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Machine Learning for Harnessing Thermal Energy: From Materials Discovery to System Optimization

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Abstract

Recent advances in machine learning (ML) have impacted research communities based on statistical perspectives and uncovered invisibles from conventional standpoints. Though the field is still in the early stage, this progress has driven the thermal science and engineering communities to apply such cutting-edge toolsets for analyzing complex data, unraveling abstruse patterns, and discovering non-intuitive principles. In this work, we present a holistic overview of the applications and future opportunities of ML methods on crucial topics in thermal energy research, from bottom-up materials discovery to top-down system design across atomistic levels to multi-scales. In particular, we focus on a spectrum of impressive ML endeavors investigating the state-of-the-art thermal transport modeling (density functional theory, molecular dynamics, and Boltzmann transport equation), different families of materials (semiconductors, polymers, alloys, and composites), assorted aspects of thermal properties (conductivity, emissivity, stability, and thermoelectricity), and engineering prediction and optimization (devices and systems). We discuss the promises and challenges of current ML approaches and provide perspectives for future directions and new algorithms that could make further impacts on thermal energy research.
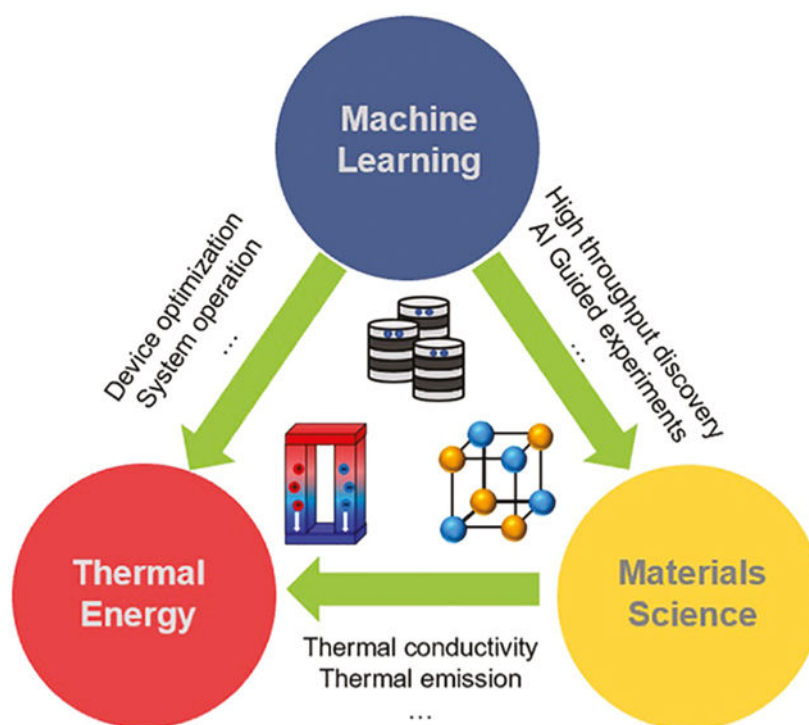
Graphical Abstract

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Author Contributions
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Thermal energy is the main form for energy conversion, storage, and thermal management: It converts to 90% of total electricity generation,[1] represents 80% of residential energy consumption,[2] and consumes 50% of the electricity used in computers and data servers for thermal management.[3] Efficient utilization of thermal energy, including conversion, storage, and thermal management, plays a key role in global sustainability while relying critically on innovations in thermal materials systems. Over the past decades, tremendous efforts have been devoted to modeling materials' structures with designed thermal properties and improved energy efficiency. Those computational approaches, from empirical to first-principles, atomistic to microscopic and multi-scales, diffusive to non-equilibrium, have made exciting progress in all aspects of thermal properties and performance. However, the significantly expanded materials database not only provides new materials with extreme properties and energy efficiency beyond the state of the art,[4–22] but also poses challenges on further analysis and development through multi-dimensional big data. In the meantime, machine learning (ML) has gained its visibility in dealing with big data such as image recognition, social media, and game contests between human and artificial intelligence and has manifested its applicability in autonomous driving, real-time language translation, and new materials discovery.[23–26] The power of ML mainly comes from its statistical analysis of big data, which also exists in thermal energy materials research such as experimental results, ab initio calculations, and molecular dynamics (MD) simulations. Therefore, our thermal energy community actively embraces the rising and development of ML approaches to accelerate the research, from the bottom-up materials design to top-down system optimizations.

The applications of ML in energy research can be indicated by the exponential growth of publication numbers with energy and energy materials focus illustrated in Figure 1. The combination between ML and energy research observed its onset around 2011, when IBM's Watson competed on Jeopardy against the two human champions and won,[27] and took its rocket around 2016 when Google's AlphaGo finally beat the top human players in the board game Go.[28] Nowadays, ML has been implemented in almost every aspect of thermal energy study. At the fundamental level, the Schrödinger equations of quantum systems are solved with the assistance of ML algorithms, such as training artificial neural networks (ANNs) for the exchange-correlation functional of density functional theory (DFT), which helps the calculation of electronic structures and interatomic interactions.[29] The thermodynamic properties such as thermal stability, entropy, and enthalpy of materials can be predicted from the quantum mechanics calculations.[30] Combined with the MD and/or Boltzmann transport equation, where ML can also play a role, the transport properties such as thermal conductivity, thermal boundary conductance, thermal emissivity, thermoelectric properties, and others can be predicted.[18,31–35] Most importantly, with the accumulation of atomistic modeling data, the high-throughput discovery of thermal materials becomes possible using ML as the key tool. The philosophy of material discovery will be revolutionized from the traditional and slow trial and error strategy to modern efficient high-throughput screening from millions of candidate materials. On the other hand, the structure and composition of materials are also decisive to their thermal performance, such as the porous structure of thermal insulation materials and components of composite materials.[36–40] It is labor-intensive and time-consuming to scan all the compositional or structural parameters to find the optimal material synthesis and manufacturing recipes. By taking advantage of the ML's power on optimization problems with limited knowledge, the efforts on material design can be significantly reduced. The structural optimization of thermal energy devices is another challenge for engineers. For instance, the fin shape and size are important factors in the performance of heat exchangers, the thermal barrier coating layer thickness to turbines, and the diameter and arrangement of pipes to boilers in power plants. It has become an emerging trend to use ML to design thermal devices. On the other hand, the instant response to real-time sensor reading is important in different applications, especially in thermal energy fields, like the ventilation, cooling and heating power control in response to the real-time temperature, and humility reading in buildings. The decision-making power of ML is suitable for these scenarios, considering their big success in games like Go.

This emerging interdisciplinary area is still expanding rapidly and should be reviewed promptly regarding the state-of-the-art development, existing opportunities, and challenges. First, we provide a brief introduction to ML concepts and several common algorithms for thermal energy research. Then we discuss the intrinsic thermophysical properties prediction of homogeneous materials, including thermodynamic properties, thermal transport properties, and thermoelectric properties. The implementations of ML in structural and compositional optimization of heterogeneous materials are also discussed from porous structures to composite materials. In addition, the applications of ML in the design of thermal devices and operation of energy systems will be highlighted, including heat exchangers and heating, ventilation, and air conditioning (HVAC) systems in buildings. We

hope that this review can serve as an inspirational reference to the thermal energy research community and encourage them to integrate ML into their own research.

MACHINE-LEARNING CONCEPTS, ALGORITHMS, AND IMPLEMENTATION: WHAT AND WHY?

Machine learning is a concept in applied statistics and was initially defined by Tom M. Mitchell as a computer program to learn from experience (E) with respect to some class of tasks (T) and performance measures (P) if its performance at tasks improves with experience.[41] Considering the continuing expansion of ML methods and our focus on its applications for scientific research, we are not ambitious to make a comprehensive discussion of ML algorithms here. Instead, we summarize the most representative and popular algorithms in Figure 2 at the balancing point of completeness and conciseness. ML can be mainly categorized into supervised, unsupervised, and reinforcement learning, depending on the computer program's interaction with humans or certain feedback designed by humans. Supervised learning is to learn a relationship between the input X = {X_1, X_2, …, X_N} and output Y = {Y_1, Y_2, …, Y_N} from a labeled training set of observations of (X, Y) under human guidance. Each element in the X is a D-dimensional vector X_i = [$X_{i,1}$, $X_{i,2}$, …, $X_{i,D}$] representing D features. For materials science, the features are usually called material descriptors. The mathematical function $f(X_i)$ to map input to output is given by humans no matter if it is explicit or implicit. Supervised learning is mainly used for classification and regression, conducted through various algorithms including the basic linear regression method and the more recent methods like ANNs and random forest. Unsupervised ML can develop learning without human guidance and the machine needs to capture certain patterns from untagged data, such as the probability density. The dimension of X in unsupervised learning can be much higher than that in supervised learning. This type of learning is usually used for clustering and dimensionality reduction, for example, searching for the principal variation directions of data in a high-dimensional space, or called principal component analysis. Reinforcement learning is to let machines learn how to interact with an environment dynamically instead of understanding the patterns or mappings behind the static data. In the reinforcement learning process, the machine can earn an immediate reward once it takes a certain action to make state transition happen. It suits decision-making to achieve optimal performance for dynamically active scenarios, like robot control and game theory. With the recent improvement of computational resources and rapid data expansion in many areas such as commercial behaviors, industrial operations, and academic research, ML has been successfully applied to handle complex and high-dimensional problems during the past decade. In the following context, we are going to introduce several popular ML methods for materials discovery.

Linear Regression.

As the most traditional supervised learning method, linear regression assumes the output **Y** is a linear function of the input data **X**, as shown in Figure 3a. Mathematically, the linear function can be expressed as

$$f(x_i) = w^T X_i + w_0 \tag{1}$$

where w^T, w_0 are the weight vector for the D features and offset from zero point. In the case that the **Y** values cannot be approximated by a linear function of the initial set of input data **X**, a new set of input data can be constructed from **X** to fulfill the linearity requirement, such as $f(X_i) = w^T G(X_i) + w_0$, where $G(\mathbf{X}_i)$ is a nonlinear function of X_i. To determine the weighting parameters, the residual sum of squares should be minimized, i.e., $min \sum_{i=1}^{N} (Y_i - w^T X_i - w_0)^2$. Due to the model's simplicity, these mathematical equations can usually be analytically determined. For simple problems, linear regression can provide fast, robust, and physically interpretable fitting results. In thermal transport, it is exemplified by the linear relationship between heat flux and temperature gradient in solids, i.e., Fourier's law. However, materials science is a complex subject, which can pose challenges to linear regression so sometimes it may not work well and cause issues, for example, overfitting, for determining materials properties.

Kernel Methods.

Under the kernel trick,[42] a kernel function is used to transform nonlinear regression problems by mapping the input data to a higher dimensional space (feature space) so that they become linear or separable. In this way, computational efficiency can be improved by using a kernel function, rather than explicitly specifying the mapping function $G(X_i)$. The most common kernel functions include radial basis function kernels, Matern kernels, Fisher kernels, String kernels, and others.[43] The kernel functions can easily calculate the inner products of data in the feature space $K(X_i, X_j) = G(X_i)G(X_j)$ without knowing the explicit form of $G(X_i)$, which essentially is the distance or similarity of two data points in the feature space. The distance can be input to various ML methods, including support vector machines, Gaussian processes, principal components analysis, relevance vector machines, and so on. The kernel methods were initially designed for pattern recognition, and recently they have been applied for calculating thermal transport properties.[44–46]

Artificial Neural Networks.

The development of ANNs is inspired by the signal transmission and processing in biological neural networks that constitute animal brains. ANNs consist of a collection of stimulating units or nodes, called artificial neurons. Each neuron receives, processes, and transmits signals to adjacent neurons. The neurons are connected to each other in various patterns via links, which determine the strength of one neuron's influence on another, mimicking the biological axon–synapse–dendrite connections. One representative ANN is the feed-forward neural network, as shown in Figure 3b, consisting of one input layer (X_i), multiple hidden layers (Z_i), and one output layer (Y_i). The input layer neurons process the input data and feed the output data into the hidden layers. After several layers are processed, until the processing of the last hidden layer is achieved, the output layer neurons generate the output data. Mathematically, the output of a certain neuron at the hidden layer can be calculated as $Z_i = \sigma(w^T X_i + w_0)$, where σ is an activation function, defining if the neuron can be activated by the excitation. Another ANN is reservoir computing as shown in Figure 3c, by passing the input signals to the neurons reservoir, where the

neurons are not distinguished by layers but form a reservoir and readout layer which is similar to the hidden layer in the feed-forward ANN to generate a useful output data set. The distinguishing feature of reservoir computing is the recurrent behavior; i.e., the current response of a neuron is affected by the stored historical information on all neurons, with different strengths. Since reservoir computing only requires training the readout layer under fixed reservoir dynamics, it can largely reduce the computational cost for time-dependent thermal operations considering the recurrent behaviors. For example, reservoir computing can be applied to design a building heating or cooling system that can automatically adapt itself by temperature and humidity mapping between room and environment or to optimize the cleaning strategy of a home robot cleaner by deep-learning image processing and recognition.

Decision Trees.

A decision tree is a flowchart-like decision-making process, where the root receives the input data, each internal node is a logical question with possible answers represented by the branches, and each leaf node is the final answer to the series of questions. The decision trees can deal with classification and operation problems accurately with explicit logic. To avoid overfitting results, a random forest of decision trees (Figure 3d) can be applied: Each decision tree receives a random sample of the input training data set, different from each other, called bagging. The trained decision trees will generate a distribution of predictions, from which the final output can be computed, for example by averaging or voting. Random forest decision trees usually require much less computational resources than the ANN while could be accurate enough for simple regression problems. One advantage of using decision trees in thermal energy materials is to evaluate the key important material descriptors to determine thermal transport properties.

