ARTIFICAL INTELLIGENCE EMPOWERED THERMAL MANAGEMENT MATERIALS DESIGN

Shenghong Ju and Bingyang Cao

Key Laboratory for Thermal Science and Power Engineering of Ministry of Education, Department of Engineering Mechanics, Tsinghua University

ABSTRACT The development of high-performance thermal management materials holds significant importance in fields such as chips, data centers and batteries. Materials informatics, which integrates big data and artificial intelligence, is emerging as the fourth paradigm for materials research. Over the past few years, our team has undertaken preliminary explorations in the development of advanced thermal management materials empowered by big data and artificial intelligence. In this work, we introduce three successful materials informatics applications on thermal management materials design, the construction of machine learning interatomic potentials for thermal property calculations, the discovery and generative design of high-thermal-conductivity materials, and the intelligent design of micro/nano structures for thermal transport. Those successful cases have shown great advantage for thermal management materials design via materials informatics.

1. INTRODUCTION

The relentless advancement of high-power electronics, data centers, electric vehicles, and battery systems, has pushed heat dissipation to the forefront of engineering challenges. Thermal management materials can effectively conduct, dissipate, or insulate heat to prevent device failure and enhance the thermal transport efficiency. Traditional approaches for thermal management materials design have heavily relied on trial-and-error experiments and simulations. However, the thermal properties of materials are governed by a complex interplay of factors across multiple scales, including atomic composition, microstructural morphology, and interfacial effects. Navigating this vast design space manually is immensely time-consuming, expensive, and often intractable.

Materials informatics (MI), which integrates big data and artificial intelligence (AI), has emerged as fourth paradigm for materials research. The necessity for AI stems from its unique ability to leverage data-driven strategies to overcome the limitations of traditional methods. Machine learning (ML) algorithms can assimilate vast datasets from experiments, simulations, and scientific literature to uncover hidden patterns and establish sophisticated relationships between materials' composition, processing parameters, and its final thermal properties. This capability allows for the rapid screening of tens and thousands of candidate materials, dramatically accelerating the discovery process. Beyond mere prediction, AI enables inverse design, where desired thermal performance criteria are inputted into generative models to propose entirely new, optimal material configurations that might be non-intuitive to human brains. By acting as a powerful surrogate for complex simulations, AI also reduces computational costs and can intelligently guide experimental efforts, creating a closed-loop, accelerated research pipeline.

In this work, we present three successful applications of materials informatics in thermal management materials design: (1) developing machine learning interatomic potentials for thermal property calculations, (2) discovering and generative designing materials with high thermal conductivity, and (3) intelligently designing micro/nano structures for thermal transport. These cases demonstrate the significant advantages of MI in advancing thermal management materials.

2. MACHINE LEARINING POTENTIALS

Recently, machine learning interatomic potentials (MLIPs) have emerged as powerful tools in computational physics and chemistry, showing great potential in providing reliable predictions of thermal transport properties with high efficiency (Liu et al., 2020 and 2023, Yang et al., 2024). The MLIPs have been attracting researchers' attention due to their computational efficiency and accuracy as a compelling alternative to Density Functional Theory (DFT). In MLIP models, a potential energy surface (PES) is constructed for the accurate prediction of energies and forces by learning from the DFT reference results. In this work, the atomic cluster expansion (ACE) potential has been selected as the paradigmatic model due to its precision with efficiency on high-performance parallel computation, meeting a range of computational requirements (Guo, et al., 2025a and 2025b).

The primary purpose of MLIPs is to model the PES of a target system, from which the total energy and

interatomic forces are derived based on a set of N atomic positions. This modeling process, represented as a regression task in mathematics, starts with the description of total energy, as the forces can be obtained by differentiating the energy with respect to the atomic positions. Unlike empirically fitted potentials, MLIPs do not impose any prior assumptions on the functional form of the PES. Instead, the shape of the potential is directly learned through a regression process from a large set of reference configurations with their corresponding energies and forces, typically obtained from DFT calculations. Collectively, these elements constitute the dataset for training and validating the ML potential.

