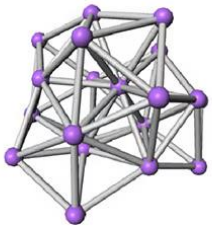
Research Article

8. Neural network to predict ^{23}Na NMR spectra of Nan clusters

Full-Text **PDF** **RIS**

Cite this article: Kaneko M, Suzaki A, Muraoka A, Gotoh K, Yamashita K. Neural network to predict ^{23}Na NMR spectra of Nan clusters. *J Mater Inf* 2023;3:8. https://dx.doi.org/10.20517/jmi.2022.39

Abstract



In order to understand the charging and discharging processes of sodium-ion batteries, we are interested in the relationship between the size of sodium clusters inserted into the hard carbon anode and the solid-state ^{23}Na NMR chemical shifts. In this study, we investigated the predictability of the size dependence of ^{23}Na NMR shielding constants by SchNet, a deep learning model that uses the distance between Na atoms without graph connection information. The data set required for training the neural network was constructed by density functional theory (DFT) calculations. This study shows that the neural network model, which only used structural data, achieved comparable accuracy in predicting the shielding constant to the Lasso model, which utilized gross orbital population predicted from DFT calculations. Moreover, by introducing a penalty term to the neural network's loss function, the neural network was able to reproduce the skewed distribution of the shielding constant without modifying its architecture.

Keywords

Neural network SchNet, ^{23}Na NMR chemical shifts, Nan clusters, DFT calculations

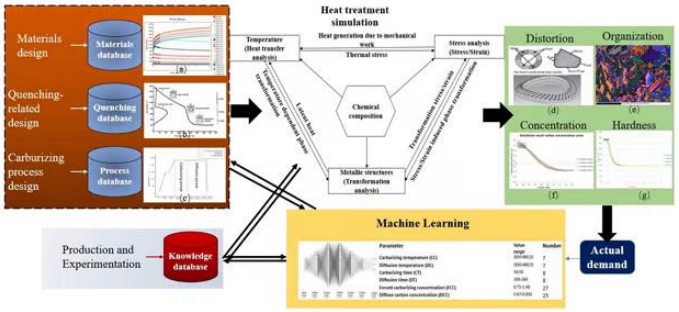
Research Article

9. Machine learning based optimization method for vacuum carburizing process and its application

Full-Text **PDF** **RIS**

Cite this article: Jia H, Ju D, Cao J. Machine learning based optimization method for vacuum carburizing process and its application. *J Mater Inf* 2023;3:9. https://dx.doi.org/10.20517/jmi.2022.43

Abstract



This paper develops an optimized prediction method based on machine learning for optimal process parameters for vacuum carburizing. The critical point is data expansion through machine learning based on a few parameters and data, which leads to optimizing parameters for vacuum carburization in heat treatment. This method extends the data volume by constructing a neural network with data augmentation in the presence of small data samples. In this paper, the database of 213 data is expanded to a database of 2,116,800 data by optimizing the prediction. Finally, we found the optimal vacuum carburizing process parameters through the vast database. The relative error of the three targets is less than that of the target obtained by the simulation of the corresponding parameters. The relative error is less than 5.6%, 1%, and 0.02%, respectively. Compared to simulations and actual experiments, the optimized prediction method in this paper saves much computational time. It provides a large amount of referable process parameter data while ensuring a certain level of accuracy.

Keywords:

Machine learning, heat treatment, neural networks, data augmentation, small sample

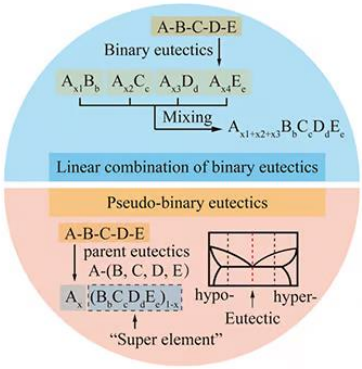
Review

10. Data-driven design of eutectic high entropy alloys

Full-Text **PDF** **RIS**

Cite this article: Chen Z, Yang Y. Data-driven design of eutectic high entropy alloys. *J Mater Inf* 2023;3:xx. https://dx.doi.org/10.20517/jmi.2023.06

Abstract



Eutectic high entropy alloys (EHEAs) have attracted tremendous research interest over the past decade due to their superior physical and mechanical properties. Given the compositional complexity, there are no well-established phase diagrams for EHEAs. Therefore, the compositional design of EHEAs has been following a trial-and-error empirical approach, which is time-consuming, costly, and ineffective. To accelerate the search for EHEAs, data-driven approaches, particularly machine learning (ML) based modeling, have recently been utilized in lieu of the traditional empirical approach. In this article, we provide a critical overview of the recent efforts in the design and development of EHEAs, which covers the various empirical methods and the state-of-the-art machine learning models developed for EHEAs. In addition, we also briefly discuss the mechanical properties and plasticity strengthening mechanisms in EHEAs which are related to their heterogeneous microstructure, such as heterogeneous deformation induced strengthening, twinning induced strengthening, and phase transformation induced strengthening.