WHY AND HOW TO IMPLEMENT MACHINE LEARNING INTO THERMAL SCIENCE

The implementation of ML into thermal science spans from the most fundamental ab initio modeling of thermal transport to the prediction of thermal performance and optimized operation of thermal energy systems. ML-assisted methods provide new opportunities in addressing complex systems or mathematically high-dimensional problems, which include the many-body problems at the electron level, the atomic arrangement at the lattice level, the imperfection and structural complexity at the nano/microscale, geometric factors at the device level and variable working conditions at the system level. Although the application potential of ML in some areas has yet to be fully demonstrated, the promise has been underscored by recent progress. For example, as illustrated in Figure 4, supervised learning finds its niche in high-throughput thermal materials screening by establishing the relationship between various materials descriptors and thermal conductivity, while unsupervised learning can function as a differential equation solver, which helps efficiently solve equations including the Schrodinger equation, Boltzmann transport equation (BTE), heat conduction equation, Navie–Stokes (NS) equation, and radiative transfer equation. In the following, we discuss in detail how ML plays an increasingly significant role in DFT, MD, and BTE.

Machine-Learning-Assisted Density Functional Theory.

In thermal materials modeling, DFT often serves to provide first-principles atomic interactions by calculating the energy and force using quantum mechanics, which can be input parameters for further calculations such as lattice dynamics, MD, and BTE. For better discussion on machine-learning-enabled DFT solutions, the basic idea of DFT is briefly revisited here. To begin with, the many-body Schrodinger equation, which is the foundation of quantum theory, in most cases is notoriously difficult to solve in practical applications. Simplification efforts have been made, with the central idea of describing an interacting electronic system via its electron density. Remarkably, Hohenberg and Kohn related ground-state properties to electronic density, which can further be explored based on the self-consistent variational method, and thus laid the foundation for a so-called orbital-free DFT (OF-DFT) method or pure DFT due to there being no need to solve the Schrodinger equation.[49] To overcome the critical shortcoming in OF-DFT methods that no accurate orbital-free kinetic energy functional can be found, Kohn and Sham proposed to study a non-interacting electronic system with the same electronic density of the original system, invoking solutions based on single-electron wave functions, so-called Kohn–Sham DFT (KS-DFT).[50] All these milestones make quantum mechanical calculations become tractable and accurate to a great extent. The core challenges for current DFT methods include the expensive computational cost for iterative calculations and the accuracy of functionals. Although commonly used approximations such as local density approximation or generalized-gradient approximation exchange correlations have been shown to work well for a broad range of materials, the form of the exact functional remains undiscovered, and these exchange-correlation approximations often fail for strongly correlated systems in particular.

The major expectation of expediating DFT calculations with ML is to reduce the computational resources required and enable simulations of larger systems. Different from the most current approximations beginning from local density approximation and failing miserably when there is a poor starting point, ML produced functionals that do not suffer the same problems if it has good examples to train on. Some strategies have been put forward to circumvent the expensive Schrodinger equation calculations and optimize computational resources without sacrificing accuracy. These strategies can be divided into two groups:[51] one is using ML to predict novel density functionals, such as exchange-correlation functionals and kinetic energy functionals, which can be used in traditional KS-DFT apparatus; the other is bypassing KS-DFT to implement OF-DFT or predicting electron density by direct mapping. Aiming to improve KS-DFT methods, Nagai et al.[52,53] developed ML mapping using an ANN from electron density to an exchange-correlation potential for a one-dimensional, two-body model system trained using accurate reference data from exact KS equations and applied their approach to small molecules. The ML-trained functions exhibited performance comparable or superior to that of the representative standard and hold promise for modeling systems that cannot be treated using existing functionals, such as those with dispersion interaction, self-interaction error, and strong correlation. On the other hand, the computational bottleneck of solving large-scale KS equations induces great interest in investigating OF-DFT. This demands accurate construction of a universal Hohenberg–Kohn functional of electrons, especially

a kinetic energy functional considering its magnitude comparable to the total energy of the system. Synder et al.[54] employed Gaussian kernel ridge regression on a kinetic energy functional and principal component analysis on functional derivatives using exact solutions at several discretized grid points as training data for non-interacting spinless fermions in a 1D box and predicted accurate results for other points that exceeded, by far, any present approximations. The same approach was demonstrated for calculating molecular-stretching and bond-breaking processes and modeling highly correlated and infinite hydrogen atom chains.[55,56] However, the aforementioned ML methods for OF-DFT are limited by sacrificed accuracy of finding functional derivatives in the Euler equation, which is important to solve for ground-state electron density and energy. Hence, to further improve the prediction accuracy for these quantities, Brock-herde et al.[57] replaced the iterative-solution-needing Euler equation by direct-learning potential–density and density– energy mapping and performed it on malonaldehyde, showing that intermolecular proton-transfer processes could be well captured. Similar works on sulfur-cross-linked carbon nano-tubes,[58] aluminum,[59] and non-covalent systems[60] demonstrated the potential of such a direct mapping method from the atomic local environment.

At present, the development of these methods is still at an early stage where only proof-of-principle works have been done. However, as they mature, solving of DFT problems could become much more efficient and enable faster force extraction and also computation on large unit cell materials which have been rarely explored hitherto, owing to the extremely high computational cost.

In addition to the DFT methods discussed above, an increasingly important effort has been made recently to develop post-DFT methods that aim to handle weak interactions, strong correlations, phase transitions, and excited-state properties in many-body systems. These include, to name a few, quantum Monte Carlo (QMC), time-dependent DFT, and GW approximations.[61] It has been reported that, through the combination with convolutional neural networks, lattice QMC can be accelerated by more than an order of magnitude,[62] and QMC can correctly identify both continuous and discontinuous quantum phase transitions, even the intermediate phases.[63,64] GW convergence with respect to basis completeness can be reached by solely relying on fast preliminary calculations with an unconverged basis set using linear regression.[65] On the other hand, statistical learning makes it possible to predict excited-state properties, such as bandgaps, directly without performing expensive quantum mechanical calculations. Na et al.[66] predicted the bandgap of a crystalline compound using tuple graph neural networks at an accuracy level of hybrid functionals and GW approximations with largely reduced computational expense; Rajan et al.[67] computed bandgaps of MXene crystals based on kernel ridges, a support vector, a Gaussian process, and bootstrap aggregating regression methods, bypassing time-consuming GW approximations; Knøsgaard et al.[68] trained a gradient boosting model and accurately predicted full GW band structures. Although relevant applications have not been extensively demonstrated in the thermal transport community yet, further efforts should be devoted to enabling calculations of phonon and electronic band structures for complex systems (i.e., strongly correlated materials) and better predicting energy carriers' coupling strengths involving excited states.

Machine-Learning-Assisted Molecular Dynamics.

MD is a widely used atomistic modeling approach to simulate the dynamical motion of atoms and molecules, including the thermodynamic and thermal transport properties. MD has the capability of modeling disordered materials such as polymers and amorphous structures,[69] defects-contained materials,[70,71] and high-temperature transport[72,73] using the interatomic potential that naturally incorporates all orders of anharmonicity and requires no lattice periodicity. Empirical MD applies Newtonian mechanics to evolve the dynamics of particles governed by forces of specific potential forms. Assorted macroscopic material properties can be further deciphered from atomic trajectories invoking statistical correlations. The key ingredient determining its simulation accuracy is the interatomic potential. Conventionally, the potential is fitted to various analytical expressions in an empirical way, such as the well-known Lennard-Jones potential, the Stillinger–Weber potential, the Buckingham potential, etc. These potentials, of simple functional forms, however, often are not able to capture the actual complicated interactions among atoms and molecules under enormous configurations. Hence, the aspiration for formalizing high-fidelity and configurationally widely held potentials necessitates new paths, where ML is one of the candidates. It does not require a rigid functional form and could adaptively learn the embedded knowledge from the ab initio energy landscape corresponding to a vast space of atomic configurations, thus improving the accuracy when computing energies and forces (error estimates: 0.1 meV/atom for energies and 0.01 eV/A for forces) in later MD simulations.

We summarize a general strategy for using machine-learning potential (MLP) to facilitate MD simulations, as shown in Figure 5: To begin with, proper descriptor vectors (i.e., Smooth Overlap of Atomic Positions descriptors,[74] moment tensor,[75] atomic orbital matrices,[76] etc.) are constructed to uniquely fingerprint atomic configurations and incorporate many-body interactions; then, a training database of energies, forces, and atomic descriptors is collected by performing ab initio MD or applying a perturbation to crystals; furthermore, the MLP is fitted employing various ML algorithms (Gaussian process regression,[77] support vector machines,[78] etc.); last, MLP is used as input to run MD in a conventional way. As MLP became available, its practicability on heat-transfer modeling started to become a hot topic among the thermal engineering community. Studies using MLP-based MD simulations on graphene, CN, MoS_2, SiP, Si, SnSe, $MoS_{2(1-x)}Se_{2x}$, diamond, BAs, Ga_2O_3, $BaAg_2Te_2$, the graphene/borophene interface, and the Ge/GaAs interface have been reported in the literature, showing a promising agreement with experiments or first-principle calculations.[70,73,79–86]

As we are pleased to see MLP-enabled high-accuracy calculations on these crystalline materials and interfaces, it is more impressive to see its promising potential to unlock prediction power that is prohibited in conventional methods owing to either high computational cost or low prediction reliability.[87] Some notable works using MLP for MD simulations in thermal transport areas include high-temperature simulations,[72,73,88] phonon–defect interactions,[70,71] and amorphous materials.[80,89] Specifically, MD can tackle high-temperature simulation by directly tracking atomic trajectories, whereas DFT based on ground-state force knowledge cannot give dynamically stable information. Second, MLP

could also contribute to thermal transport modeling on defects-included materials by fitting potential energy surfaces over a vast landscape of atomic configurations due to flexibility, disregarding conventional mean-field assumptions. Third, MLP can also be applied to amorphous materials where heat carriers are propagons, locons, and diffusons rather than phonons.

Machine-Learning-Assisted Boltzmann Transport Equation and Other Partial Differential Equations.

ML can be used to assist in solving governing thermal transport equations, for example BTE. BTE is an essential tool to bridge microscopic phonons or electrons transport to macroscopic properties. It provides the quantification of a distribution function evolving in the spatial and temporal spaces, as well as an external force, collisions and scattering, and drifting terms. Solving the phonon BTE has been widely used to determine temperature distribution, heat flux, and other thermal properties; however, it can be challenging due to its nonlinearity and high dimensionality. In the past, gray models assuming all modes have the same properties have always been used, which suffers inaccuracy, for example, due to the fact that different modes could have a wide span of mean free paths and, therefore, behave differently at a given physical length scale. Recent progress in numerical schemes like the Monte Carlo method, lattice Boltzmann methods, and deterministic discretization-based methods has been proposed to solve mode-resolved BTEs, but with increased computational challenges such as slow convergence and large memory requirements, as well as induced uncertainties and accuracy issues. This dilemma calls for easier and more efficient high-dimensional solvers.

According to the universal approximation theorem that a deep neural network possesses the potential to accurately approximate any continuous functions, it is natural to apply ML for solving partial differential equations (PDEs) such as BTEs. The incorporation of the governing PDEs' residuals and initial/boundary conditions with a regularization term into the cost function converts the problem from solving PDEs to neural network optimization. The parameters that minimize such a cost function correspond to a solution in the form of a physics-informed neural network. In this way, a solution can be learned in a physics-constrained unsupervised manner, with small uncertainty and less computational cost of discretization. Progress has been made to use ML for solving phonon BTEs. For example, a physics-informed neural network framework has been developed by Li et al. to predict phonon energy distribution with improved calculation speed under a steady state[90] and temperature gradient.[91] With preliminary success, such an early-stage physics-informed neural network framework can be augmented for capturing transient thermal transport, solving phonon and electron BTEs simultaneously, and modeling complex structures. Some works also deal with BTEs to tailor to other systems (entropy closure of the momentum system, fluids, etc.) and properties.[92–95] Moreover, the framework of using ML to solve BTEs can be readily extended to other macroscopic PDEs in thermal transport (i.e., heat conduction equation,[96] NS equation,[97] radiative transfer equation[98]) and replace the current slow trial-and-error finite element methods as well. ML has been shown to efficiently provide accurate results in contrast to conventional methods.

THERMAL ENERGY MATERIALS GENEALOGY

The family of thermal energy materials consists of countless members, which can hardly be exhaustively reviewed. Here, we aim to discuss several representative categories of materials that form the principal components of thermal energy systems like electronics thermal management, thermoelectrics, solar cells, high-temperature engineering, and so on. The common materials descriptors for machine-learning thermophysical properties of these materials are summarized in Figure 6.

Semiconductors.

Semiconductors are materials with large electrical conductivity tunability under field and the foundation of our modern technologies, including computers, mobiles, electric vehicles, robots, and everything with programmable electrical circuits. For example, silicon, germanium, and gallium arsenide are the most common semiconductors, while gallium nitride and gallium oxide are rising stars. During the past decades, the number of transistors per area on chips has been doubled about every 2 years, famous as Moore's law, unintentionally introducing the thermal management challenge due to the increased power density.[99,100] Developing new semiconductors with high thermal conductivity is the most straightforward way to overcome the heat management challenge and save a large amount of energy for device cooling. On the other hand, semiconductors are the energy conversion materials in solar cells and thermoelectric power generators, where the bandgap, charge carrier lifetime, electrical conductivity, Seebeck coefficient, thermal conductivity, and thermal stability are the key properties. All these properties are essentially determined by the atomic structures, regardless of the defect and boundary effects, and can be predicted from ab initio calculations with only lattice structure and atom types as input, as illustrated in Figure 6. Computation-guided development of new semiconductors can be best exemplified by boron arsenide, which was experimentally synthesized with thermal conductivity up to 1300 W/mK, 5 years later after the initial motivation from ab initio calculations.[4,15] ML approaches have been recently applied to accelerate the computational prediction process. Fast and accurate materials screening of different types of semiconductors has been demonstrated with various ML algorithms for both thermal conductors and thermal insulators.[101–103] The electronic properties of semiconductors, including bandgap and carrier mobility, can be efficiently predicted with ML methods,[104,105] which are critical to quickly evaluate their potential applications in electronics, thermoelectrics, and solar cells. Moreover, the dynamical evolution of structure and properties of semiconductors under extreme conditions can be modeled with ML-assisted atomistic simulations, for example, the insulator-to-metal transition of amorphous silicon under high pressure.[106] Semiconductors in solar cells have also benefited from ML methods, including the accelerated search for stable, efficient, and eco-friendly perovskites.[107–109] In addition, the manufacturing of semiconductors is another area where ML has played a role for decades. By training the process-to-product data set with decision-making trees, the manufacturing parameters for semiconductors can be optimized.[110]

Polymers.