As illustrated in Fig. 1, the perturbation method begins with structures positioned at energy minima and then introduces random displacements to atoms in their supercells to generate reference configurations. However, structures generated by this stochastic approach might sometimes exhibit large interatomic forces due to the possibility of atoms being placed very close together, resulting in significant repulsive forces. To address this issue, constraints on a minimum atomic distance can be added via a Monte Carlo (MC) process, where configurations with short atomic distances below a threshold are only accepted with low probability. Moreover, to ensure that the potential accurately forecasts forces, it might sometimes be necessary to subject the lattice to stress through tension or compression. After acquiring these reference structures, they are subsequently employed to produce a reference dataset via DFT calibration.

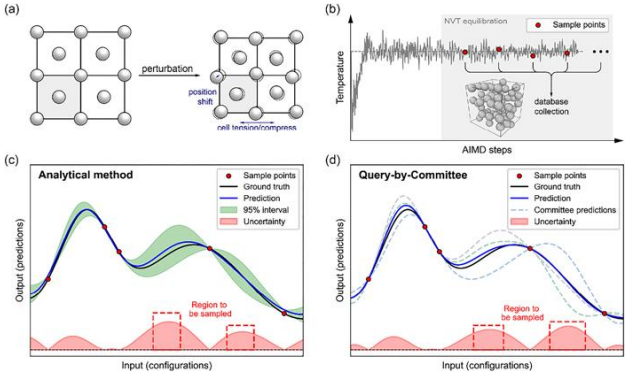

Fig. 1. Approaches for data collection. (a) Perturbation method. (b) *Ab Initio* Molecular Dynamics (AIMD) method. (c) Analytical definition of uncertainty in active learning. (d) Query-by-Committee definition of uncertainty in active learning.

As demonstration, we applied the machine learning approach to calculate the thermal conductivity of amorphous carbon. Using the same time step of 1 fs, we start with a 512-atom orthogonal box held at 8,000 K and then cooled down to 5,000 K for 100 ps. We then perform a rapid quench from 5,000 to 300 K within 1 ps. Finally, the system is equilibrated at 300 K for 100 ps, followed by an energy minimization process for the equilibrium structure. We compare the radial distribution function (RDF) of the final generated structure with those from AIMD and the Tersoff potential. As shown in Fig. 2, the RDF of ACE shows good agreement with the result of AIMD simulation, whereas the Tersoff potential does not capture the right locations and values of the second and the third RDF peaks. The simulations accelerated by MLIPs show a speed of 3 to 4 orders of magnitude faster than AIMD, with linear scaling relative to the system size and the number of CPU cores used in the calculation. In contrast, the computational cost of AIMD grows exponentially with the number of atoms, leading to a sharp increase in computational expense, which restricts its application to large systems.

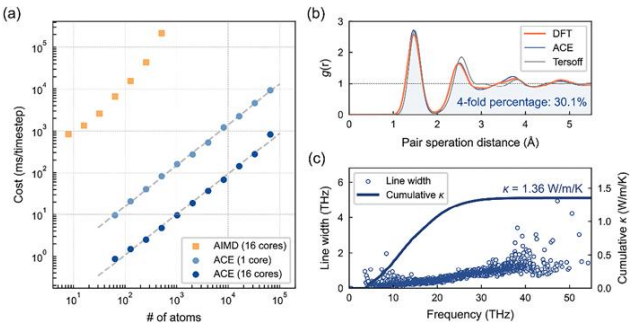

Fig. 2. (a) Comparison of computation efficiency on AIMD and MLIP MD. (b) RDF of a-C. (c) Scattering rate distribution and cumulative thermal conductivity of a-C.

As illustrated in Fig. 2(c), the thermal conductivity of a-C is 1.36 $Wm^{-1}K^{-1}$, which is close to the value of 1.61 $Wm^{-1}K^{-1}$ using the linear fit to experimental data reported, demonstrating the capability of MLIPs in thermal calculations for complex systems. We noted that the propagation contribution is likely to be underestimated due to the limitation of the quasi-harmonic Green's function method and a proper extrapolation is needed for the case in which propagation mechanism matters, like a-C with higher density and amorphous silicon.