Keywords:

Eutectic alloys, high entropy alloys, machine learning, alloy design, mechanical properties

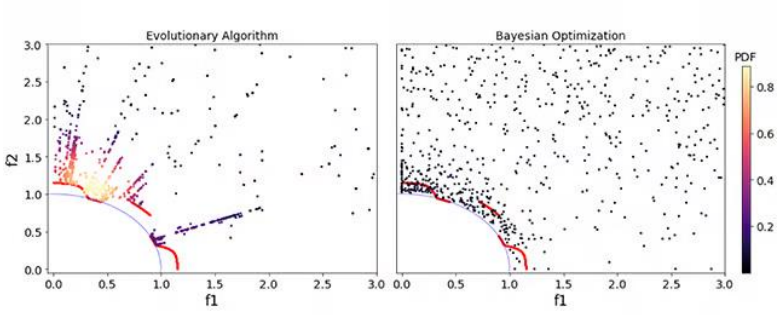
Research Article

11. Mapping pareto fronts for efficient multi-objective materials discovery

Full-Text **PDF** **RIS**

Cite this article: Low AKY, Vissol-Gaudin E, Lim YF, Hippalgaonkar K. Mapping pareto fronts for efficient multi-objective materials discovery. *J Mater Inf* 2023;3:11. https://dx.doi.org/10.20517/jmi.2023.02

Abstract



With advancements in automation and high-throughput techniques, we can tackle more complex multi-objective materials discovery problems requiring a higher evaluation budget. Given that experimentation is greatly limited by evaluation budget, maximizing sample efficiency of optimization becomes crucial. We discuss the limitations of using hypervolume as a performance indicator and propose new metrics relevant to materials experimentation: such as the ability to perform well for complex high-dimensional problems, minimizing wastage of evaluations, consistency/robustness of optimization, and ability to scale well to high throughputs. With these metrics, we perform an empirical study of two conceptually different and state-of-the-art algorithms (Bayesian and Evolutionary) on synthetic and real-world datasets. We discuss the merits of both approaches with respect to exploration and exploitation, where fully resolving the Pareto Front provides more knowledge of the best material.

Keywords

Bayesian optimization, constrained multi-objective optimization, evolutionary algorithm, materials science

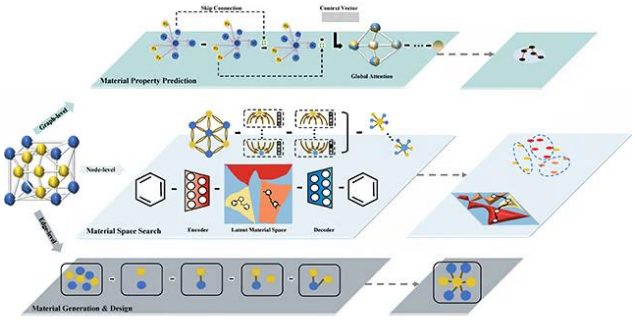
Review

12. Graph neural networks for molecular and materials representation

Full-Text **PDF** **RIS**

Cite this article: Wu X, Wang H, Gong Y, Fan D, Ding P, Li Q, Qian Q. Graph neural networks for molecular and materials representation. *J Mater Inf* 2023;3:12. https://dx.doi.org/10.20517/jmi.2023.10

Abstract



Material molecular representation (MMR) plays an important role in material property or chemical reaction prediction. However, traditional expert-designed MMR methods face challenges in dealing with high dimensionality and heterogeneity of material data, leading to limited generalization capabilities and insufficient information representation. In recent years, graph neural networks (GNNs), a deep learning algorithm specifically designed for graph structures, have made inroads into the field of MMR. It will be instructive and inspiring to conduct a survey on various GNNs used for MMR. To achieve this objective, we compare GNNs with conventional MMR methods and illustrate the advantages of GNNs, such as their expressiveness and adaptability. In addition, we systematically classify and summarize the methods and applications of GNNs. Finally, we provide our insights into future research directions, taking into account the characteristics of molecular data and the inherent drawbacks of GNNs. This comprehensive survey is intended to present a holistic view of GNNs for MMR, focusing on the core concepts, the main techniques, and the future trends in this area.

Keywords:

Material molecular representation, material property, reaction prediction, graph neural networks, expressiveness, adaptability

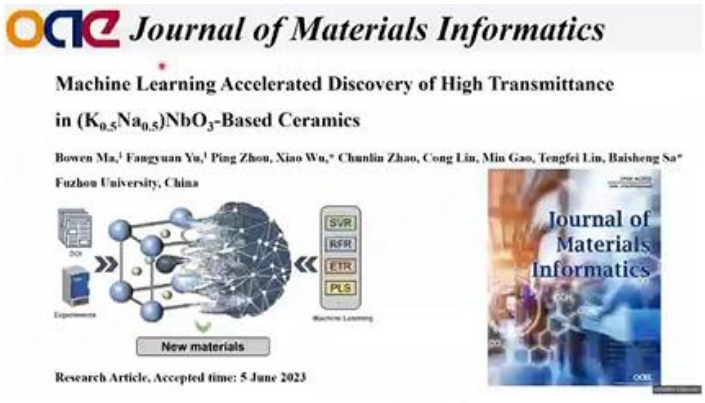
Research Article

13. Machine learning accelerated discovery of high transmittance in $(K_{0.5}Na_{0.5})NbO_3$-based ceramics

Full-Text PDF RIS

Cite this article: Ma B, Yu F, Zhou P, Wu X, Zhao C, Lin C, Gao M, Lin T, Sa B. Machine learning accelerated discovery of high transmittance in $(K_{0.5}Na_{0.5})NbO_3$ -based ceramics. *J Mater Inf* 2023;3:13. https://dx.doi.org/10.20517/jmi.2023.09