Polymers consist of macromolecules with huge numbers of repetitions of monomers and have the highest volume of manufacture in modern society due to their light weight and low-cost advantages for packaging applications.[111] The properties of polymers vary a lot with the atomic structure, functional groups, and morphology, exemplified by the complex functions of numerous proteins in biological system. The high-dimensional structure–property relationship has been partially learned by living beings during evolution and stored in our genes, now waiting for explicit interpretation and smart utilization with the help of ML.[112,113] A recent breakthrough is the successful prediction of protein folding with unprecedented accuracy by Deep Mind's AlphaFold2.[114] The major challenge for polymer informatics comes from the coupling between long-range, van der Waals, or Coulombic forces and the complicated morphologies, resulting in countless hierarchical materials descriptors from the atomic information on the polymer units and the molecular information such as topological polar surface area, ring numbers, and functional groups, to structural information like alignment, twisting, branching, and others. For example, Kim et al. constructed a platform for a polymer genome using a collection of 229 polymer descriptors and predicted the variation of properties over a large range, e.g., band gap from 0.7 to 10.2 eV and dielectric constant from 2.61 to 9.09.[115] Polymers can also be encoded into sequences of tokens regardless of their morphology, such as the simplified molecular input line entry system,[116,117] which is similar to the genetic code system of life. The genetic algorithm could be a powerful tool for predicting polymers' properties and behaviors in the future.[118]

The major limitations of polymers in thermal management applications are the low thermal conductivity (usually ~0.2 W/mK) and relatively low melting temperature (usually less than 400 °C), partially due to the weak intermolecular interactions. Additionally for thermal conductivity, due to the competition between the conformational entropy and chemical potential,[118] the structure of the polymer is much more disordered (than crystals) and forbids the collective thermal transport of lattice waves (phonons). Therefore, it is expected that improvement of the polymer chain's alignment can increase its thermal conductivity,[119,120] which had been experimentally verified by mechanical stretching, electrical spinning, and other methods.[121–123] The design of polymeric materials with dynamically tunable and enhanced thermal conductivity can be the next research opportunity in this area. In addition, the ML approach may help search for polymers that are useful for organic photovoltaic, radiative cooling, and other energy systems. For instance, Sahu et al. learned the power conversion efficiency from experimental results of 300 molecules using a gradient boosting regression tree and ANN and applied the ML model to screen 32 structures from ~10 000 molecules in the Harvard Clean Energy Project.[124,125] The hierarchical structural polymers are promising radiative cooling materials due to their spectrally selective emission properties,[126,127] which could be optimized with ML in the future.

Alloys.

Alloys are one type of important materials in high-temperature machines such as turbines, engines, and boilers due to their high mechanical strength and thermal stability. Alloys also represent several top thermoelectric materials.[20,128,129] The current design of alloy systems

usually relies on phase diagrams to characterize the phase–composition relationships. Therefore, multi-alloy systems, or high-entropy alloys, which are proposed as single-phase multi-component alloys of five or more elements in approximately equal proportions,[130] and later to include intermetallics, nanoprecipitation, ceramic compounds, and non-equiatomic materials,[131–133] have provided high-dimensional composition and tenability.[134] However, a complete experimental scan of concentrations of more than 10 different elements is challenging, severely impeding the construction of a phase diagram of high-entropy alloys. Similar to semiconductors, the structural homogeneity of alloys enables relatively clean and simple material descriptors for ML training, mainly including atomic information and some easy-to-access proproteins, especially the molar concentration of each element.[135] The Al-Ni-Zr glass-forming ability phase diagram was predicted using the ML method with descriptors derived from stoichiometric ratio, elemental property, orbital information, and ionic bonding.[136] The ANN was proven to have a test accuracy of ~75% for phase prediction of high-entropy alloys with a training data set of 401 alloys.[137] The calculation of phase diagrams using thermodynamic theory, also known as CALPHAD, is one of the widely used tools. CALPHAD gives geometric descriptions of the system at thermal equilibrium, which can further be used for compositional design. With the development of various ML methods, researchers are able to seek help from data science and try to use limited data and ML algorithms to predict the alloy phase at any compositional combination, which is essentially a classification problem. For example, Zeng et al.[138] combined CALPHAD calculations and the XGBoost method to predict 213 new single-phase BCC and FCC high-entropy alloys and established new high-fidelity phase selection rules; Liu et al.[139] integrated a support vector machine with CALPHAD to quickly locate two new eutectic compositions in Ni-Co-Cr-Al high-entropy alloy systems and confirmed their designs by experiments. In addition to the phase diagram prediction, other properties of alloys can also be predicted from the stoichiometric ratio–properties relationships trained from ML, including formation enthalpy, hardness, toughness, thermal conductivity, electronic conductivity, Seebeck coefficients, etc.[107,140,141] The hardness of Al-Co-Cr-Cu-Fe-Ni alloys can be calculated from a ML model trained with experimental data using molar concentration and elemental information as descriptors.[142] The ML approach can also help optimize the catalytic efficiency of high-entropy alloys for CO_2 and CO reduction reactions by learning the results from ab initio calculations.[143] A more detailed discussion of ML-driven high-entropy alloys studies can be found elsewhere.[144]

Composites.

Composites are heterogeneous materials with a wide range of energy applications, from thermal interface materials[19,145] to electrodes and electrolytes in batteries.[146] Different from alloys, where the elements are soluble in the matrix, the component materials in composites are insoluble in the matrix. The intrinsic properties of the component materials are often known. The properties of composites are determined by the percentage, shape, size, and arrangement of each component, and sometimes the interface interaction between them, as illustrated in Figure 6. For porous structures like aerogels, the key descriptors are porosity, pore size, wall thickness, pore arrangement, pore shape, and so on.[38–40] Effective medium approximation was the most used tool to predict the thermal conductivity of composites, but unsatisfied due to the lack of consideration of the detailed fillers' structures. Finite element

analysis of the heat diffusion equation is a common tool to consider the exact structures of composites. For instance, by including the shape, loading, and alignment of fillers in the finite element analysis, Cui et al. illustrated the heat-transfer mechanism of their boron arsenide/polymer thermal interface composites with thermal conductivity up to 21 W/mK and elastic compliance less than 100 kPa.[19] However, the rigorous numerical calculations based on finite element analysis, lattice Boltzmann method, or others usually take too much time for material design, which undoubtedly can benefit from the ML approach to speed up the computations for composites. By taking the structure–properties relationships from experiments and/or rigorous numerical calculations, multiple algorithms have been applied to learn the thermal conductivity of composites, such as support vector regression, Gaussian regression, and neural networks.[45,46] In addition, ML methods have also been applied to design functional composites for thermal cloaking,[147] energy storage,[148,149] and additive manufacturing.[150]

THERMOPHYSICAL PROPERTIES OF MATERIALS

The ideal performance of thermal energy systems is essentially limited by key materials properties, such as thermal conductivity, critical temperatures, emissivity, and so on. During the past 2 decades, numerous materials properties have been measured and accumulated, especially computational results from different simulation approaches. The ML methods start to manifest their power in searching for materials with desired properties. In this section, we will focus on the efforts and progress regarding ML applications in the study of thermal stability, thermal conductivity, thermal boundary resistance, thermal emission, and thermoelectrics.

Thermal Stability.

Thermal stability is a major consideration for high-temperature applications, like thermal barrier coating of turbines and sharp leading-edge materials of hypersonic vehicles, and an important factor for the lifetime and performance of most devices, also involved in the high-throughput prediction of other physical properties as a prerequisite screening process. Experimentally, the thermal stability of materials is usually characterized by differential scanning calorimetry and thermal gravimetric analysis, measuring critical temperatures such as the phase change temperature and decomposition temperature. However, in materials with high-dimensional variations, like numbers of monomers and conformational variations of organic materials and alloys with multiple components, the complete measurement of overall variable dimensions is almost impossible, leaving much space for ML methods. Many molecular features can serve as descriptors for ML training for organic materials, including molecular mass, atom types, topological charge, and so on. For example, Zhao et al. applied a light gradient boosting algorithm to construct a prediction platform of the critical temperatures of organic light-mitting materials using the existing experimental results of 1944 molecules and revealed that the hydrogen bonding, molecular polarity, and size were the most important features for these molecules' thermal stability.[151] Sifain et al. used a group of group-constitutive and gradient boosting decision trees to predict the melting temperature of over 47k organic molecules.[152] The other properties coupled with thermal stability can also be analyzed with ML. Shen et al. studied the stability of polymer

dielectric materials at different temperatures and electric fields using dielectric constant, electrical conductivity, and Young's modulus as descriptors and least-squares regression.[149] The light output degradation of Eu^{3+}-substituted phosphors with temperature can also be predicted using support vector regression training of reported experimental data.[153] Phase diagram construction of alloy systems traditionally requires substantial experimental efforts along three dimensions, i.e., temperature, pressure, and element concentration, which can also be significantly reduced with ML. Balachandran et al. accelerated the experimental search for high-temperature ferroelectric perovskites by using classification learning methods to identify the perovskite phase in the phase diagram and regression methods to predict the Curie temperature, as illustrated in Figure 7.[154] On the other hand, the atomistic modeling with MLPs helps reveal new fundamental insights on the phase change of materials, such as the discovery of a transient phase during the amorphous-to-crystalline silicon transition.[106,155]

Thermal Conductivity.

Thermal conductivity is a phenomenological metric defined by Fourier's law to relate heat flux and temperature gradient in a medium and is probably the most important thermal transport property for thermal engineering. As mentioned before, ab initio calculation of thermal conductivity has been standardized as the most accurate prediction method; however, it requires much computational resources, only possible for case-by-case modeling but formidable for an exhaustive search for thermal materials. With the rise of ML algorithms, so-called high-throughput thermal transport prediction has become popular during the past decade, which can be hardly defined as more than a purpose efficiently realized with the assistance of ML methods, instead of any specific workflow, framework, or even protocol.

The most straightforward strategy to integrate ML algorithms into the prediction of thermal transport properties is to design physically insightful descriptors and take advantage of the existing database of materials' properties as training data to develop accurate and computation affordable correlations for thermal conductivity. conductivity from the atoms' mass, Debye temperature, Gruneisen number, bond length, and atom numbers in the unit cell of materials.[156] The physical understanding of thermal transport plays a much heavier role than statistical analysis, and the accessible descriptors were quite limited in the early attempts. Nowadays, with the rapid growth of computing power, more and more calculations have been accumulated of materials' properties such as formation enthalpy, bond strength, phonon dispersion, and specific heat. Millions of material compounds have been recorded on open databases like AFLOW, Materials Project, NOMAD, and so on, making ML over a large volume of input data possible together with the existing experimental results, as shown in Figure 4. Carrete et al. predicted 10 promising low-thermal-conductivity half-Heusler semiconductors from 79 000 initial entries in the AFLOW database by combining random forest regression and ab initio calculations of 32 compounds using a group of descriptors including chemical information, compound information, and accessible thermal information like specific heat and scattering phase space, as shown in Figure 8.[101] A similar approach was also performed using different input data such as entries in Materials Projects and different ML algorithms like Gaussian process regression, random forest, transfer learning,

and principal component analysis to map thermal conductivity with different descriptor sets.[47,102,103,157,158] Different from inorganic crystals, the descriptors for ML training of the thermal conductivity of polymers are more complicated, for example, the vectors of binary digits representing the chemical units. The search for high-thermal-conductivity polymers is underway but far from satisfactory considering the current progress.[120,159] The thermal conductivity of alloys can also be predicted by adding composition as another dimension for ML training.[160,161] In addition, ML can also assist the ab initio calculations of thermal conductivity, especially for high-temperature calculations, which are usually much more computationally expensive than ab initio calculation at 0 K. By performing principal component analysis and regression analysis, a correlation between 0 K force constants and 1000 K force constants can be built to accelerate the phonon scattering calculations.[48]

In addition to homogeneous materials, the effects of compositional and structural factors on thermal conductivity can also be efficiently predicted with ML algorithms, mainly for nanostructures, composites, and porous materials. By using period and layer thickness as material descriptors and MD simulation results as training data for ANN, the thermal conductivity of superlattice can be minimized.[162,163] The thermal transport in a porous medium can be modeled with the finite element method and heat diffusion equation once the porous structure size is much larger than the heat carriers' mean free path. By training a limited data set of finite element method simulation results with appropriate structural features like shape and bottleneck thickness, the structure–thermal conductivity relationship can be found.[46] Similarly, the thermal conductivity of composites can also be predicted from ML methods and training data from finite element method simulations with properties and geometric factors of fillers.[45,164] When the grain size or pore size approaches the heat carriers' mean free path, the solutions to BTEs are obtained first as training data.[165] Thermal resistance at the interface in heterogeneous materials is another important consideration, which will be discussed later.

Thermal Transport Physics.

ML methods can also be applied to study fundamental thermal transport physics. Hydrodynamic phonon transport is a heat-transfer regime much less studied than ballistic and diffusive heat conduction, existing only in limited materials at appropriate temperature windows. Torres et al. determined promising materials for hydrodynamic thermal transport by training the ab initio calculated hydrodynamic length of 131 materials using neural networks.[82] Thermal transport in amorphous materials is another long-standing problem due to the complicated structures with short-range, medium-range, and long-range disorders. Ab initio modeling of amorphous materials is extremely challenging because of the lack of symmetry. MLPs from ab initio calculation of small systems (less than 1000 atoms) can be used for MD simulations of large systems (more than 10 000 atoms), approximating the real amorphous structure.[80,88,166] On the other hand, the thermal transport of materials such as zirconium compounds at high temperatures can also be modeled with MLPs.[72,167,168] Otherwise, the ab initio calculation of high-order force constants to include anharmonicity requires too many computational resources.

Thermal Boundary Resistance.