3. HIGH THERMAL CONDUCTIVE MATERIALS

3.1 Crystals with high thermal conductivity

Ultrahigh lattice thermal conductivity materials hold great importance since they play a critical role in the thermal management of electronic and optical devices. Models using machine learning can search for materials with outstanding higher-order properties like thermal conductivity. However, the lack of sufficient data to train a model is a serious hurdle. Herein we show that big data can complement small data for accurate predictions (Ju, et al., 2021) when lower-order feature properties available in big data are selected properly and applied to transfer learning. The connection between the crystal information and thermal conductivity is directly built with a neural network by transferring descriptors acquired through a pretrained model for the feature property, as shown in Fig. 3. The transfer learning bridges “big data” (harmonic three-phonon scattering phase space of 320

crystals) and "small data" (thermal conductivity of 45 crystals) to search for ultrahigh lattice thermal conductivity crystals. All neurons (circles) are activated by ReLU (Rectified Linear Unit). Dropout (dash circles and lines) range (0.1 or 0.2) in each hidden layer is randomly chosen. Numbers at the bottom indicate the number of neurons used in each layer of the neural network and random forest model.

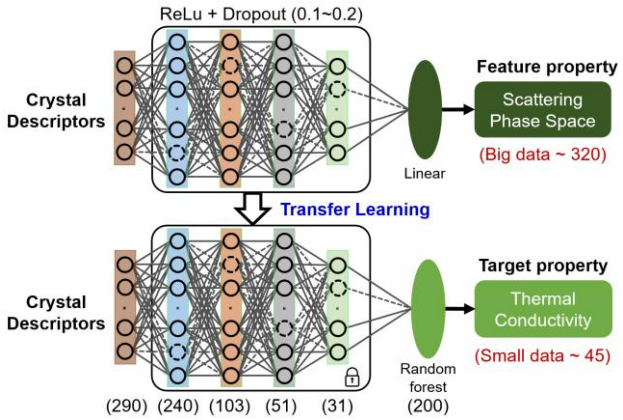

Fig. 3. Schematics of feature-based transfer learning.

Successful transfer learning shows the ability of extrapolative prediction and reveals descriptors for lattice anharmonicity. The training and validation results of the pre-trained and transferred models are shown in Fig. 4. The transferred model successfully predicts the 14 crystals even though their κ_L lie in the ultrahigh region of 1,000-3,000 $Wm^{-1}K^{-1}$. It should be noted that the κ_L of the 45 training crystals reside in the region smaller than 370 $Wm^{-1}K^{-1}$, which is much lower than the prediction. This indicates that the transferred model exhibits extrapolative predictive power.

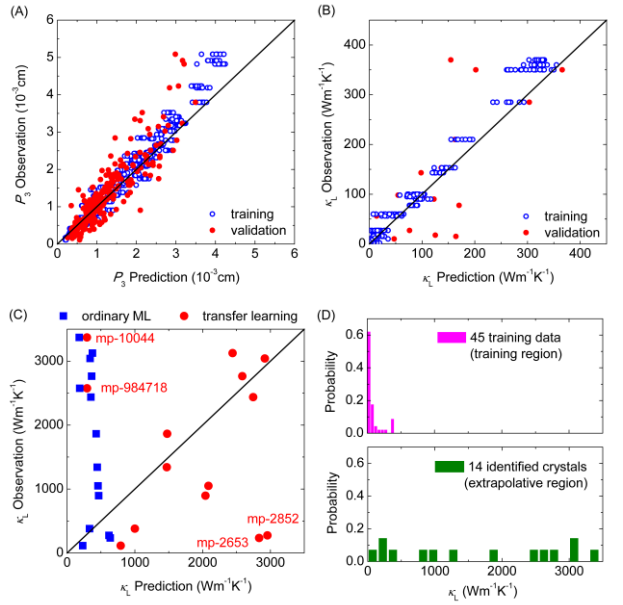

Fig. 4. Training and validation for (A) the pre-trained P_3 model, (B) transferred κ_L model. (C) Comparison of ordinary machine learning and transfer learning. (D) κ_L distribution of 45 training and 14 identified crystals.

The resulting model is employed to screen over 60,000 compounds to identify novel crystals that can serve as alternatives to diamond. Even though most materials in the top list are superhard materials (Fig. 5), we reveal that superhard property does not necessarily lead to high lattice thermal conductivity. Large hardness means high elastic constants and group velocity of phonons in the linear dispersion regime, but the lattice thermal conductivity is determined also by other important factors such as the phonon relaxation time. What is more, the average or maximum dipole polarizability and the van der Waals radius are revealed to be the leading descriptors among those that can also be qualitatively related to anharmonicity.