Abstract



High optical transmittance (*T%*) has always been an important indicator of transparent-ferroelectric ceramics for optoelectronic coupling. However, the pathway of pursuing high transparency has been at the experimental trialand-error stage over the past decades, manifesting major drawbacks of being time-consuming and resourcewasting. The present work introduces a machine learning (ML) accelerated development of highly transparentferroelectrics by taking potassium-sodium niobate (KNN)-based ceramics as the model material. It is highlighted that by using a small data set of 118 sample data and four key features, we predict the *T%* of un-synthesized KNNbased ceramics and evaluate the importance of key features. Meanwhile, the screened $(K_{0.5}Na_{0.5})_{0.956}Tb_{0.004}Ba_{0.04}$ NbO_3 ceramics were successfully realized by the conventional solid-state synthesis, and the experimental measured *T%* is in full agreement with the predicted results, exhibiting a satisfactory high *T%* of ~78% at 800 nm. In addition, ML is also used to explore the best experimental parameters, and the prediction results of *T%* are particularly sensitive to changes in sintering temperature (ST). Eventually, the predicted optimal ST is highly consistent with the experimental one. This study constructs a new avenue for exploring high *T%* ferroelectric KNN ceramics based on ML, ascertaining optimal process parameters, and guiding the development of other transparent-ferroelectrics in optoelectronic fields.

Keywords:

Machine learning, KNN-based ceramics, transmittance, sintering temperature

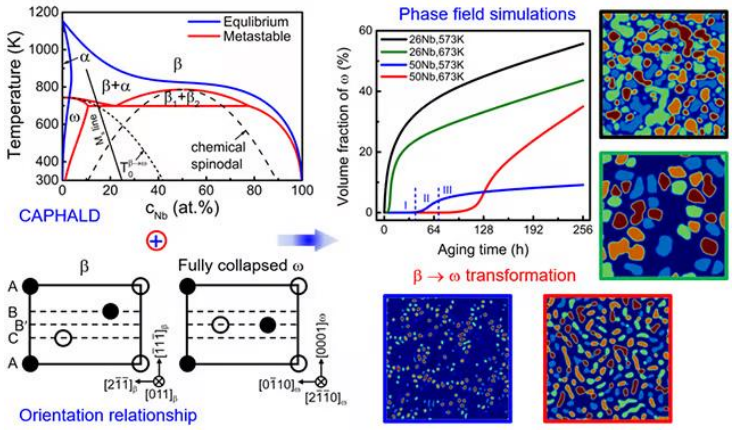
Research Article

14. Composition- and temperature-dependence of β to ω phase transformation in Ti-Nb alloys

Full-Text **PDF** **RIS**

Cite this article: Su Y, Liang C, Wang D. Composition- and temperature-dependence of β to ω phase transformation in Ti-Nb alloys. *J Mater Inf* 2023;3:xx. https://dx.doi.org/10.20517/jmi.2023.12

Abstract



ω phases have shown great effects on the superelasticity and modulus of metastable β-Ti alloys. In this study, the microstructure evolution during cooling and aging for β → ω phase transformation is investigated by integrating a thermodynamic database with phase field simulations. Our CALPHAD calculations based on an available thermodynamic database give the Gibbs energies of metastable β (Nb-lean β_1 + Nb-rich β_2 produced via spinodal decomposition) and ω phases in Ti-Nb. Informed by the results, our phase field simulations show that the formation mechanisms of ω exhibit dependence on the composition and temperature. The ω can form in Ti-26 at.% Nb without the assistance of spinodal decomposition. Further analysis shows that the precursory spinodal decomposition in the β phase occurs in Ti-50 at.% Nb, and could induce geometrically confined ω. The novel transformation pathway could create unique morphology of ω. This study could elucidate new insights into the ω phase transformation in Ti-Nb alloys and metastable β-Ti alloys having spinodal decomposition.

Keywords

Omega phase, Ti-Nb, microstructural evolution, spinodal decomposition, phase field simulation

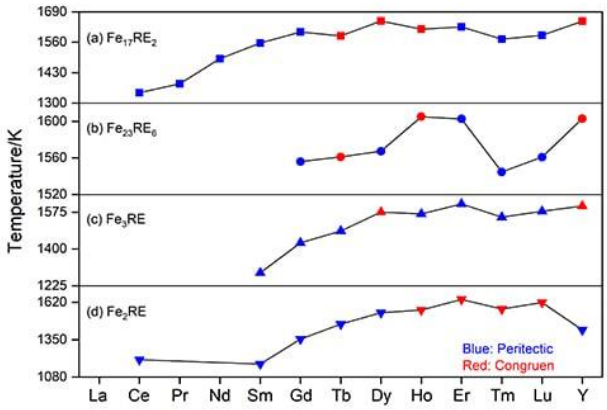
Research Article

15. Assessment of phase equilibria and thermodynamic properties in the Fe-RE (RE = rare earth metals) binary systems

Full-Text PDF RIS

Cite this article: Ye H, Rong M, Chen Q, Yao Q, Wang J, Rao G, Zhou H. Assessment of phase equilibria and thermodynamic properties in the Fe-RE (RE = rare earth metals) binary systems. *J Mater Inf* 2023;3:15. https://dx.doi.org/10.20517/jmi.2023.08