Thermal resistance is not only contributed by the intrinsic thermal properties of component materials but also contributed by their interfaces, especially in heterogeneous structures, known as thermal boundary resistance (TBR).[169] TBR is a decisive factor in the performance failure of high-power electronics, the efficiency of nanostructured thermoelectric materials, and the thermal properties of composites, to name a few. TBR results from the breakdown of coherent vibrational waves at the interface. The physical process can be pictured as wave transmission and reflection, as illustrated in Figure 9a and mathematically described by the Laudaur formula.[145,170] Due to the lack of symmetry at the interface, the modeling of TBR requires a large atomic system, making first-principles calculations computationally challenging, compared to the widely used methods such as acoustic mismatch models, diffuse mismatch models, and molecular dynamics simulations.[145] On the other hand, classical MD simulation is an ideal approach to deal with interface thermal transport by modeling the exact interface structure, defects, and anharmonicity, though the output mainly relies on the accuracy of empirical potentials. One of the major examples of progress comes from the MD simulations with MLPs, which provides a balance between modeling accuracy and cost. For example, Kang et al. constructed a potential for boron arsenide by training the force and energy data from DFT calculations using linear regression and calculated the TBR between boron arsenide and gallium nitride, which was in good agreement with their experimental measurements, as shown in Figure 9b.[18] Following their work, Wu et al. applied the deep-learning method to build another potential to study the thermal transport of this heterostructure.[171] A similar approach was also applied to the thermal resistance at the grain boundary of silicon and hence the thermal conductivity of polycrystalline silicon.[172]

On the other hand, the high throughput of TBR is also under development and has already achieved better prediction accuracy at least than mismatch models. Since phonon waves' transmission is related to the intrinsic phonon properties of interface materials, multiple physical properties can serve as descriptors for ML training of TBR data, such as specific heat, thermal conductivity, Debye temperature, melting temperature, sound speed, bulk modules, and so on. Wu et al. used these descriptors and three different ML algorithms—regression tree ensembles of LSBoost, support vector machines, and Gaussian regression process—to train 1317 data entries from experimental measurements and achieved coefficients of determination around 0.9.[44] Even for the same pair of interface materials, ML can also be applied to study the dependence of interface conditions such as temperature, defects, bonding strength, etc. Vu et al. constructed the mapping between the TBR of a glass/steel interface and descriptors including temperature, pressure, and surface roughness by using linear regression, decision tree, and random forest algorithm to train their own experimental results and achieved a coefficient of determination up to 0.99, as illustrated in Figure 9c.[173] In addition, ML algorithms can also be combined with classical MD simulations to accelerate the optimization of fine structure at the interface for thermal transport.[174–176]

Thermal Emission.

The emission and absorption of electromagnetic waves is one of major ways heat is exchanged, called radiative heat transfer. Any object above 0 K is emitting electromagnetic waves due to the movement of charge carriers. Thermal emission is extremely important for high-temperature objects and objects without direct contact, for example, our Earth and sun, between which thermal energy is transferred only through radiative heat transfer. The control of thermal emission properties is critical to various applications including daytime radiative cooling, thermophotovoltaics, metallurgy, turbines, and others. During the past 2 decades, nanostructure engineering of surfaces has opened up new directions for light–matter interactions, i.e., emissivity control with metasurfaces.[177,178] However, the spectral dependence of emissivity and temperature dependence of electromagnetic waves' emission complicate the inverse design of metasurfaces. Although the emissivity of metasurfaces can be precisely calculated with the Maxwell equation, it requires substantial efforts to scan different material properties and geometrical parameters to achieve desired thermal emission properties. For example, the emissivity of the pillar structure illustrated in Figure 10 can be affected by the height, period, shape, length, and width of the pillars. This high-dimensional problem can also be addressed with ML methods. Instead of solving Maxwell equations case by case, the structure–property mapping can be established more efficiently by training a limited data set from rigorous calculations. For instance, the light scattering of core–shell nanoparticles can be tuned by changing the thickness of each shell and shell material. Peurifoy et al. applied ANN to train 50 000 rigorous calculation results from Maxwell equations and reduced the inverse design time by up to 2 orders,[179] as shown in Figure 10. Dielectric and metallic particles with different shapes like spheres, cylinders, parallelepipeds, and triangular prisms were also studied with decision trees and random forests to address the inverse design of emissivity.[180] The narrow-band thermal emitters with a quality factor higher than 200 are promising for high-performance thermophotovoltaic devices, making it possible to convert the broad-band solar spectrum to narrow-band light, where the photovoltaic cells have the maximum efficiency.[181–183] Additionally, beyond the optimization of geometric parameters, it is also expected that the emerging ML approaches could be built on high-fidelity fundamental results, i.e., a database of ab initio calculations, to further enhance modeling capability by having a larger design space with much cheaper computational cost. Since ML methods have just been introduced to the thermal radiation, photonics, and plasmonics communities, relevant research is still deficient in the literature.[184]

Thermoelectrics.

Thermal energy can also be directly converted into electricity via thermoelectric effects due to the diffusion of charger carriers under a temperature gradient. Thermoelectric devices are regarded as ideal power generators without complicated mechanical components and moving parts, though they are significantly limited by the low energy conversion efficiency, which can be characterized with a ZT value, $ZT = \sigma S^2 T/\kappa$, where σ, S, κ, and T are electrical conductivity, Seebeck coefficient, thermal conductivity, and temperature, respectively. The maximum efficiency of a thermoelectric generator working between 300 and 400 K heat reservoirs is 4.7% and 11.3% with ZT values of 1 and 5, respectively.[185] The state-of-the-art ZT value had remained less than 1 for more than 50 years until the

nanoengineering of material structures was introduced,[8,20,186] opening up new directions for improving thermoelectric performance. With the new hope accompanies new challenges, i.e., searching for optimal materials with additional dimensions, such as impurity, doping, grain boundary, and so on, especially considering the modeling complexity of electron and phonon transport in nanostructures. ML tools have been applied to speed up the search for high-performance thermoelectric materials, either by guiding the exploration of σ, s, and κ values separately or the overall ZT value.[104] For instance, the electronic band structure and lattice thermal conductivity of half-Heusler compounds were analyzed with ML separately.[101,105] The selection criteria (large lattice parameter and effective mass of holes) for high-ZT half-Heusler thermoelectric materials were identified by Carrete et al. by analyzing their ab initio calculation results from 75 compounds using decision trees.[187] However, the family of thermoelectric materials is huge, as illustrated in Figure 11, requiring more general material descriptors for ZT values, either physics-inspired or data-driven.[188,189] Xu et al. applied the random forest method to train thermoelectric data from 204 materials and obtained coefficients of determination higher than 0.9 by using four descriptors from the information entropy evaluation of an ExtraTree-based model.[189] Some better descriptors could be found from the several visualization databases for properties relevant to thermoelectrics.[190–192] Moreover, structural design and material manufacturing methods such as chemical mixing and thermal processing can also be optimized with ML.[193–195]

PERFORMANCE PREDICTION AND DESIGN OPTIMIZATION OF THERMAL ENERGY APPLICATIONS

Beyond mechanistic modeling and high-throughput searching for materials' properties as discussed in the above section, ML can also assist the design of architectures and performance, ranging from thermal devices to large-scale systems, which we exemplify in Figures 12 and 13, below.

Device Level.

On the level of thermal device optimization, ML methods could provide advantages for a broad range of applications, including thermophotovoltaics, thermal desalination, heat pumps, heat exchangers, solar water heaters, steam turbines, additive manufacturing, etc. Recent works employ various ML models to tune multiple geometric and physical parameters in a way to comprehensively search in hyper-dimensional design space, which is generally restrained by the formidable computational cost of conventional manual sweep. Numerous discoveries of unorthodox practical structures away from previous intuition and prior selected topologies have been made via computer algorithms, and these ML approaches are expected to play a vital role for device optimization in the future. For this review, we highlight this progress by focusing on three typical devices involving thermal energy, i.e., heat exchangers, thermophotovoltaics, and solar water heaters.

Several commonly used heat exchangers have been optimized using ML algorithms. The input parameters for these heat exchangers generally include total tube number, total baffle number, baffle pitch, diameter of the center tube, flow rate, Reynolds number, inlet

and outlet temperatures, fin dimensions, fin spacing, materials, etc., and the objectives are performance prediction, efficiency (and effectiveness, if applicable), and economical optimization.

Specifically, an early-day investigation on fin tube heat exchangers using ML was initiated by Zhao et al.,[198] where they introduced ANN to the prediction of the performance of heat exchangers. The ANN model they trained based on a very limited amount of experimental data showed the prediction of heat rate with error in the same order as the uncertainty of the measurements under different operating conditions. Pacheco-Vega et al. later considered condensation in their ANN model in the case of humid-air flow and demonstrated better performance than conventional correlations.[199] The promising prediction capability paved the way for further optimization along the map of ML. Besides ANN, Peng et al. used support vector regression with different hyperparameters for predicting the thermal-hydraulic performance of fin tube heat exchangers and claimed better prediction performance than using ANN with shorter computational time.[200] As prediction becomes more accurate, design optimization based on these approaches appears naturally. Recently, Krishnayatra et al. studied the thermal performance of fins for a novel axial fin-tube heat exchanger invoking k-nearest neighbor regression, and the designed structure shows high efficiency, confirmed by numerical simulations of ANSYS.[201] To take into account total cost on top of heat-transfer effectiveness, Xie et al. used a genetic algorithm for minimization of total annual cost and total weight.[202] By combing a genetic algorithm design and additive manufacturing, Moon et al. fabricated a heat exchanger with optimal fin geometry and achieved a power density of 26.6 W/cm^3, as shown in Figure 12b.[196]

On the other hand, based on a small set of experimental data on shell-tube heat exchangers, Luo et al. trained ANN using normal backpropagation and different architectures for the prediction of heat-transfer rates in segmental baffles and continuous helical baffles.[203] Their results show a better prediction of heat-transfer rate than empirical correlations, which is the preliminary stage for ML-enabled optimization. Thanikodi et al. furthered their methods by incorporating teaching learning (dividing training data into a few chunks and using in order) to make a hybrid ANN based on the same set of training data and confirmed reduced learning error.[204] More than ANN, Krzywanski developed an ML model using a genetic algorithm and ANN on a large falling-film evaporator and optimized the heat exchanger regarding the total heat-transfer rate by tuning the kind of tubes and tube pass arrangements under the specific number of tube rows and the refrigerant mass flow rate.[205] Ocło et al. invoked particle swarm optimization and continuous genetic algorithms for optimizing flow distribution and effectively reducing thermal stresses.[206] Explorations in flat-tube multi-louvered fin compact heat exchangers,[207] plate-fin heat exchangers,[208] and wavy fin-and-elliptical tube heat exchangers[209] are also documented in the literature.

As for thermophotovoltaic applications, Kudyshev et al. optimized a metasurface thermal emitter by adapting the topology optimization method with deep-learning algorithms (i.e., adversarial autoencoders) for unorthodox compact hyper-parametric representations and showed substantial improvement in the optimization process, 3 times faster with higher efficiency (98%) than previously used adjoint-based topology optimization design as shown in Figure 12c.[182,210] Zhang et al. demonstrated that a highly selective aperiodic

thermal emitter made of silicon, silica, and tungsten can be achieved under the framework of Bayesian optimization and a transfer matrix method.[211] Integrated with a gallium antimonide (GaSb) photovoltaic cell, such an optimal emitter is fabricated, and the measured emission spectrum shows agreement with the predicted figure of merit, notably better than previously designed multi-layers with similar material. Silva-Oelker et al. explored two structures (a planar multi-layer stack and a grating) of tungsten–hafnia ($W-HfO_2$) selective thermal emitters with high hemispherical emittance.[212] Through optimization using a genetic algorithm and rigorous coupled wave analysis, the design of high thermal emittance with low directional sensitivity can be obtained. On top of genetic algorithms and adversarial autoencoder networks which require large data sets and are based on exploitation only, particle swarm optimization that also includes exploration was proposed by Wang et al.[213] They optimized solar-to-power conversion efficiency for multi-layer solar thermal absorber made of tungsten, SiO_2 and Si_3N_4 multilayer thin films by theoretical design and experimentally demonstrated excellent spectral selectivity.

With regard to solar heaters, Kalogirou et al. first used ANN to predict useful energy extracted from domestic hot water systems,[214] instantaneous efficiency,[215] and temperature level[216] for the storage tank by the end of the daily operation cycle. Lecoeuche et al. then used ANN to predict in situ outlet temperature of the collector based on solar radiation and thermal heat loss coefficients.[217] However, accurate determination of heat collection rate and heat loss coefficients is difficult. Liu et al. proposed using ANN and a support vector machine to predict these two quantities based on portable instrument measurable parameters and improved their prediction accuracy of heat loss coefficients with an extreme learning algorithm, as shown in Figure 12d.[197] Afterward, Liu et al. applied ANN-driven high-throughput screening for designing a promising water-in-glass evacuated tube solar water heater (WGET-SWH) with a high heat conduction rate using billions of combinations of extrinsic properties (tube length, tube numbers, center distance, tank volume, collector area, final temperature, tilt angle).[218] Two novel designs generated by this approach were installed experimentally for validation and showed higher average heat collection rates than all existing cases in the previous measurement database. Li et al. then presented the predictive power of ML methods and generalized an ANN-based high-throughput screening framework by providing vital details about the modeling and high-throughput screening process.[219] The success of designing a new SWH with optimized performance without knowing the complicated physical relationship between SWH settings and target performance is highlighted.

System Level.

In addition to material structure and device configuration, ML methods can also be applied at system level for a variety of purposes, including, to name a few, energy demand forecast, fault detection, and optimal control and scheduling of a system. Here we draw attention to ML applications in the modulation of district heating networks and indoor HVAC systems.