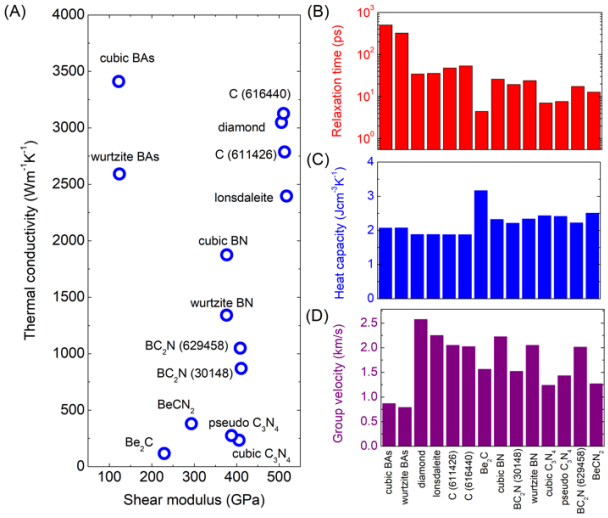

FIG. 5. Hardness versus thermal conductivity and comparison of parameters related with thermal conductivity. (A) Thermal conductivity versus shear modulus for the top-14 materials. (B)-(D) Average group velocity, heat capacity, and relaxation time of the top-14 materials.

The recent development of generative models and ML holds great promise for predicting new functional materials. Here, we show how combining deep generative models of crystal structures with quantum-accurate, fast ML interatomic potentials can accelerate the prediction of materials with ultrahigh lattice thermal conductivity while ensuring energy optimality. We exploit structural symmetry and similarity metrics derived from atomic coordination environments to enable fast exploration of the structural space produced by the generative model. Additionally, we propose an active-learning-based protocol for the on-the-fly training of ML potentials to achieve high-fidelity predictions of stability and lattice thermal conductivity in prospective materials, as shown in Fig. 6. Starting with the initial crystalline structures, an SE(3)-equivariant crystal diffusion variational autoencoder (CDVAE), is trained to produce synthetic structures. The synthetic structures then undergo optimization with pre-trained MLIP models. Complex unit cells with low symmetry are filtered out based on the

empirical rule, leaving a refined dataset of candidate materials. Subsequently, we select the most diverse m structures using the farthest points sampling (FPS) algorithm as benchmarks and assess their κ_L via an accurate evaluation of lattice thermal conductivity (ETC) protocol. Next, we cluster the candidate materials into m groups based on their structural similarity with benchmarks. All materials in those groups containing benchmarks with $\kappa_L \geqslant 800$ $Wm^{-1}K^{-1}$ are further screened with the same ETC protocol. During the ETC process, MLIP models will be improved on the fly using an active learning strategy, ensuring high-fidelity κ_L predictions. Finally, the identified potential materials with ultrahigh κ_L are validated by either DFT calculations or experimental measurements.

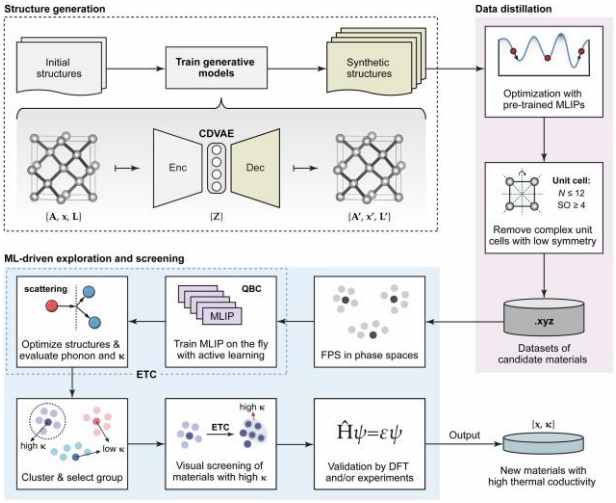

Fig. 6. Generative deep learning for predicting ultrahigh lattice thermal conductivity materials.