Abstract



This study focuses on investigating phase equilibria and thermodynamic stability of intermetallic compounds made of the transition metal Fe and rare earth (RE) elements. By using the CALPHAD method and reliable experimental information from the literature, the binary systems of Fe-Y, Fe-Er, and Fe-Lu were reassessed. To improve our previous calculations of Fe-RE (RE = Tb and Dy) binary systems, the Gibbs energy expressions of intermetallic compounds Fe_2Tb and Fe_2Dy were modified to avoid artificial breaks in their heat capacity curves. Thermodynamic parameters obtained are self-consistent, and the Gibbs energies of the Fe-RE (RE = Tb, Dy, Er, Lu, and Y) phases were accurately expressed to reappear available both thermodynamic data and phase equilibria. This work was further combined with the previous calculations of the Fe-RE (RE = La, Ce, Pr, Nd, Sm, Gd, Ho, and Tm) systems to discuss thermodynamic characteristics and phase equilibria of Fe-RE binary systems in detail. A trend was noticed for the change of thermodynamic

properties and phase equilibria of the Fe-RE binary systems with RE atomic number. Generally, as the RE atomic number increases, the formation temperatures of the Fe-RE intermetallic compounds increase gradually, and the enthalpy of mixing of liquid Fe-RE (apart from Fe-Y and Fe-Ce) alloys and the enthalpy of formation of the Fe-RE (apart from Fe-Y, Fe-Ce, Fe-Gd, and Fe-Dy) intermetallic compounds become increasingly negative. The results provide a thorough set of thermodynamic parameters of thirteen Fe-RE binary systems, which could serve as a sound basis for developing a thermodynamic database of Fe-RE-based alloy systems.

Keywords

Fe-RE binary systems, Phase equilibria, Thermodynamic

Review

16. Virtual sample generation in machine learning assisted materials design and discovery

Full-Text PDF RIS

Cite this article: Xu P, Ji X, Li M, Lu W. Virtual sample generation in machine learning assisted materials design and discovery. *J Mater Inf* 2023;3:16. https://dx.doi.org/10.20517/jmi.2023.18

Abstract

Virtual sample generation (VSG), as a cutting-edge technique, has been successfully applied in machine learningassisted materials design and discovery. A virtual sample without experimental validation is defined as an unknown sample, which is either expanded from the original data distribution for modeling or designed via algorithms for predicting. This review aims to discuss the applications of VSG techniques in machine learning-assisted materials design and discovery based on the research progress in recent years. First, we summarize the commonly

used VSG algorithms in materials design and discovery for data expansion of the training set, including Bootstrap, Monte Carlo, particle swarm optimization, mega trend diffusion, Gaussian mixture model, random forest, and generative adversarial networks. Next, frequently employed searching algorithms for materials discovery are introduced, including particle swarm optimization, efficient global optimization, and proactive searching progress. Then, universally adopted inverse design methods are presented, including genetic algorithm, Bayesian optimization, and pattern recognition inverse projection. Finally, the future directions of VSG in the design and discovery of materials are proposed.

Keywords

Materials machine learning, virtual sample generation, searching algorithms, inverse design

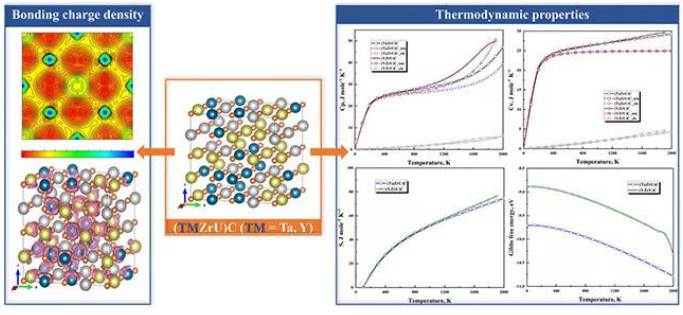
Research Article

17. Effects of solutes on thermodynamic properties of (TMZrU)C (TM = Ta, Y) medium-entropy carbides: a first-principles study

Full-Text PDF RIS

Cite this article: Liu Y, Lu Y, Wang WY, Li J, Zhang Y, Yin J, Pan X, Gao X, Chen Y, Song H, Li J. Effects of solutes on thermodynamic properties of (TMZrU)C (TM = Ta, Y) medium-entropy carbides: a first-principles study. *J Mater Inf* 2023;3:17. https://dx.doi.org/10.20517/jmi.2023.19

Abstract



High entropy carbide ceramics have garnered significant interest as a novel class of ultra-high temperature and superhard metallic materials. In the present work, a comparative investigation was conducted for the first time on the stability, mechanical, and thermodynamic properties of two medium entropy carbides

(MECs), (TaZrU)C and (YZrU)C, using high-throughput first-principles calculations. Additionally, data from groups IV and V transition metal monocarbides were employed for comparison. The temperature-dependent thermodynamic properties, including bulk modulus (B), constant volume/constant pressure heat capacity (Cv/Cp), Gibbs free energy, volume, entropy, and thermal conductivity, were evaluated using the Debye-Gruneisen model. The results demonstrate that (TaZrU)C and (YZrU)C exhibit similar trends in their thermodynamic properties, with (YZrU)C displaying slightly superior performance as the temperature rises. This work provides valuable insights into the design of innovative high entropy fuels, holding significant implications for the advancement of MEC ceramic fuels in advanced nuclear power systems and nuclear thermal propulsion systems.