District heating is a widely used way to transmit thermal energy in the form of hot water or hot steam to end users (i.e., households, offices, shops, industry, etc.), which can be further employed for heating and hot water production. Central energy plants and multiple

buildings in a district heating system are connected through miles of insulated underground pipes where the thermal energy carrier is distributed. It becomes popular in major cities due to its low overall economic cost and high energy efficiency. However, the long delivery distance and long delay time from producer to consumer are inherent problems for such a large transmission system. The decision to change the transmission status may come hours later than the relevant report is made. Some forms of forecast and prediction must be made, which currently are based on statistical knowledge and experience. Accurate demand prediction can help utilities to plan and shield against uncertainties. ML comes into the picture given its potential for high-fidelity forecast on energy demand. If a prediction can be made far in advance, then the exact amount of thermal energy can be transferred to the users after some distribution time. However, the prediction of energy load is not simple. It invokes not only weather conditions (temperature, dew points, solar radiation, wind speeds, etc.) but also social behaviors. Ordinary systems that only monitor the current state of the system fail to take into account the historical records and possible future events. The application of ML, on the other hand, exhibits potential for high-accuracy energy load prediction and further leads to the complete digitalization of tomorrow's district heating systems. ML methods can learn the patterns of heating load from a large database consisting of previous customer data, operational data, and holiday activities as well as weather reports, and thus are able to schedule the heat production and storage dynamics in advance and correspond to evolving conditions (uncertainties in weather forecasts and human behaviors) so as to handle peak load properly. Even economic data, such as prices of electricity, natural gas, and other sustainable resources, can be integrated into the whole analysis to achieve higher efficiency at a broader scope. The first work invoking ML for energy load prediction was done by Dotzauer et al., who developed a simple heat demand prediction model by considering outdoor temperature and human activities.[220] As the computational power improves, many ML models have been proposed for the sake of energy load prediction, such as online ML algorithms,[221] ensembles of online ML algorithms,[222] ridge regression,[223] support vector machines,[223] random forest,[223] ANN,[224] linear regression,[224] etc. Deep-learning methods,[225] which are extended from ANN and capable of modeling complex nonlinearity, are becoming attractive and have been tested many times. Xue et al. investigated heat prediction using a long short-term memory model and feature fusion long short-term memory,[226] which outperformed other models. A recursive strategy embedded with extreme gradient boosting for multi-step-ahead forecasting of the heat load is also highlighted in Figure 13.[227]

ML methods can be used to design optimal structures of transmit networks. Feng et al. used a genetic algorithm to optimize the structural design of the pipeline of a district heating system, with the objective of minimizing annual total cost but maintaining hydraulic stability.[228] Similarly, Li et al. further included a variety of heating and cooling loads throughout a year and employed a genetic algorithm based on a least-annualized-cost global optimal mathematical model for a design that could avoid hydraulic unbalance, resulting in increased running efficiency and reduced operation cost compared with conventional design methods.[229] ML can also help with fault detection (i.e., leakage, insufficient heating, malfunction of individual components) in streaming data. Such diagnosis can be achieved from retrieved real-time customer data and other data from the network, replacing manual

inspection and reducing the time needed between fault detection and repair. Given the universally reported fact that no single anomaly detector that is ultimately superior in all cases exists, Calikus et al. proposed a framework integrating separate unsupervised components that address the fundamental tasks as separate concerns.[230] Unlike unsupervised methods, Bode et al. created supervised models and studied the transferability from an experimental training data set to a real-world building test data set.[231] Abghari et al. further proposed a robust higher order mining approach to detect deviating and sub-optimal operational behaviors.[232] To build a predictive model for pipe deterioration, Winkler et al. found that a boosted decision tree approach with random under-sampling enables higher precision extrapolation for the prediction of current and future states of the pipe network.[233] What's more, ML methods can satisfy the need for the development of intelligent monitoring and control frameworks for district heating systems. Current control systems are primarily based on manual tuning of network operators using conventional proportional-integral-derivative (PID) controllers, and thus automation is needed to avoid human errors and guarantee optimal management with reduced cost. Static models not capturing the time evolution of energy vectors are commonly used for control. To overcome the shortcoming of static optimization models, Moustakidis et al. proposed a hierarchical control framework that breaks the overall decision problem down to sub-problems using multiple decision layers: the high-level layer deals with tactical decisions and seasonally/ monthly/daily load changes; the middle-level layer is responsible for the slow time scale adjustment of the continuous variables at production sites; and the lower layer handles the fast time scale regulation of the aforementioned continuous variables at the substation/ building level.[234] Reynolds et al. built up optimal scheduling of distributing heat subsystems using genetic algorithms and found a 44.88% increase in profit compared with a rule-based conventional priority order scheme.[235] A multi-stage–multi-level ANN with three different variants has also been implemented by Arat et al. for optimum control strategy of a geothermal heat-pump-aided distributing heat system and yielded improved efficiency.[236]

HVAC is another area where ML applications make a crucial difference. It is responsible for continuous regulation of the artificial environment so that the indoor climate remains constantly comfortable while the outside weather changes. In recent years, the concept of smart buildings contingent on building automation has arisen. In accordance with the fast evolution of AI and ML techniques, smart buildings are further advanced with systems capable of predicting, monitoring, and adjusting in response to the dynamics of outside variables.

Energy demand prediction is the essential foundation for building energy management and can be enhanced by employing various ML methods. Specifically, supervised ML algorithms, such as ANN,[237] support vector machines,[238] decision trees,[239] and ensemble learning,[240,241] are widely used to forecast building heating/cooling load and total energy consumption load. Numerous test results showed improved accuracy better than simulation software results. However, these methods are usually built on shallow structures and thus cannot extract highly complex patterns from training data. That is why deep-learning approaches, which feature multiple layers of structures and thus a higher order of sophistication, are proposed to learn greater abstraction and render higher accuracy of prediction. Berriel et al. showed solutions of deep-learning algorithms, such as convolutional

and short-term memory neural networks, that were applied to the problem of monthly energy consumption forecasts and outperformed the baseline reference of historical average consumption.[242] Deep-learning models combined with ensemble techniques,[243] generative adversarial nets,[244–246] sequence-to-sequence models,[247] and transfer-learning models[248] have also been explored. Recently, to couple prediction with actuation, deep learning has further been devised to connect with reinforcement learning to become so-called deep reinforcement learning (DRL),[249–251] which encapsulates the perceptual power of deep learning and the decision-making capability of reinforcement learning. DRL controllers are proposed for optimally controlling space heating to achieve low-exergy buildings. Liu et al. compared three commonly used DRL techniques with popular supervised models and concluded that DRL can improve prediction performance with the cost of more computation time.[252]

In addition, ML helps detect and diagnose faulty operations and equipment (i.e., water valves, air dampers, filters, chillers, pumps, and fans) failures that often remain undiscovered for a long period due to the difficulty of manually deciphering complex information in building management systems. By analyzing the trends of data collected by sensors, statistical ML methods can deliver high-accuracy detection for complex systems and be easily transferred to different systems, overcoming the limitations in existing rule-based physical models. West et al. proposed a novel fault detection and diagnosis technique using hidden Markov models embedded with inter-sensor relationships from historical data under normal and faulty conditions.[253] The comparison between real-time data stream and learned historical patterns yields accurate operation diagnosis for a few fault types in a real building. Later in the past decade, various aspects of ML methods were intensely explored to characterize occurrences of faults, detect abnormal operating conditions, and classify fault types, such as adaptive thresholds, using t-statistic approach,[254] fuzzy logic,[255] ANN,[256] Gaussian process regression,[257] support vector machine,[258,259] gradient boosting regression,[260] and generative adversarial network.[261] However, these methods rarely captured temporal dependencies and dynamics of faults. To close such a loophole, deep recurrent ANNs, which can also learn implicit nonlinear relationships, are proposed. Topology optimization among diverse deep recurrent ANN configurations and relevant hyperparameters have been explored.[262–264] The improved effectiveness and advantages of deep recurrent ANN compared to other non-recursive methods, namely higher accuracy, transparency to substantial noise, and incorporating time dependency, have been reported.[265]

Moreover, ML methods, especially DRL, enable automatic smart adjustments with continuous sensor readings and actuator controls. Gupta et al. introduced DRL heating controllers to a simulation model of a house to remove deviation of the indoor temperature from a set point to ensure thermal comfort while reducing energy consumption under dynamic conditions.[266] Brandi et al. implemented both static and dynamic DRL to control supply water temperature for heating units, and they both outperformed rule-based and climatic-based control schemes, given a careful selection of input variables.[267] Rahimpour et al. demonstrated the superiority of actor–critic DRL methods on tuning buildings with phase change materials whose nonlinearities cannot be handled by conventional controllers.[268] Beyond temperature control, Yoon and Moon considered optimizing relative humidity,[269] whereas Chen et al. further included natural ventilation.[270] Zou et al. devised a framework

to optimally control air handling units using DRL with a training environment of long short-term memory network approximation for historical building automation system data.[271]

During the past several years, the explosion of big data toolboxes and the urgent need for efficient and clean energy technologies have opened up a new interdisciplinary area focused on ML-assisted energy materials development, thermal device design, optimization, and operational improvement of energy systems. At the most fundamental level, atomistic modeling of thermal energy materials can benefit from the ML-accelerated numerical solution of quantum mechanics and highly accurate MLP-assisted MD simulations. High-throughput material discovery for ideal thermal conductivity, thermoelectric coefficient, emissivity, and other properties will largely reduce the cost of the traditional trial-and-error process. At the mesoscale, the transport dynamics of electrons and phonons can be more efficiently addressed. Inverse design of functional materials with desirable properties by combing nanoengineering and ML training of existing experimental and modeling data becomes possible. Automated design of thermal devices with ML and additive manufacturing will become a new industrial strategy. Moreover, the large thermal systems will be operated more efficiently by ML-improved energy demand forecasts, fault detection, and optimal control and scheduling. We expect that ML can find its future opportunities in different directions, including but not limited to computationally efficient first-principles materials modeling, materials with extreme thermal transport properties and high energy conversion efficiency, novel thermal materials, or devices with variable thermophysical properties, operation, and control of distributed energy systems.