The ML-driven exploration of ultrahigh κ_L materials is conducted on the 1361 candidates. The visualization of the entire candidate set is illustrated in Fig. 7 mapped by Smooth Overlap of Atomic Positions (SOAP) descriptors. It highlights some well-known carbon allotropes, such as diamond, graphite, and Bct-C12, which have been reproduced through the generative process. We first use the FPS algorithm to select the 50 most diverse structures as benchmarks, as indicated by the green squares. In addition, five reported ultrahigh κ_L materials are included as benchmarks to further enhance the search process. Note that by executing FPS, we identify 53 benchmarks, among which diamond and AA T12-carbon are included. Applying this method to carbon materials, we screen 100,000 candidates and identify 34 carbon polymorphs, approximately a quarter of which had not been previously predicted, to have lattice thermal conductivity above 800 $Wm^{-1}K^{-1}$, reaching up to 2,400 $Wm^{-1}K^{-1}$ aside from diamond. Figure 7d shows the distribution of κ_L values for the entire set of candidate materials identified through our workflow. These findings provide a viable pathway toward the ML-assisted prediction of periodic materials with exceptional thermal properties.

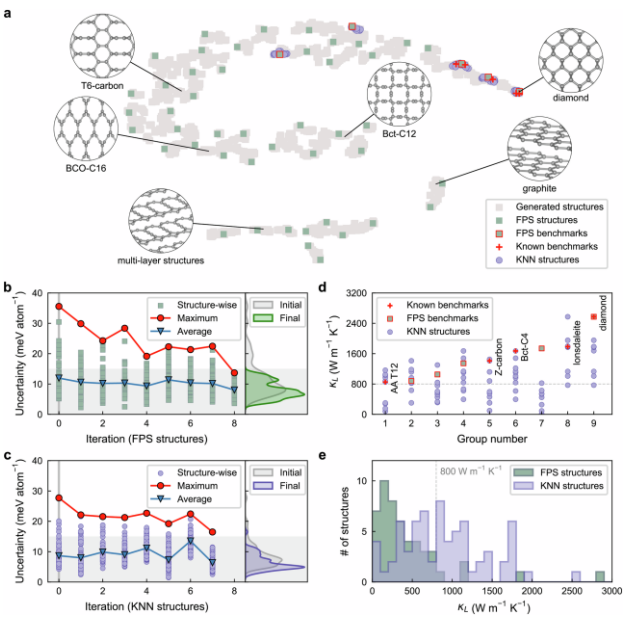

Fig. 7. Machine learning-driven exploration of ultrahigh κ_L materials.

3.2 High thermal conductive polymers

The efficient and economical exploitation of polymers with high thermal conductivity (TC) is also essential to solve the issue of heat dissipation in organic devices. Currently, the experimental preparation of functional polymers with high TC remains a trial-and-error process due to the multi-degrees of freedom during the synthesis and characterization process. Polymer informatics equips ML as a powerful engine for the efficient design of polymers with desired properties. However, available polymer TC databases are rare, and establishing appropriate polymer representation is still challenging. Herein, we propose a high-throughput screening framework for polymer chains with high TC via interpretable ML and physical feature engineering, as shown in Fig. 8 (Huang, et al., 2023a and 2023b). The hierarchical down-selection process stepwise optimizes the 320 initial physical descriptors to the final 20 dimensions and then assists the ML models to achieve a prediction accuracy R^2 over 0.80, which is superior to traditional graph descriptors.

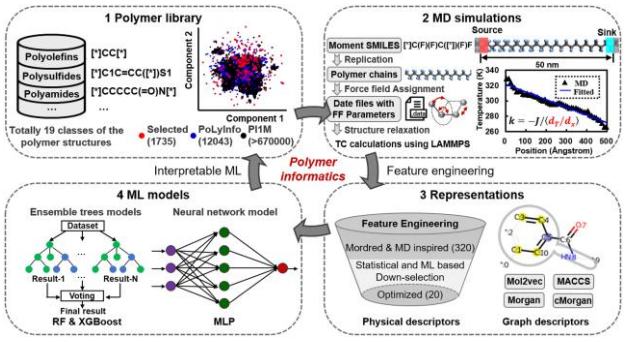

Fig. 8. High-throughput screening of polymers with high TC via interpretable machine learning.