Keywords

Medium entropy carbide ceramics, first-principles calculations, thermodynamic properties, transition metal monocarbides, nuclear thermal propulsion (NTP) systems

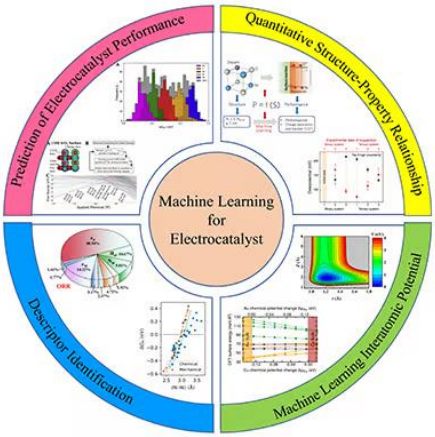
Review

18. Recent advances and applications of machine learning in electrocatalysis

Full-Text **PDF** **RIS**

Cite this article: Hu Y, Chen J, Wei Z, He Q, Zhao Y. Recent advances and applications of machine learning in electrocatalysis. *J Mater Inf* 2023;3:18. https://dx.doi.org/10.20517/jmi.2023.23

Abstract



Electrocatalysis plays an important role in the production of clean energy and pollution control. Researchers have made great efforts to explore efficient, stable,

and inexpensive electrocatalysts. However, traditional trial and error experiments and theoretical calculations require a significant amount of time and resources, which limits the development speed of electrocatalysts. Fortunately, the rapid development of machine learning (ML) has brought new solutions to scientific problems and new paradigms to the development of electrocatalysts. The combination of ML with experimental and theoretical calculations has propelled significant advancements in electrocatalysis research, particularly in the areas of materials screening, performance prediction, and catalysis theory development. In this review, we present a comprehensive overview of the workflow and cutting-edge techniques of ML in the field of electrocatalysis. In addition, we discuss the diverse applications of ML in predicting performance, guiding synthesis, and exploring the theory of catalysis. Finally, we conclude the review with the challenges of ML in electrocatalysis.

Keywords

Machine learning, electrocatalysis, performance prediction

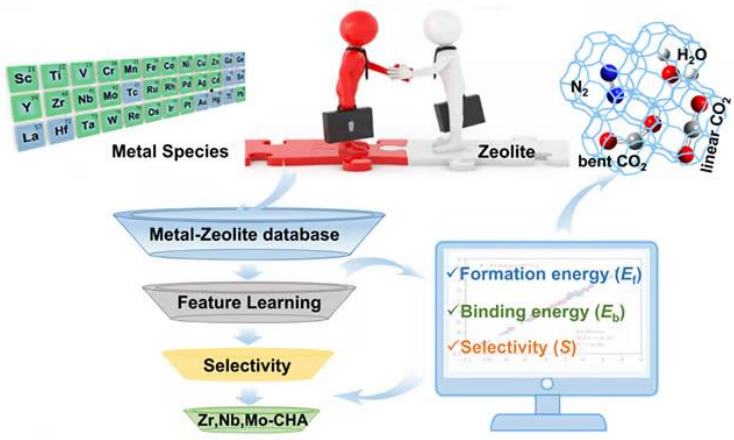
Research Article

19. Machine learning for prediction of $CO_2/N_2/H_2O$ selective adsorption and separation in metal-zeolites

Full-Text PDF RIS

Cite this article: Gu YT, Gu YM, Tao Q, Wang X, Zhu Q, Ma J. Machine learning for prediction of $CO_2/N_2/H_2O$ selective adsorption and separation in metal-zeolites. *J Mater Inf* 2023;3:19. https://dx.doi.org/10.20517/jmi.2023.25

Abstract



Carbon dioxide (CO_2) capture, utilization, and storage technologies are crucial in

reducing global warming and producing various high-value chemicals and fuels. It is challenging to effectively separate the molecules of CO_2, N_2, and H_2O, whose kinetic diameters are close to each other. Although zeolites have garnered considerable attention in gas separation, the huge chemical space of metal-doped zeolites (metal-zeolites) coming from the combination of different metal active sites, topology, and Si/Al ratios poses a difficulty in finding an optimal material for selectively trapping CO_2. In this study, we build machine learning (ML) models to predict the selective adsorption of $CO_2/N_2/H_2O$ on metal-zeolites through the regulation of electrostatic polarization interaction. The stability of 208 metal-zeolites encompassing five distinct topological structures is estimated through the formation energy (Ef), indicating the potential accessibility in the experiment for most of the studied systems, especially for Sc-, Y-, and Zr-zeolites. Adsorption of CO_2 on metal sites has two possible configurations: linear vs. bent CO_2, depending on different embedded metals. The concerted binding of CO_2 with both carbon and oxygen atoms on the metal center leads to the bent geometry and larger binding energies on metal-zeolites (Zr-, Nb-, Mo-zeolites). Accessible descriptors associated with the zeolites, adsorbates, and metals are selected to train the adsorption strength index (I), showing good performance [mean absolute error (MAE) = 0.04, R^2 = 0.88]. The predicted adsorption selectivity is in agreement with the experimental systems (Co-, Zn-, Cu-, Fe-SSZ-13). It is found that medium-poresized zeolites [pore limiting diameter (PLD) = ~7 Å] anchored with Zr, Nb, or Mo are promising materials for the CO_2 adsorption and separation. The proposed ML scheme may also be applicable to give a fast prediction of CO_2 adsorption and separation ability in other porous metal-organic frameworks or amorphous materials.