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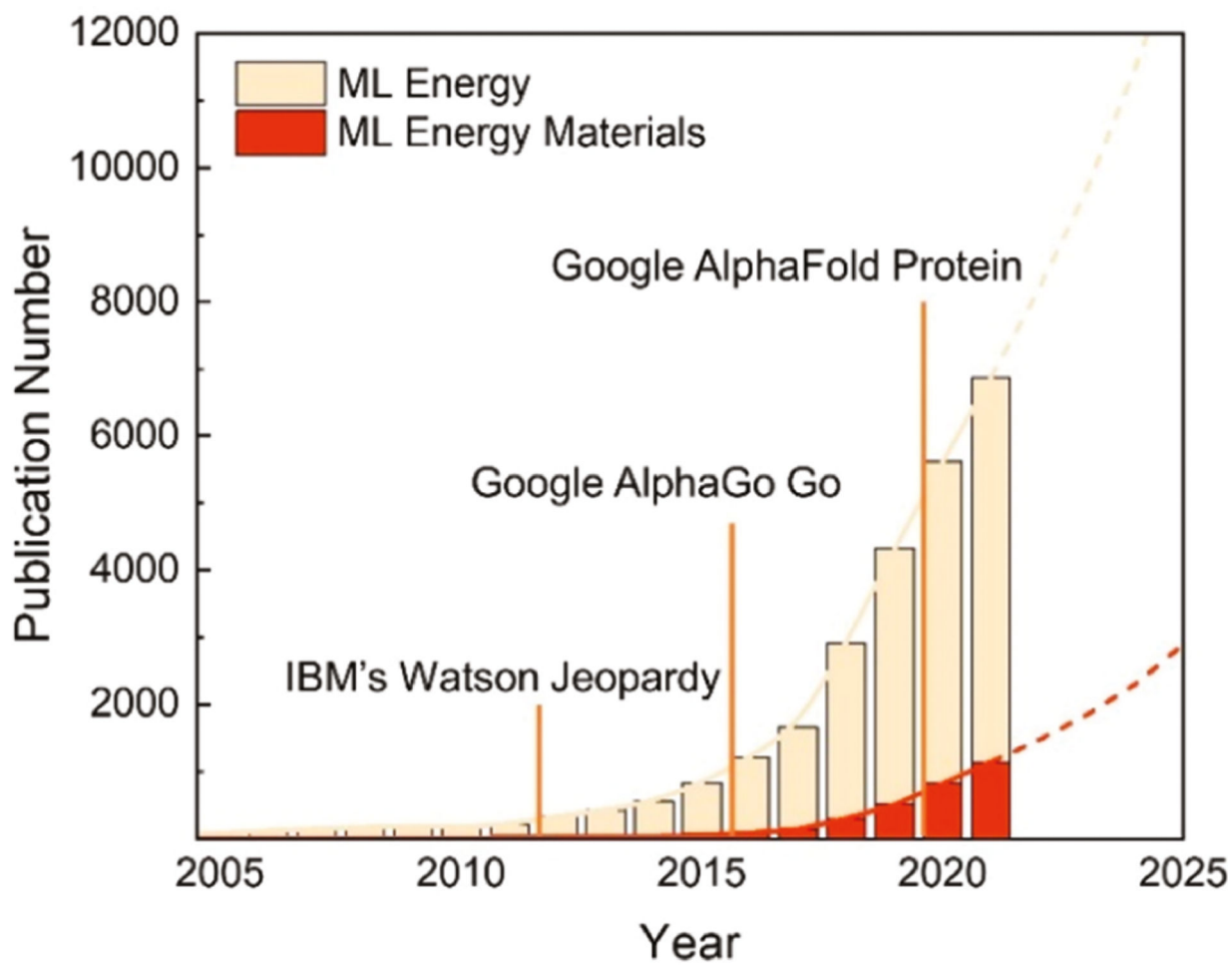
Figure 1.
Number of machine learning publications per year with energy and energy materials focus since 2005, highlighted with the milestone achievements.
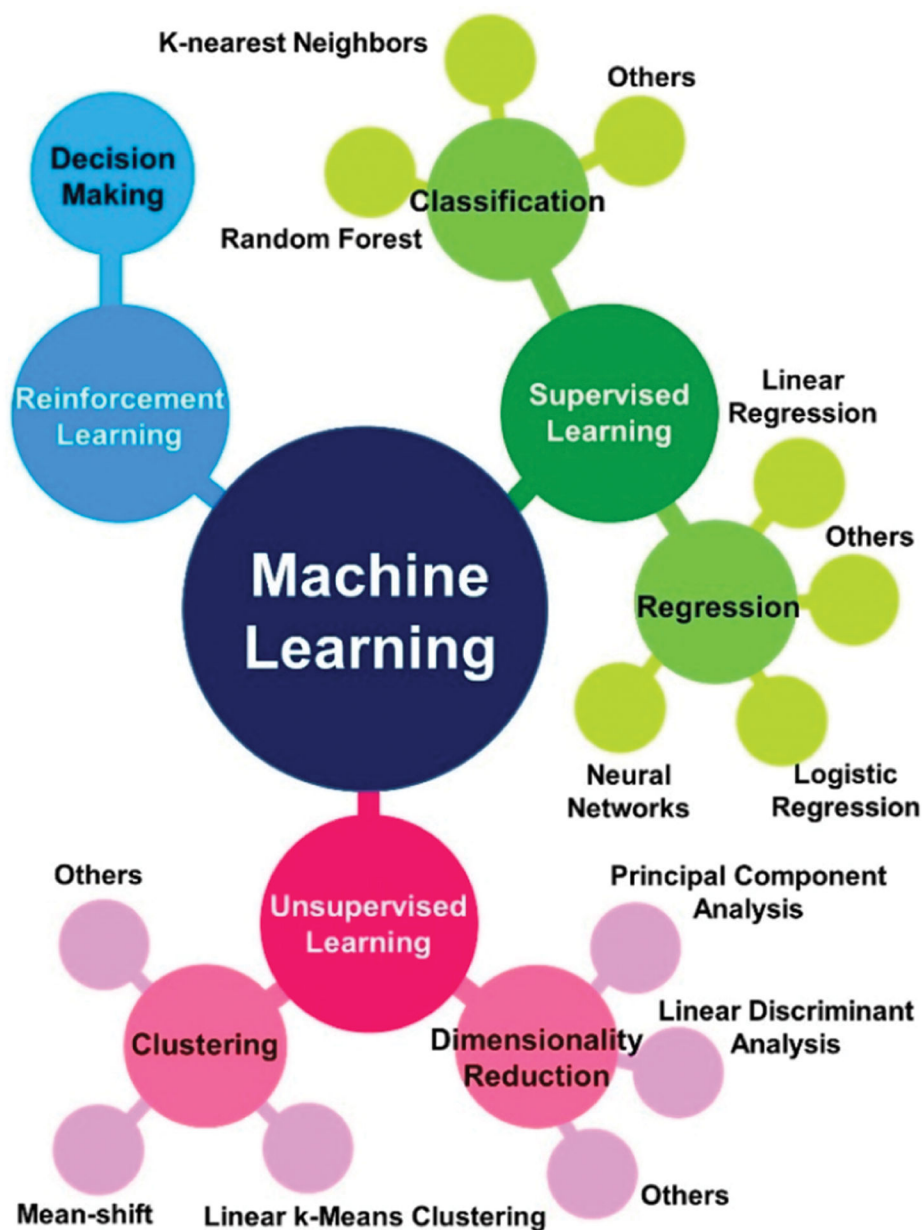
Figure 2.
Categories of machine-learning algorithms, including supervised, unsupervised, and reinforcement learning. Under each type of learning, there are multiple algorithms, specialized for targeted problems.
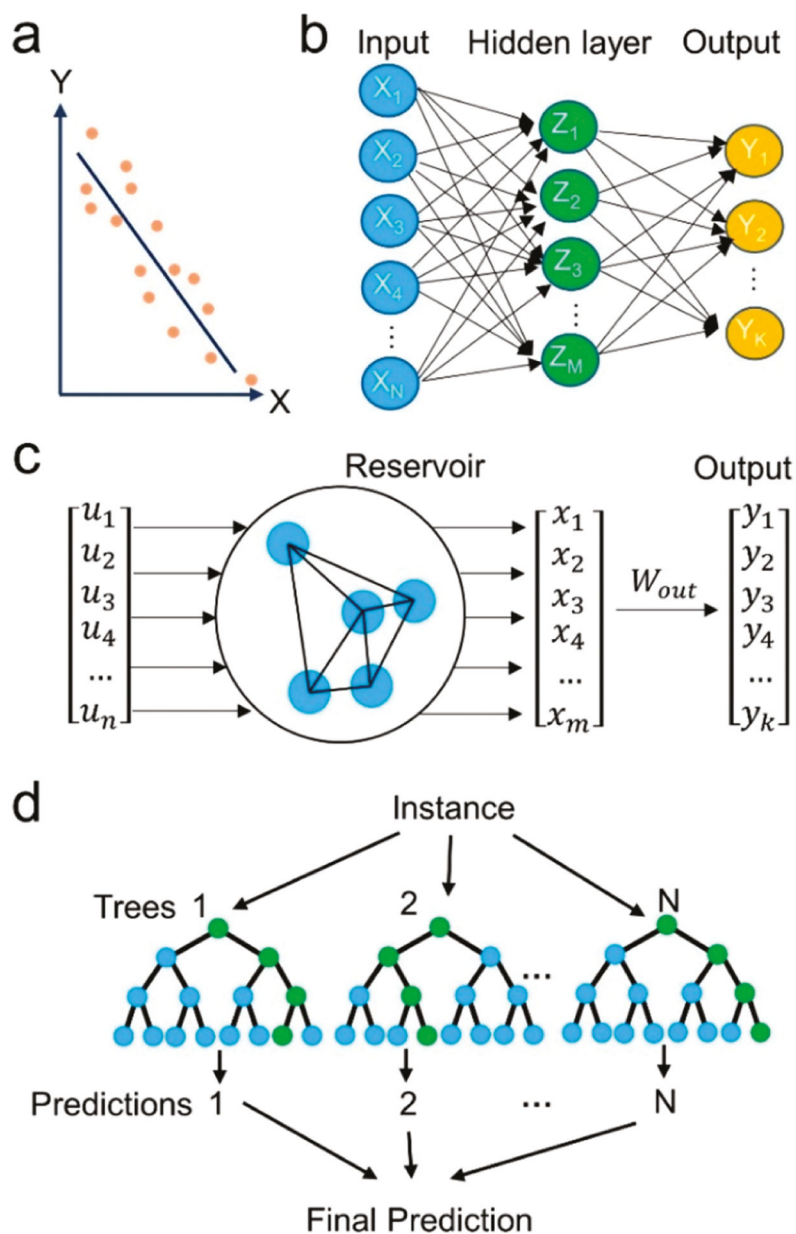
Figure 3.
Representative machine-learning algorithms. Examples to illustrate (a) linear regression, (b) feed forward neural network, (c) reservoir computing, and (d) random forest.
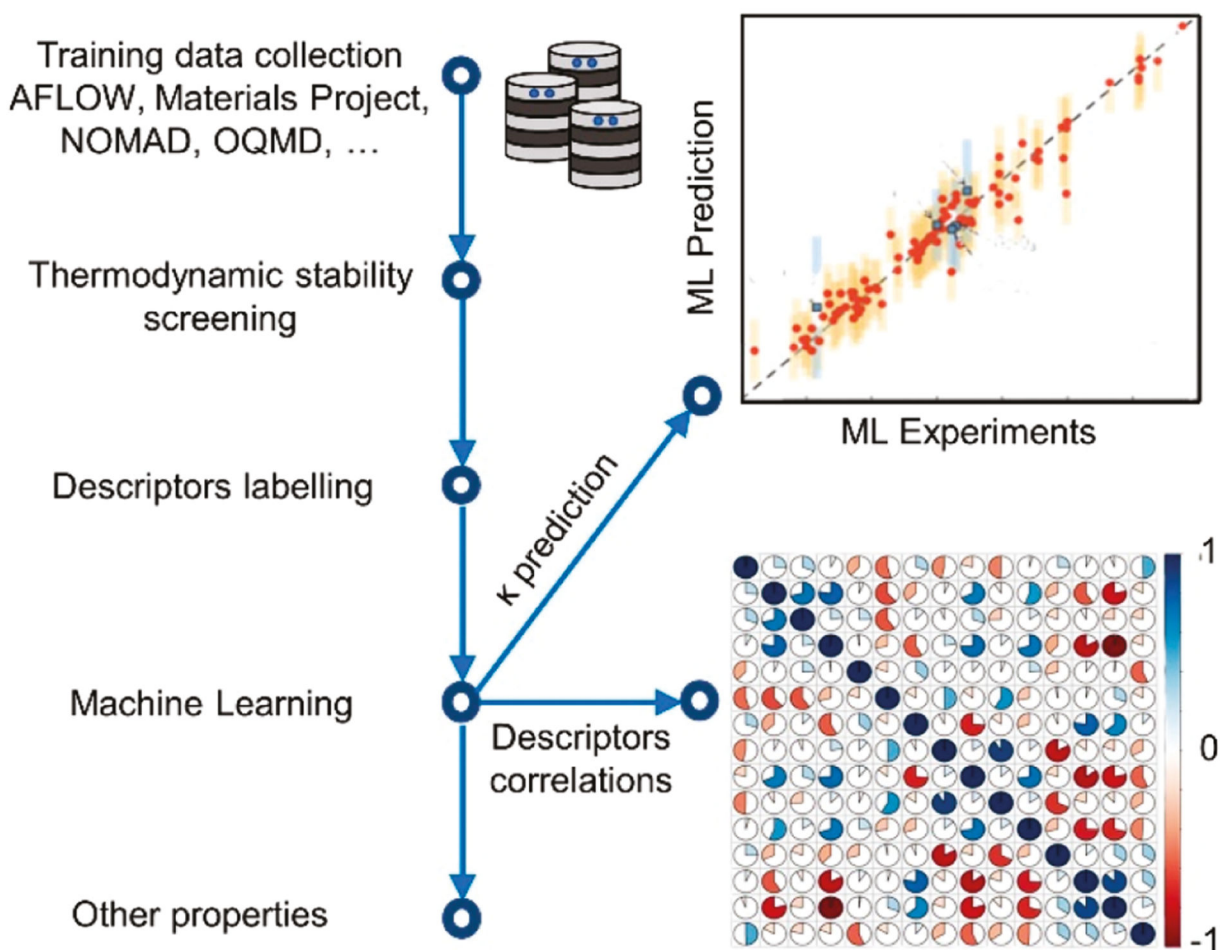
Figure 4.
General workflow of machine-learning-assisted high-throughput thermal energy materials discovery. Machine-learning relationships between materials descriptors and thermophysical properties from the existing experimental and modeling big data in various databases can help predict properties of unexplored materials and distinguish the important materials' descriptors. Reprinted with permission from refs 47 and 48. Copyright 2016 Elsevier and 2016 American Physical Society.
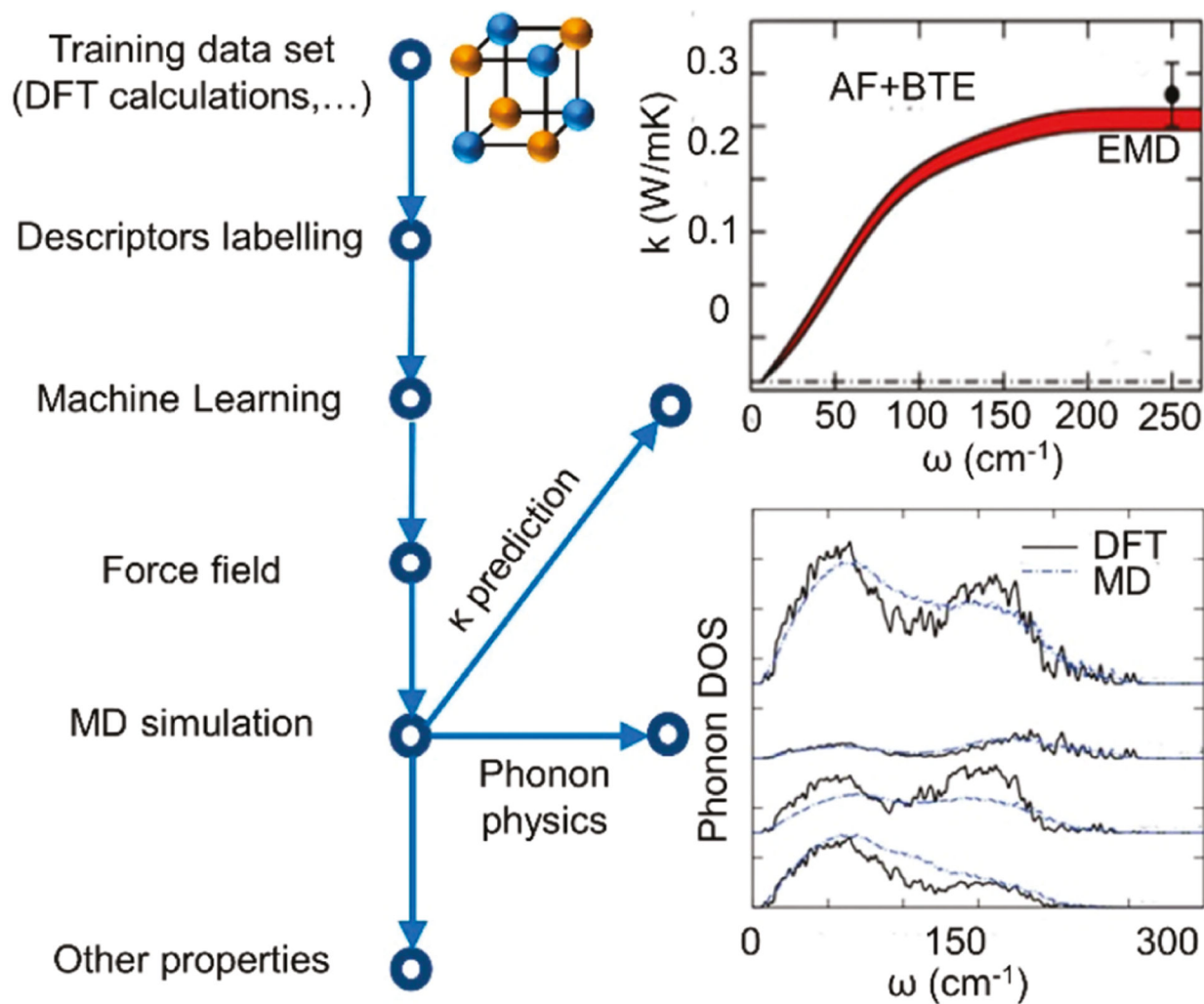
Figure 5.
General workflow of atomistic modeling of thermal properties accelerated or improved by novel functionals for density functional calculations, accurate force fields for molecular dynamics, and numerical solutions for partial differential equations assisted by machine learning. Reprinted with permission from ref 88. Copyright 2012 American Physical Society.
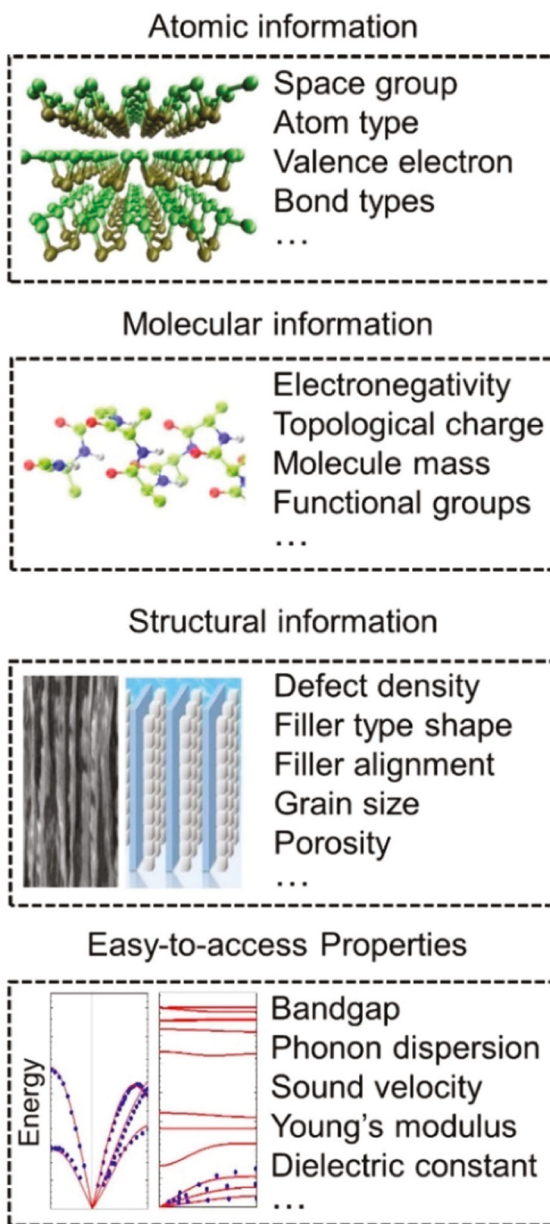
Figure 6.