Using the trained ML models, we discovered 107 promising polymers with TC greater than 20.00 $Wm^{-1}K^{-1}$, and 29 of which have SA scores of no more than 3.00. These polymer structures have been validated through high-fidelity MD simulations. Further, we used SR with optimized descriptors to fit the TC of promising polymers, and the derived mathematical formulas enable a preliminary fast screening of high TC polymers without relying on ML models, which is friendly for experimental studies. In closing, we calculated phonon dispersion relations for four typical polymer structures via phonon spectral energy density analysis to reveal the underlying TC mechanisms, as shown in Fig. 9. Notably, most of these structures are π-conjugated polymers, whose overlapping p-orbitals enable easy maintenance of strong chain stiffness and large group velocities. Ultimately, we establish the connections between the individual chains and the amorphous state of polymers. Polymer chains with high TC have strong intra-chain interactions, and their corresponding amorphous systems are favorable for obtaining a large radius of gyration and causing enhanced thermal transport. The proposed data-driven framework should facilitate the theoretical and experimental design of polymers with desirable properties.

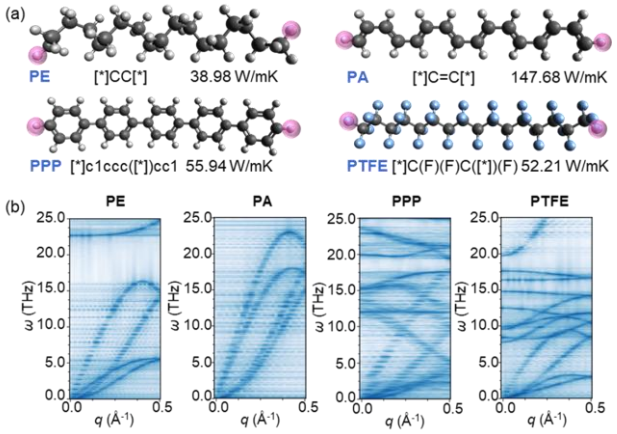

Fig. 9. Structure (a) and phonon dispersion relations (b) for four promising polymers.

4. STRUCTURE DESIGN AND OPTIMIZATION

The rapid development of nanotechnology has introduced unprecedented opportunities in designing nanostructures for energy transport in the forms of phonons, electrons, and photons. Take thermal transport in semiconductors as example, the phonon transport becomes more ballistic when the material length scale is reduced to the nanoscale. Forming the appropriate nanostructure to tune the phonon transport is challenging because phonon transport is highly sensitive to the detailed atomistic configurations. Among the various machine-learning algorithms, the Bayesian optimization employing Gaussian processes is well established as a prediction model for black-box optimizations. The combined process for the Bayesian optimization and the thermal-transport-property calculator is shown in Fig. 10 (Ju, et al., 2020). Suppose the candidates are represented as d-dimensional vectors $\boldsymbol{x} = (x_1, \ldots, x_m) \in \mathbf{R}^d$, which are candidate descriptors. The dimensional size is typically smaller than 20 in most successful applications. In the Bayesian optimization process, the transport properties of n candidates are initially calculated. Then, the next one to calculate is chosen. The purpose of the Bayesian optimization is to find the candidate with an optimal transport property using as few calculations/experiments as possible. A Bayesian regression function is learned from n pairs of descriptors and transport properties. This statistical prediction model is invariably a Gaussian process, which provides a Bayesian posterior probability distribution that describes the potential thermal conductance values for candidate point x. The best candidates are chosen based on the expected improvement criterion, a widely used acquisition function that can explicitly encode a trade-off between exploitation (evaluating points with low mean) and exploration (evaluating points with high uncertainty). Besides the expected improvement, the maximum probability of improvement and upper confidence bound are two other popular acquisition functions used in Bayesian optimization. Finally, the exact thermal transport properties values are calculated for the chosen candidate and added to the training set. By repeating this procedure, the calculation of thermal transport property is scheduled optimally, and the best candidate can be found quickly.

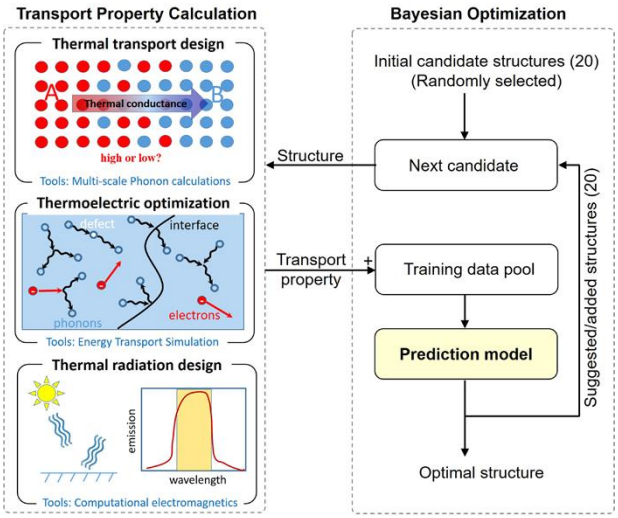

Fig. 10. General workflow of the optimal material design for thermal functions such as phonon transport, thermoelectrics, and thermal radiation.