Keywords

Metal-zeolites, machine learning, separation, selective adsorption

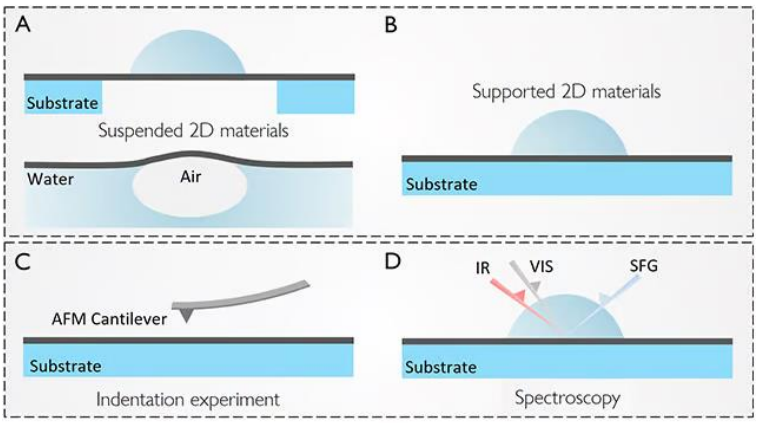
Review

20. Characterizing the wetting behavior of 2D materials: a review

Full-Text **PDF** **RIS**

Cite this article: Yu C, Dai Z. Characterizing the wetting behavior of 2D materials: a review. *J Mater Inf* 2023;3:20. https:/ /dx.doi.org/10.20517/jmi.2023.27

Abstract



A comprehensive understanding of the interaction between liquids and two-dimensional (2D) materials is pivotal for the manipulation, transfer, and assembly of 2D materials across a wide range of applications, from liquid cell microscopy to hydrovoltaics. This review discusses this interaction by surveying the intrinsic wettability of suspended 2D materials and the apparent wettability of substrate-supported 2D materials, both of which have recently been revealed through water contact angle (WCA) experiments. We discuss important factors that can affect the apparent WCA, including thin film elasticity, surface contamination, and the microstructure and electronic state of the underneath substrate. We also discuss some microscopic-level insights into the 2D materialliquid interface that have recently been provided via spectroscopy characterizations and surface energy measurements. By discussing the latest experimental advancements in characterizing the interaction between 2D materials and liquid droplets, this review aims to inspire future theoretical progress capable of unraveling the intricate and occasionally contradictory wetting behavior observed in 2D material systems.

Keywords

2D materials, wettability, water contact angle, elastocapillarity, surface energy

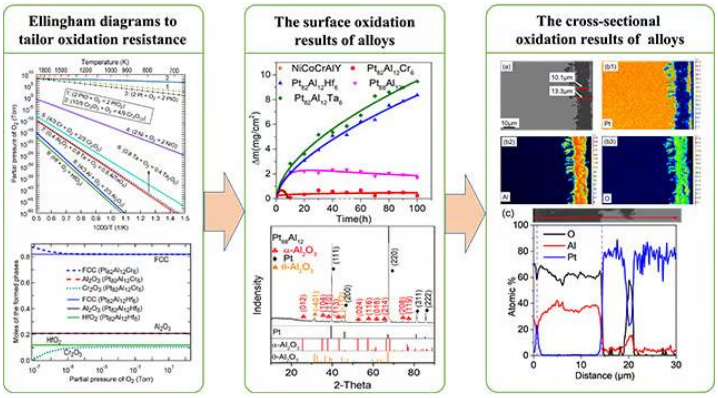
Research Article

21. Understanding oxidation resistance of Pt-based alloys through computations of Ellingham diagrams with experimental verifications

Full-Text PDF RIS

Cite this article: Chong X, Yu W, Liang Y, Shang SL, Li C, Zhang A, Wei Y, Gao X, Wang Y, Feng J, Chen L, Song H, Liu ZK. Understanding oxidation resistance of Pt-based alloys through computations of Ellingham diagrams with experimental verifications. *J Mater Inf* 2023;3:21. https://dx.doi.org/10.20517/jmi.2023.17

Abstract



Thermodynamic calculations of Ellingham diagrams and the forming oxides have been performed relevant to the Pt-based alloys $Pt_{82}Al_{12}M_6$ (M = Cr, Hf, Pt, and Ta). The predicted Ellingham diagrams indicate that the elements Hf and Al are easy to oxidize, followed by Ta and Cr, while Pt is extremely difficult to oxidize. Oxidation experiments characterized by X-ray diffraction (XRD) and electron probe micro-analyzers verify the present thermodynamic predictions, showing that the best alloy with superior oxidation resistance is $Pt_{82}Al_{12}Cr_6$, followed by $Pt_{88}Al_{12}$ due to the formation of the dense and continuous α-Al_2O_3 scale on the surface of alloys; while the worse alloy is $Pt_{82}Al_{12}Hf_6$ followed by $Pt_{82}Al_{12}Ta_6$ due to drastic internal oxidation and the formation of deleterious HfO_2, $AlTaO_4$, and Ta_2O_5. The present work, combining computations with experimental verifications, provides a fundamental understanding and knowledgebase to develop Pt-based superalloys with superior oxidation resistance that can be used in ultrahigh temperatures.

