https://doi.org/10.1038/s43588-023-00433-2

# Guiding element mixing



**Materials design has largely expanded to multiple compositions, which requires the mixing of an increasing number of elements. In this joint Focus issue with *Nature Materials*, we take a closer look at the role of computational methods for guiding exploration within such vast chemical spaces.**

There is no doubt that compositionally complex materials (CCMs) — which are formed by mixing multiple elements — are of great interest to the materials science and engineering communities. The availability of a large number of blended elements in material lattices greatly expands the chemical space for materials design. Correspondingly, this expansion can help materials scientists to access previously unexplored physical domains, thus potentially enabling improved and exotic materials properties and allowing researchers to explore unprecedented applications.

This issue presents a Focus, in collaboration with *Nature Materials*, that highlights recent developments within the burgeoning field of complex element coupling, bringing together experts' opinions on the opportunities in designing CCMs for expanding materials capabilities. Notably, we at *Nature Computational Science* present a collection of manuscripts that provide insights into critical issues in computational method development for guiding element mixing in CCMs.

It goes without saying that the field of computational materials science has seen tremendous growth over the past several decades when it comes to steering materials design. For instance, first-principles methods at the atomic- and electronic-scale have enabled the calculation of defect energetics and electronic structures, offering insightful knowledge for dopant design in semiconductor applications, such as transistors and photovoltaics[1]. As another example, meso-scale computational methods, such as phase-field methods[2], have been widely used to investigate materials properties related to kinetics and microstructural evolution. However, these conventional techniques can be ineffective when dealing with the new complexities that arise with CCMs, such as low crystal symmetry, an increased number of competing phases, and imbalance in interactions among various atomic pairs. Thus, there is a quest in the computational science community to effectively utilize the available computational power in order to guide the design of CCMs.

Physics-based models continue to provide essential advances for the materials design process, but not without facing obstacles: the central computational challenge is to accurately model complexity and simultaneously keep the calculation affordable. One essential task in materials engineering, for example, is to predict materials defect properties and to further link these properties to application design. When modeling defects in CCMs — such as vacancies and interstitials — it is computationally expensive to sample and calculate the increased number of inequivalent defect sites within different local chemical environments. In a Perspective, Xie Zhang and colleagues provide an overview of the challenges and opportunities for extending conventional defect physics models to CCMs. They argue that conventional defect energetic models can be extended to CCMs by defining an effective formation energy with the help of advanced computational tools, such as statistical methods, sampling techniques, and configuration generation tools. Zhang and colleagues further point out that the calculation of energies for such a vast configuration space by using purely quantum mechanical methods — such as density functional theory (DFT) — is very expensive, and thus, new interatomic surrogate potential models that can reproduce the quantum-level accuracy are required.

To address some of the challenges faced by conventional physics-based models, artificial intelligence (AI)-based techniques that learn models from data have been identified as a promising venue in the field. For instance, as introduced in a Review by Alberto Ferrari and colleagues, the widely-used classical potentials become infeasible to accurately describe the ubiquitous and technically-relevant short-range order (SRO) — a type of local element ordering — in CCMs, since the various blended elements require a vast number of parameters to reliably mimic the high-dimensional interatomic relations. Ferrari and colleagues argue that machine learning interatomic potentials, such as low-rank potentials and moment tensor potentials, could be used to effectively investigate SRO in CCMs. Similarly, Dierk Raabe and colleagues examine in a Perspective how AI models can consider more constraints during the optimization processes for element selection and composition design in order to provide better guidance for the control of impurity during the manufacturing process. As one illustration, constraints related to the recyclability of the mixed elements can be taken into account for more sustainable materials manufacturing. The importance of

trace impurity control in alloy design is also highlighted in a *Nature Materials* Q&A with Zhi-Wei Shan.

It is worth highlighting that AI-based models can further complement, rather than simply replace, physics-based models. On the one hand, AI approaches can greatly expand the search space for identifying more complex physical relations for the design of CCMs, but this large dimension in the search space can impact efficiency. On the other hand, physics-based models rely on established functional forms that can somewhat restrict new discoveries, but that can more efficiently guide the design process. As highlighted by Raabe and colleagues, incorporating physical relations — such as thermodynamics laws and DFT predictions — into AI models as constraints is a promising strategy in the field that can improve the optimization and search efficiency through a careful balance of exploration and exploitation.

This Focus also features primary research articles, published at *Nature Materials*, that exemplify how exotic properties can be achieved through a sophisticated engineering of element mixing. For example, the Article by Hang Xue and colleagues demonstrates an interstitial solute stabilizing strategy to produce high-density, highly stable coherent nanoprecipitates in Sc-added Al–Cu–Mg–Ag alloys, enabling the Al alloy to reach an unprecedented creep resistance as well as an exceptional tensile strength at high temperatures. In another Article, Jinlong Du and colleagues report a reversible local disordering–ordering transition of precipitates by a careful element design in multi-component metallic alloys that enables high radiation tolerance at high temperatures. Finally, an Article by Jiadong Zhou and colleagues reports the synthesis of various two-dimensional CCMs that achieve tunable materials properties such as ferromagnetism and superconductivity. We believe similar successful stories will continue to excite our community, especially with guidance from computational and theoretical insights.

Finally, we would like to highlight the fact that the design of CCMs requires multidisciplinary collaboration between experimentalists, theorists, and computational scientists. While theoretical and computational insights can help experimentalists to better navigate through the vast design space, theoretical mechanisms need new experimental data to validate the findings and to provide constructive feedback for experimentalists. We hope that this joint Focus between *Nature Computational Science* and *Nature Materials* will inspire new collaborations that will accelerate new discoveries in materials engineering.

Published online: 31 March 2023

## References

1. Freysoldt, C. et al. *Rev. Mod. Phys.* **86**, 253 (2014).
2. Chen, L.-Q. *Annu. Rev. Mater. Res.* **32**, 113–140 (2002).