4.1 Nanostructure for phonon transport

We demonstrate optimization of Si-Si and Si-Ge interfacial thermal conductance (ITC) across nanostructures by combining atomistic Green's function and Bayesian optimization, as shown in Fig. 11 (Ju, et al.,

2017). With an aim to minimize and maximize the ITC across Si-Si and Si-Ge interfaces by means of the Si/Ge composite interfacial structure, the method identifies the optimal structures from calculations of only a few percent of the entire candidates (over 60,000 structures). The obtained optimal interfacial structures are nonintuitive and impacting: the minimum ITC structure is an aperiodic superlattice that realizes 50% reduction from the best periodic superlattice. The physical mechanism of the minimum ITC can be understood in terms of the crossover of the two effects on phonon transport: as the layer thickness in the superlattice increases, the impact of Fabry-Pérot interference increases, and the rate of reflection at the layer interfaces decreases. An aperiodic superlattice with spatial variation in the layer thickness has a degree of freedom to realize optimal balance between the above two competing mechanisms. Furthermore, the spatial variation enables weakening the impact of constructive phonon interference relative to that of destructive interference. The present work shows the effectiveness and advantage of material informatics in designing nanostructures to control heat conduction, which can be extended to other nanostructures and properties.

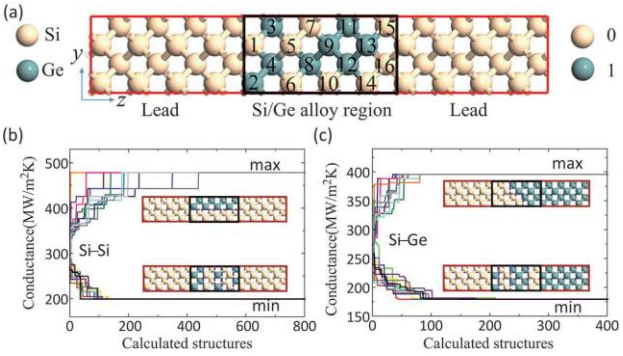

Fig. 11. Bayesian optimization of interfacial Si/Ge alloy structure for maximum and minimum thermal conductance. (a) System for atomistic Green's function calculation, (b) and (c) show the 10 optimization runs with different initial choices of candidates for Si–Si and Si–Ge cases, respectively. The insets show the corresponding optimal structures for maximum and minimum thermal conductance.

4.2 Thermal radiation materials

We also develop a hybrid materials informatics approach which combines the adversarial autoencoder (AAE) and Bayesian optimization to design narrowband thermal emitters at different target wavelengths (Zhu, et al., 2022). The schematic of the hybrid optimization framework is shown in Fig. 12, which combines AAE-assisted BO with the electromagnetic solver rigorous coupled wave analysis (RCWA). The narrowband thermal emitters are composed of 36 cell layers of Ge and SiO_2 materials. The materials are chosen from commonly used semiconductors with high refractive index and dielectric materials with low refractive index, while the substrate material uses tungsten that can be considered opaque. To make the input of the AAE model intuitive and generic, binary values are used to indicate the material selected for each layer, with "0" and "1" representing the Ge and SiO_2 layers, respectively. Each unit layer of the multilayer structure has a thickness of 0.11 μm. Following this way, 36-dimensional vectors represent different possible multilayer structures. According to combinatorial theory, the total number of candidate structures is 2^{36}, which composes a huge candidate structure space. The goal of the optimization is to determine the selection of the material sequence that enables the target thermal emission properties with a working band ranging from 4 to 7 μm.