Common materials descriptors for machine-learning thermophysical properties of various materials, including semiconductors, polymers, alloys, and composites. Atomic information is of paramount importance for materials with simple structure, like semiconductors. Molecular information is indispensable for evaluation of the properties of organic systems, like polymers. For heterogeneous materials such as composites, the structural information is critical to their apparent properties. The easy-to-access properties, for instance sound velocity and Young's modulus, can be correlated with thermal properties for most materials. Reprinted with permission from refs 19 and 34. Copyright 2021 Springer Nature and 2019 John Wiley & Sons.
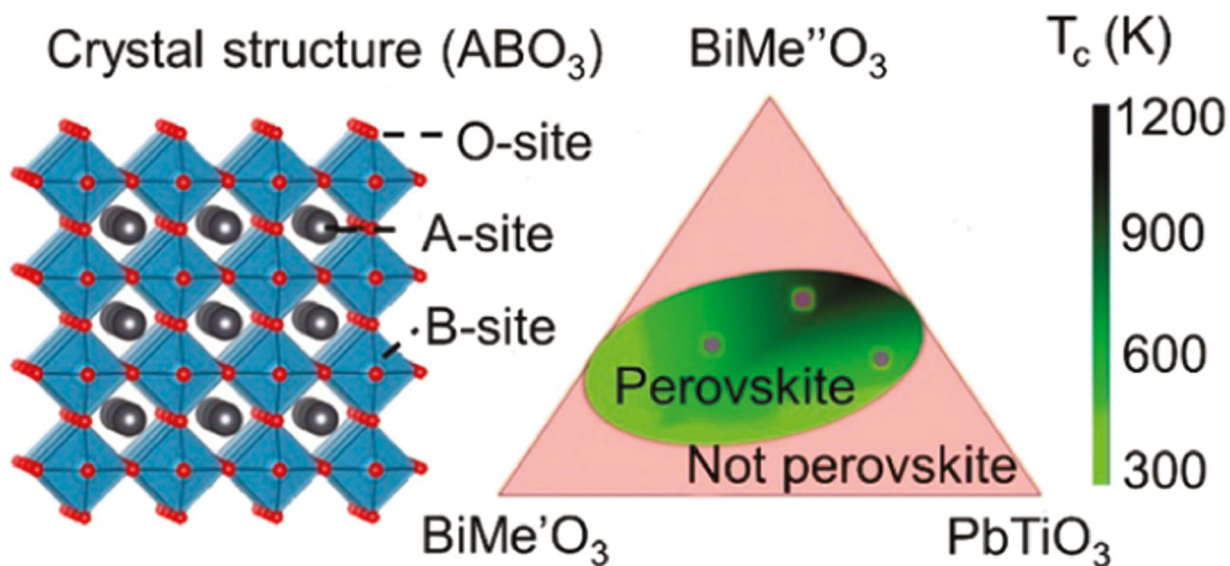
Figure 7.
Thermal stability prediction of perovskite crystals with variable elements such as Mo, W, Nb, Ta, etc. and stoichiometric ratios using classification learning and regression. Reprinted with permission from ref 154. Copyright 2018 Springer Nature.
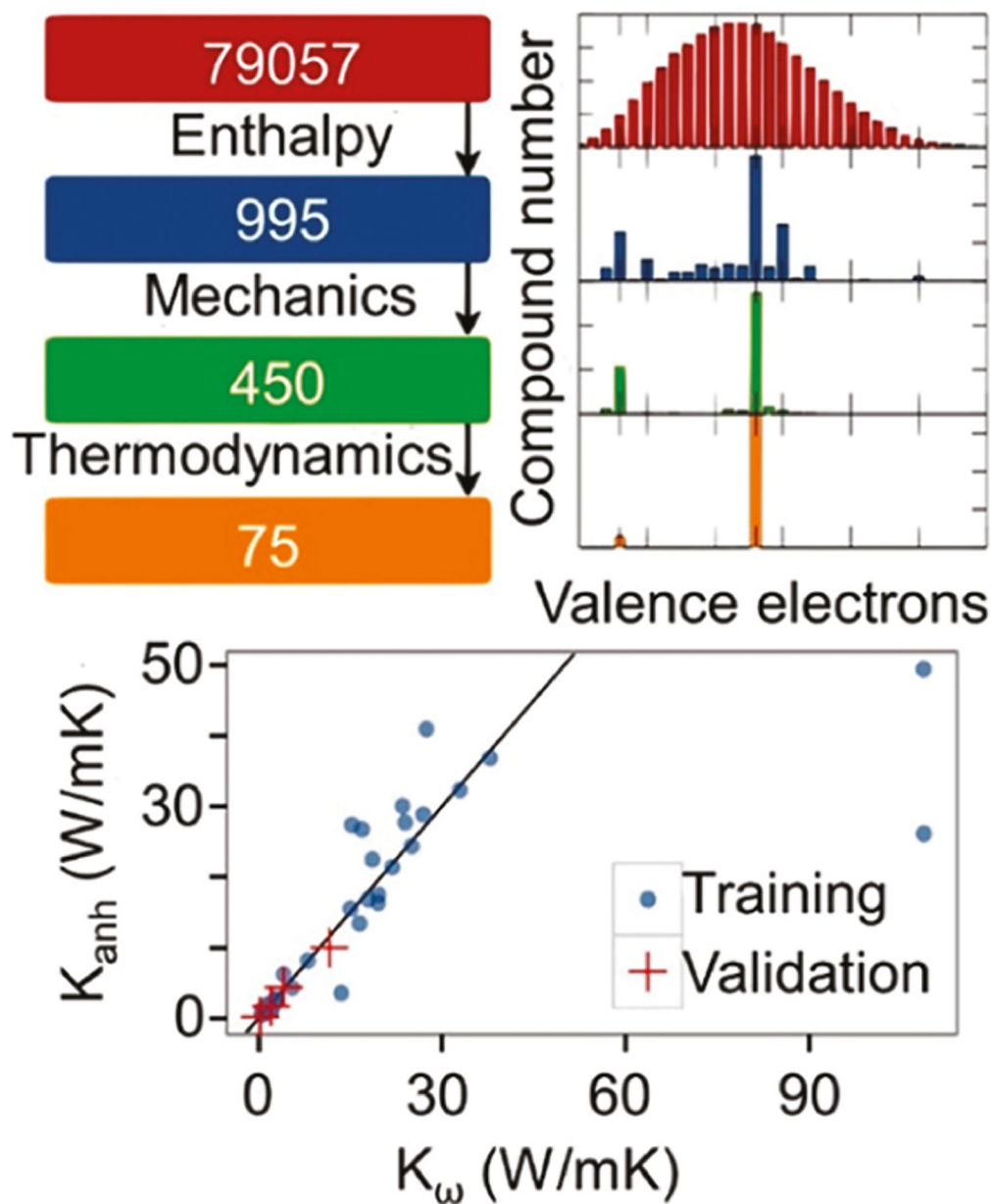
Figure 8.
High-throughput, low-thermal-conductivity half-Heusler semiconductors discovery from 79 000 initial entries in the AFLOW database by combining random forest regression and ab initio calculations. Reprinted with permission from ref 101. Copyright 2014 American Physical Society.
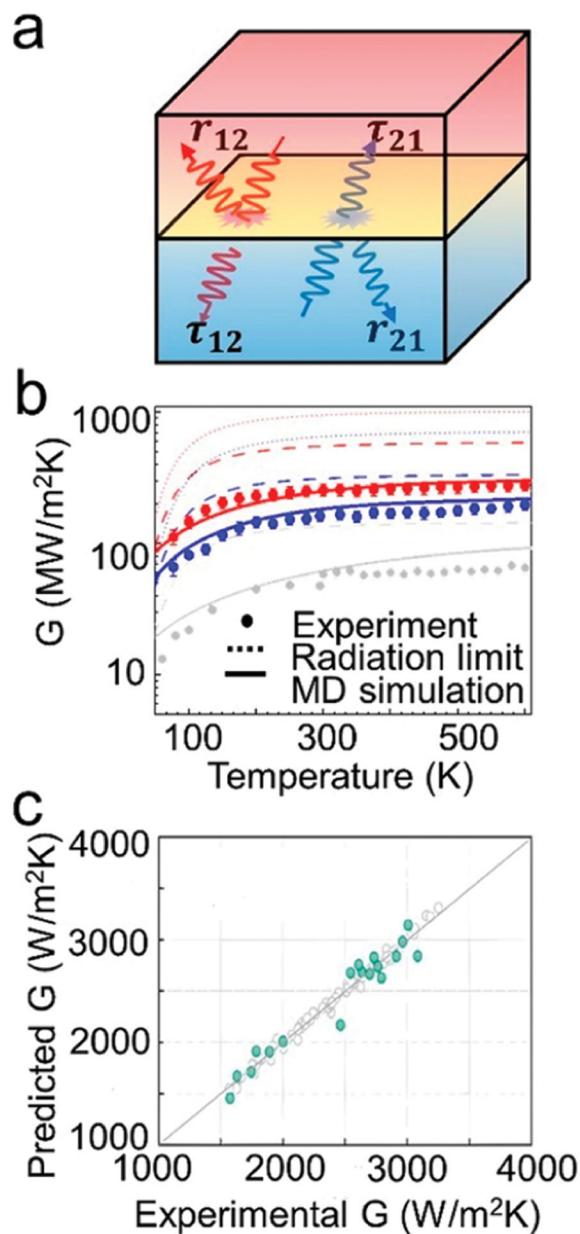
Figure 9.