Keywords

Ellingham diagrams, Pt-based alloys, oxidation resistance, XRD, EPMA

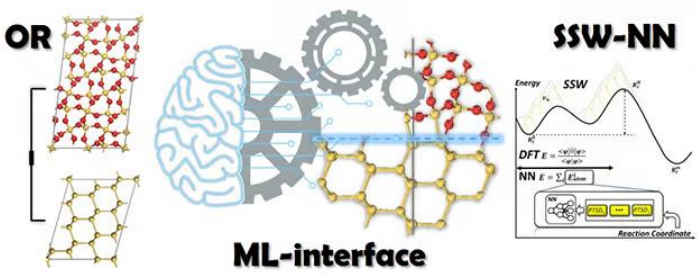
Review

22. Recent advances in the interface structure prediction for heteromaterial systems

Full-Text PDF RIS

Cite this article: Li JL, Li YF. Recent advances in the interface structure prediction for heteromaterial systems. *J Mater Inf* 2023;3:22. https://dx.doi.org/10.20517/jmi.2023.24

Abstract



The atomic structures of solid-solid interfaces in materials are of fundamental importance for understanding the physical properties of interfacial materials, which is, however, difficult to determine both in experimental and theoretical approaches. New theoretical methodologies utilizing various global optimization algorithms and machine learning (ML) potentials have emerged in recent years, offering a promising approach to unraveling interfacial structures. In this review, we give a concise overview of state-of-the-art techniques employed in the studies of interfacial structures, e.g., ML-assisted phenomenological theory for the global search of interface structure (ML-interface). We also present a few applications of these methodologies.

Keywords

Solid-solid interfaces, machine learning, ML-interface, interface structure prediction

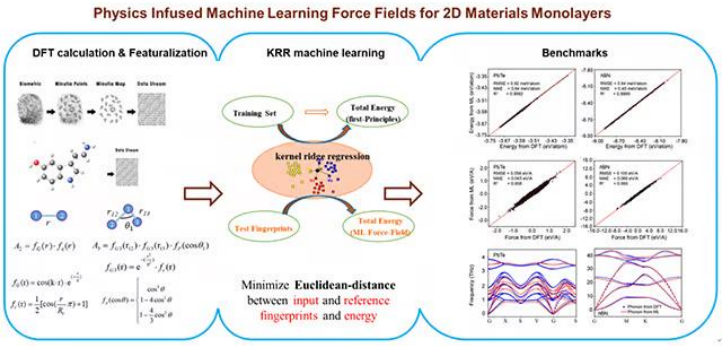
Research Article

23. Physics infused machine learning force fields for 2D materials monolayers

Full-Text **PDF** **RIS**

Cite this article: Yang Y, Xu B, Zong H. Physics infused machine learning force fields for 2D materials monolayers. *J Mater Inf* 2023;3:23. https://dx.doi.org/10.20517/jmi.2023.31

Abstract



Large-scale atomistic simulations of two-dimensional (2D) materials rely on highly accurate and efficient force fields. Here, we present a physics-infused machine learning framework that enables the efficient development and interpretability of interatomic interaction models for 2D materials. By considering the characteristics of chemical bonds and structural topology, we have devised a set of efficient descriptors. This enables accurate force field training using a small dataset. The machine learning force fields show great success in describing the phase transformation and domain switching behaviors of monolayer Group IV monochalcogenides, e.g., GeSe and PbTe. Notably, this type of force field can be readily extended to other non-transition 2D systems, such as hexagonal boron nitride (hBN), leveraging their structural similarity. Our work provides a straightforward but accurate extension of simulation time and length scales for 2D materials.

Keywords

2D materials, mechanical properties, machine learning force fields, structural evolution

Research Article

24. Regulating the electrocatalytic performance for nitrogen reduction reaction by tuning the N contents in Fe_3@N_xC_{20-x} (x = 0~4): a DFT exploration

Full-Text PDF RIS

Cite this article: Han B, Li F. Regulating the electrocatalytic performance for nitrogen reduction reaction by tuning the N contents in Fe_3@NxC_{20-x} (x = 0~4): a DFT exploration. *J Mater Inf* 2023;3:24. https://dx.doi.org/10.20517/jmi.2023.32

Abstract

The Haber-Bosch (H-B) process, which is widely used in industry to synthesize ammonia, leads to serious energy and environment-related issues. The electrochemical nitrogen reduction reaction (eNRR) is the most promising candidate to replace H-B processes because it is more energy-efficient and environmentally friendly. Atomic-level catalysts, such as single-atom and double-atom catalysts (SACs and DACs), are of great interest due to their high atomic utilization and activity. The synergy between the metal atoms and two-dimensional (2D) support not only modulates the local electronic structure of the catalyst but also controls the catalytic performance. In this article, we explored the eNRR performance of 2D $Fe_3@N_xC_{20-x}$ (x = 0~4), whose structure was based on the experimentally synthesized $Ag_3@C_{20}$ sheet, by means of density functional theory calculations. Through calculations, we found that the 2D $Fe_3@N_4C_{16}$ with Fe_2 site coordinated with four N is a promising eNRR catalyst: the limiting potential is as low as -0.45 V, and the competing hydrogen evolution reaction can be effectively suppressed. Our work not only confirms that the coordination environment of the metal site is crucial for the electrocatalytic activity but also provides a new guideline for designing low-cost eNRR catalysts with high efficiency.