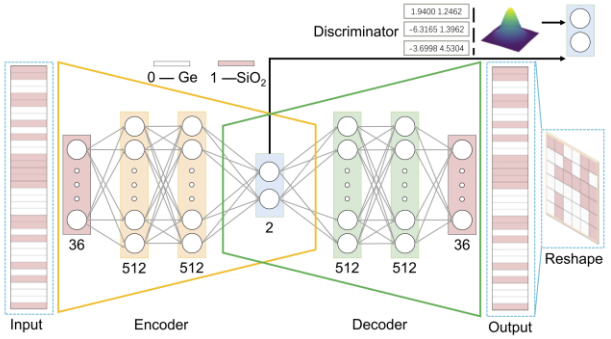

Fig. 12. Schematics of thermal radiation metamaterials design via a hybrid adversarial autoencoder and Bayesian optimization.

Figure 13 shows the emittance of the best multilayer structures designed by the AAE+BO framework for three different target wavelengths, where the dashed, dashed–dot, and solid curves represent the optimal designs with FOM of 0.87, 0.89, and 0.84, respectively. The inset of Fig. 13(a) shows the corresponding material selection sequence reshaped to 6 × 6 pixels. According to the optimization result, the high emission at the target wavelength and the rapid decay of emission at the non-target wavelength are realized. Although there is still room for further improving the emission spectra, the structures found here already satisfy the design target with less than 10,000 calculations, and the optimization efficiency is considerable for a search problem with a candidate space of 68.7 billion. In addition, less than 2,000 iterations per round enables a prevention of the exponential increase of time for BO to store the computed structural information. Figure 13(b) shows the comparison of the FOM kernel density estimation with two optimizations. With only several hundreds of training data sets, new structures with optimal properties can be quickly determined in a compressed two-dimensional latent space. This enables the optimal design by calculating far less than 0.001% of the total candidate structures, which greatly decreases the design period and cost. The proposed design framework can be easily extended to other thermal radiation metamaterials design with higher dimensional features (Liao, et al., 2024).

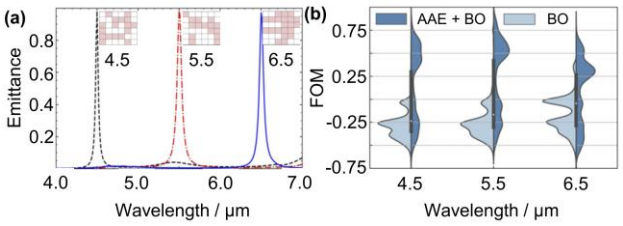

Fig. 13. (a) Emittance of the best designs searched by the AAE+BO framework. The inset depicts the structure design corresponding to each emissivity. (b) Violin plot of the optimization process for the three target wavelengths.

5. CONCLUSION AND OUTLOOK

From the various examples presented, it's clear that artificial intelligence and data science provide a powerful tool for thermal science research and is even transforming the entire field of computational materials science. However, there are still several challenges to be solved and discussed in the future. The first challenge is the automated training of machine learning potentials. Training general-purpose machine learning potentials requires extensive domain knowledge and effort. To minimize human effort and cost, developing automated workflows can be beneficial. Such workflows would also aid in developing universal machine learning potentials. The second challenge is developing universal machine learning potentials. If we can figure this out, there would be no need to train a new model for every material, significantly reducing the material development cycle. The third challenge is fine-tuning large models. Once we have universal machine learning potentials, fine-tuning them for specific material systems will make them more applicable. However, fine-tuning large models is still in its early stages. Lastly, the application of generative models is another challenge. While generative models can accelerate the development of new materials, they currently cannot directly generate thermodynamically stable materials due to the lack of physical constraints. This remains a significant hurdle. Despite these challenges, we can foresee that artificial intelligence will play an increasingly important role in the thermal science field. If above challenges are addressed, the development of new thermal management materials with superb properties will be greatly accelerated. This, in turn, will have a significant impact on both industrial applications and academic research.

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Shenghong Ju received the B.E. (2008) from Nanjing University of Aeronautics and Astronautics, and Ph.D. (2014) from Tsinghua University. He is associate professor at Dept. of Eng. Mechanics, Tsinghua University. His current interests include AI-driven materials design, and nanoscale thermal transport.

Bingyang Cao received his B.S. (1998) and M.S. (2001) from Shandong University, and Ph.D. (2005) in engineering thermophysics from Tsinghua University. He then joined Tsinghua University, and is currently a full professor and dean at the School of Aerospace Engineering, Tsinghua University. His research interests include micro-/nano-scale heat transfer, thermal functional materials, advanced thermal management technologies etc.