Prediction of thermal boundary resistance by using linear regression, decision tree, random forest algorithm, and machine-learning potential-driven molecular dynamics simulations. Reprinted with permission from refs 18 and 173. Copyright 2021 Elsevier and 2021 Springer Nature.
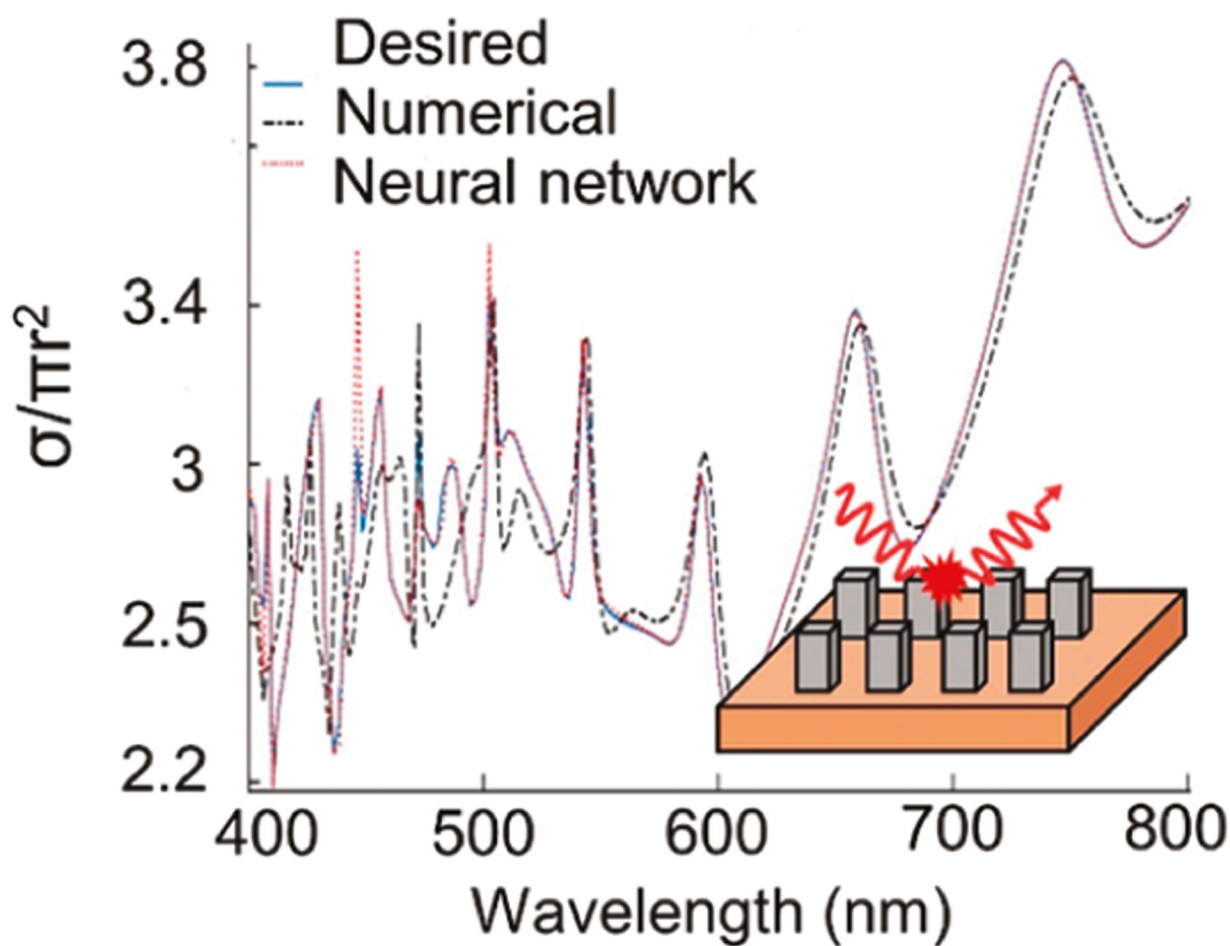
Figure 10.
Inverse design of emissivity of materials by machine learning the structure–property mapping from a training data set of rigorous calculation results of Maxwell equations using artificial neural networks. Reprinted with permission from ref 179. Copyright 2018 American Association for the Advancement of Science.
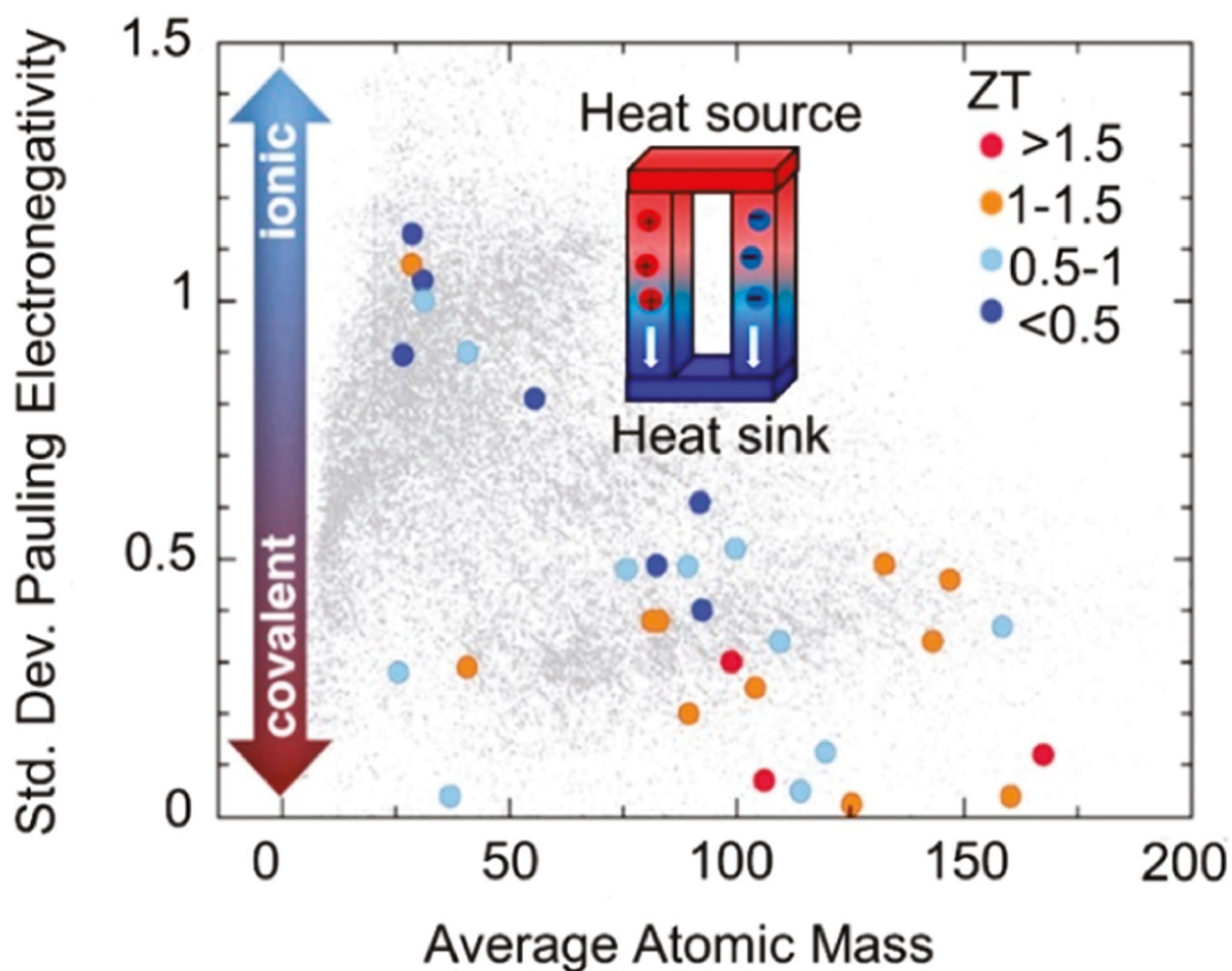
Figure 11.
Evaluation of thermoelectric properties can be accelerated with machine learning by selecting good material descriptors, including but not limited to the average atomic mass and standard deviation of Pauling electronegativity. Reprinted with permission from ref 188. Copyright 2015 Royal Society of Chemistry.
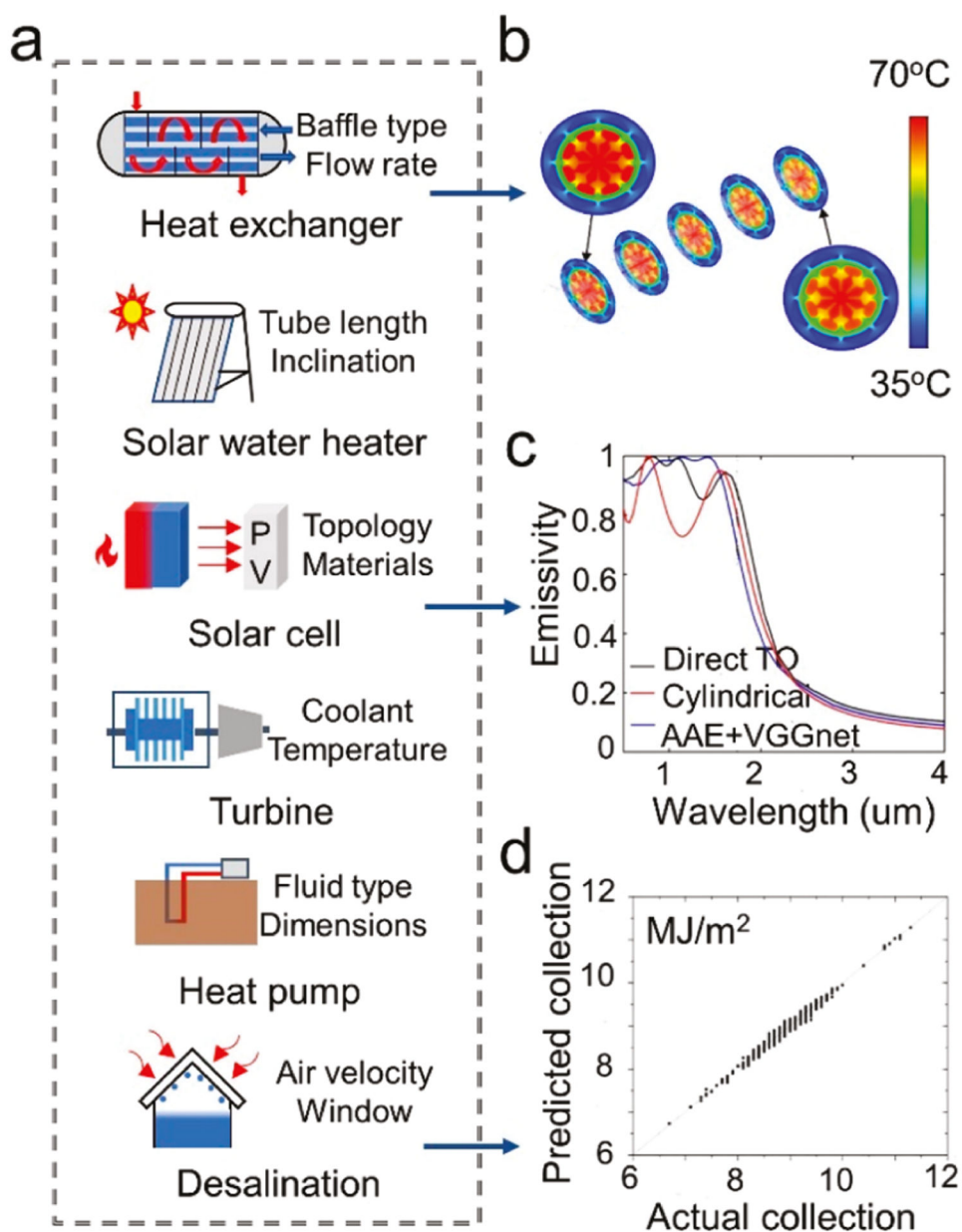
Figure 12.
Machine-learning applications in performance prediction and design optimization at the device levels, mainly including heat exchanger, thermal emitter, and heat collector. Reprinted with permission from refs 196, 182, and 197, respectively. Copyright 2021 Elsevier, 2020 AIP Publishing, and 2015 Multidisciplinary Digital Publishing Institute.
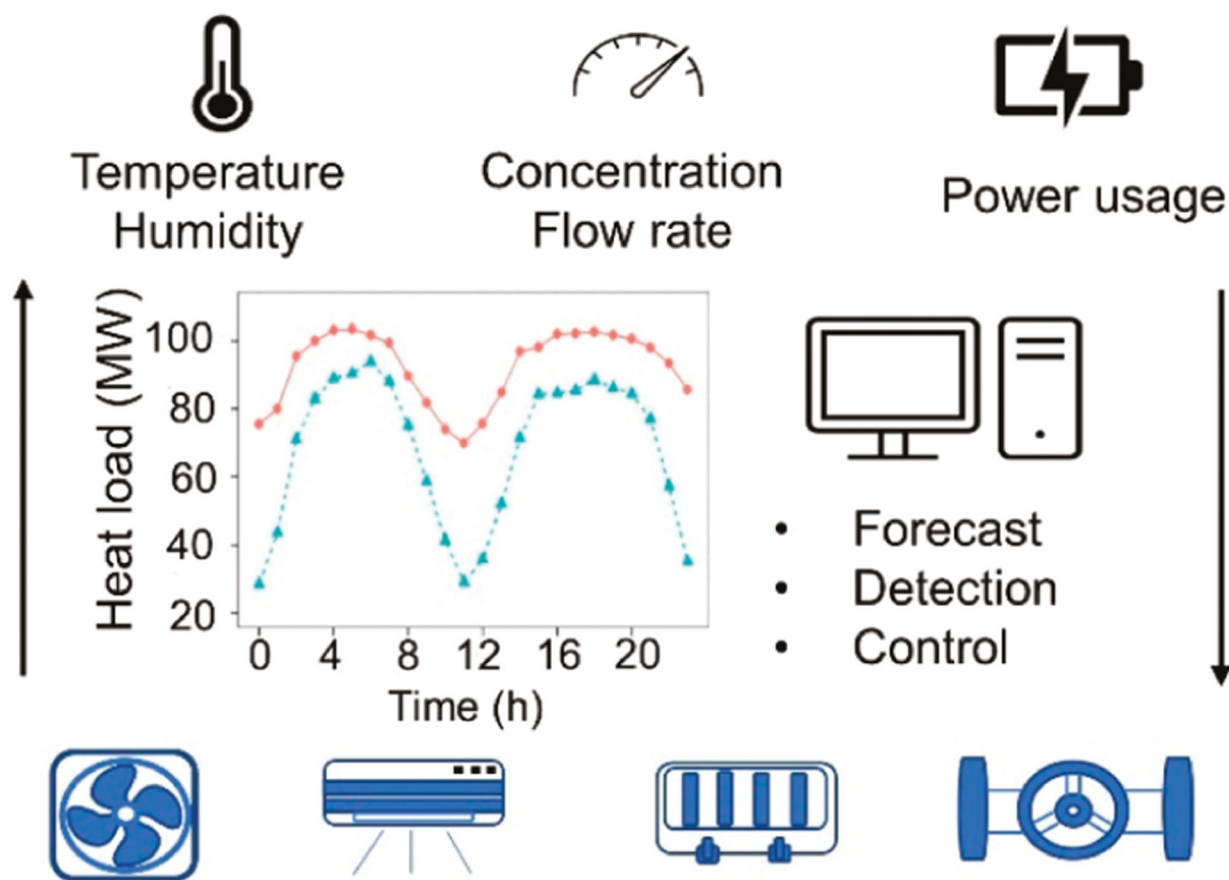
Figure 13.
Machine-learning applications in performance prediction at the system level, mainly
including the energy demand forecast, fault detection, and in situ control. Reprinted with
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