Keywords

Electrochemical nitrogen reduction reaction, two dimensions, single-atom and double-atom catalysts, active site, coordination, density functional theory

Research Article

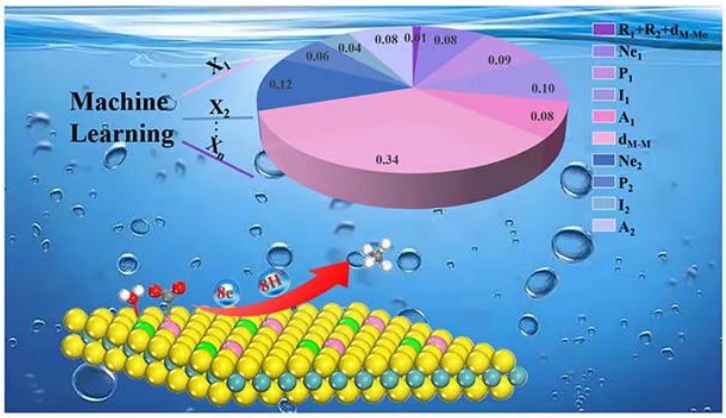
25. Investigation of dual atom doped single-layer MoS_2 for electrochemical reduction of carbon dioxide by first-principle calculations and machine-learning

Full-Text PDF RIS

Cite this article: Li H, Deng C, Li F, Ma M, Tang Q. Investigation of dual atom

doped single-layer MoS_2 for electrochemical reduction of carbon dioxide by first-principle calculations and machine-learning. *J Mater Inf* 2023;3:25. https://dx.doi.org/10. 20517/jmi.2023.29

Abstract



The exploration of efficient electrocatalysts for carbon dioxide reduction reaction (CO_2 RR) with viable activity and superior selectivity remains a great challenge. The efficiency of CO_2 RR over traditional transition metal-based catalysts is restricted by their inherent scaling relationships, so breaking this scaling relationship is the key to improving the catalytic performance. In this work, inspired by the recent experimental progress in the synthesis of dual atom catalysts (DACs), we reported a rational design of novel DACs with two transition metal atoms embedded in defective MoS_2 with S vacancies for CO_2 reduction; 21 metal dimer systems were selected, including six homonuclear catalysts (MoS_2-M_2, M = Cu, Fe, Ni, Mn, Cr, Co) and 15 heteronuclear catalysts (MoS_2-M_1 M_2). First-principles calculations showed that the MoS_2-NiCr system not only breaks the linear relationship of key intermediates but also possesses a low overpotential of 0.58 V and superior selectivity in the process of methane generation, which can be used as a promising catalyst for methane formation from CO_2 electroreduction. Notably, by combining random forest regression machine learning study, we found that the CO_2 RR activity of DACs is essentially controlled by some fundamental factors, such as the distance between metal centers and the number of outer electrons in the metal atoms. Our findings provide profound insights for the design of efficient DACs for CO_2 RR.

Keywords

Electrocatalysis, CO_2 RR, dual atom catalysts, random forest regression

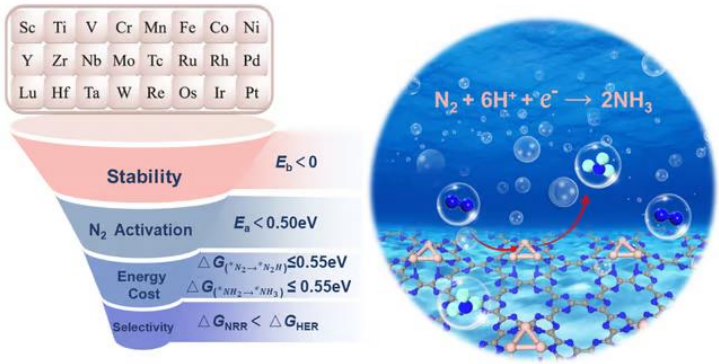
Research Article

26. Computational design of spatially confined triatomic catalysts for nitrogen reduction reaction

Full-Text **PDF** **RIS**

Cite this article: Pei W, Zhang W, Yu X, Hou L, Xia W, Wang Z, Liu Y, Zhou S, Tu Y, Zhao J. Computational design of spatially confined triatomic catalysts for nitrogen reduction reaction. *J Mater Inf* 2023;3:26. https://dx.doi.org/10.20517/jmi.2023.35

Abstract



The electrocatalytic process of nitrogen reduction reactions (NRR) offers a promising approach towards achieving sustainable ammonia production, acting as an environmentally friendly replacement for the conventional Haber-Bosch method. Density functional theory calculations have been utilized to design and investigate a set of catalysts known as triple-atom catalysts (TACs) for electrochemical NRR, which are supported on graphite-C_3N_3 nanosheets. Herein, we have systematically evaluated these TACs using stringent screening to assess their catalytic performance. Among the candidates, supported Pt_3, Re_3, and Ru_3 trimers emerged as highly active with decent selectivity, involving a limiting potential range of -0.35~-0.11 V. According to analysis of electronic properties, we determined that high NRR activity stems from the *d*-π* electron-accepting and -donating mechanism. Significantly, the correlation between chemical activity of TACs and electronic structure was established as a pivotal physical parameter, which has led to the conclusion that we can precisely control the catalytic behavior of transition metal trimer clusters by selecting appropriate metal elements and designing moderate cluster-substrates interactions. In summary, these theoretical studies not only enhance our understanding of how catalytic properties are governed by metal-support interactions, regulating stability, activity, and selectivity, but also offer a

useful method for screening and designing novel TACs for NRR.

Keywords

Density theory calculation, triple-atom catalysts, nitrogen reduction reaction, metal-support interactions