

**【Review Paper】****Material informatics for heat transfer**

Junichiro SHIOMI\*\*\*\*\*

\*Institute of Engineering Innovation, The University of Tokyo, 7-3-1 Hongo, Bunkyo, Tokyo, 113-8656, Japan

\*\*Department of Mechanical Engineering, School of Engineering, the University of Tokyo, 7-3-1 Hongo, Bunkyo, Tokyo, 113-8656, Japan

\*\*\*AIP Project, RIKEN, Nihonbashi 1-chome Mitsui Building, 1-4-1 Nihonbashi, Chuo, Tokyo, 103-0027, Japan

\*\*\*\*Institute of Statistical Mathematics, 10-3 Midori-cho, Tachikawa, Tokyo, 190-8562, Japan

E-mail: shiomi@photon.t.u-tokyo.ac.jp

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This review paper summarizes the research for which the author has received the Nukiyama Memorial Award in 2022. The key essence of the research is “materials informatics (MI) for heat transfer” entailing the combination of nanoscale thermal science and data science. Various MI studies carried out at the Thermal Energy Engineering Lab with the collaborators on nanostructure design for heat conduction and thermal radiation are introduced. The MI method coupling heat transfer calculations and black-box optimization exhibits high efficiency to optimize nanostructures for target heat transfer properties. The method enabled the computational design and experimental realization of aperiodic superlattices that optimally impede coherent thermal transport and multilayer metamaterials with wavelength-selective thermal radiation.

**Keywords :** Materials informatics, Heat transfer, Machine learning, Optimization, Phonon engineering, Thermal radiation, Metamaterial

**1. Introduction**

This review paper is written to summarize the research for which the author has received the Nukiyama Memorial Award in 2022. The key essence of the research is “materials informatics (MI) for heat transfer” entailing the combination of nanoscale thermal transport science with machine learning. MI is an academic field dedicated to developing and studying materials using informatics, particularly through data-driven methods and machine learning. A typical approach involves training a black box model to relate basic descriptors (e.g., structure, composition) to target properties and predict or design materials with the best or good performance. The general methodology underlying MI originated from bioinformatics and chemoinformatics, where high-throughput screening of large databases was performed before the emergence of MI. MI developed later due to the limited availability of material data, but its growth over the past decade has been fueled by increasing accessibility of computational and experimental material datasets, such as the Materials Project (Jain et al., 2013), AFLOW (Curtarolo et al., 2012), ICSD (Belsky et al., 2002), OQMD (Saal et al., 2013), and AtomWork (Xu et al., 2011).

The field of MI gained momentum in 2011 with the Materials Genome Initiative in the US, followed by many initiatives and projects worldwide. In Japan, the Material Research by Information Integration Initiative (MI<sup>2</sup>I) was launched in 2015 under the Japan Science and Technology Agency (JST), which aimed to connect material researchers with informatics researchers. A unique characteristic of this project was its focus on “heat transfer materials” alongside battery materials and magnetic materials. The Thermal Energy Engineering Lab (TEEL) at the University of Tokyo joined the project, and since then, we have collaborated with others to advance “MI for heat transfer,” mainly in predicting and controlling materials for thermal conduction and radiation properties. MI<sup>2</sup>I ended successfully in 2020, particularly fostering collaborations between informatics and materials researchers.

One of the first reports to apply MI for predicting and high-throughput screening of material thermal conductivity was conducted by Carrette et al. (2014). They used random regression to model and screen 79,057 half-Heusler compounds, identifying materials with extremely low thermal conductivity. Subsequently, Seko et al. (2015) reported

Bayesian optimization with Gaussian process regression of crystal compounds to identify compounds using extremely low thermal conductivity with the Materials Project database.

Our research at TEEL began by expanding the search space for thermal conductivity optimization (we have also worked on modeling and screening crystal compounds for thermal conductivity using transfer learning (Ju et al., 2021)). In collaboration with Koji Tsuda's group at the University of Tokyo, we initially designed a binary multilayered nanostructure to minimize or maximize thermal conductance by coupling thermal transport calculations and Bayesian optimization, which showed excellent efficiency (Ju et al., 2017, 2020). Subsequently, we expanded the search space further by utilizing quantum annealing (Yamawaki et al., 2018). This approach enabled the computational design and experimental realization of aperiodic superlattices that optimally impede coherent thermal transport (Hu et al., 2020) and multilayer metamaterials with wavelength-selective thermal radiation (Sakurai et al., 2019).

These studies leveraged recent advancements in the science and engineering of nanoscale thermal transport. Over the past few decades, significant advancements have been made in developing thermally functional materials via nanostructuring. Nanostructures with dimensions comparable to or smaller than the characteristic length of phonon transport can significantly decrease thermal conductivity, which benefits applications such as thermoelectrics and thermal insulation. When phonons are considered as particles, their characteristic length corresponds to the intrinsic phonon mean free path (p-MFP) during incoherent collisions. Nanostructured surfaces and interfaces shorten the p-MFP, thereby impacting heat conduction. Alternatively, when phonons are considered as waves, their characteristic length is their coherence length. Nanostructures with surface/interface roughness smaller than the phonon wavelength can cause interference, thereby hindering phonon propagation. The impact of nanostructures on phonon transport depends on the phonon frequency, wavevector, and polarization, enabling the spectral control of heat conduction. Further details on the control of phonon transport and heat conduction by nanostructures can be found in previous reviews (Ju and Shiomi, 2019; Hu and Shiomi, 2021; Guo and Shiomi, 2024). Thermal radiation is comparatively simpler than heat conduction, as its wavelength and coherence length are significantly larger. This allows for more facile coherent and spectral control of photon transport compared to phonon transport.

Nanostructure-enabled control of heat transfer greatly enhances the flexibility of structural design for thermally functional materials. However, identifying the optimal nanostructure to maximize the desired figure of merit (FOM) remains a significant challenge. MI has proven invaluable in this regard, and MI for heat transfer has demonstrated increasing potential and popularity.

In the following section, we provide examples of MI applications for heat transfer, specifically focusing on a collaborative study carried out at TEEL on nanostructure design for heat conduction and thermal radiation.

## 2. Designing nanostructures for heat conduction

The first study of research group sought to develop a framework that combines phonon transport calculations with a black-box optimization method (Ueno et al., 2016). For this purpose, the atomistic Green's function (AGF) was employed to calculate phonon transport, while Bayesian optimization (BO) with Gaussian regression was used for machine learning. The AGF calculated the phonon transmission spectrum through a "channel region" sandwiched by the two leads, as illustrated in Fig. 1(a). By introducing nanostructures into the channel region—such as allowed or multilayer structures—phonon transmission through these nanostructures can be determined. Using the Landauer formula, the corresponding thermal conductance can then be calculated. In this implementation, the AGF used only harmonic interatomic force constants, meaning inelastic phonon scattering was ignored. This simplification facilitated faster calculations and data collection, which are important for the effectiveness of machine learning. This approach is physically justified because, for the very short channel explored in our research, which is much shorter than the phonon mean-free-paths, phonons are transported ballistically without inelastic phonon-phonon scattering, and the system can be approximated as harmonic.

The actual system is composed of Si and Ge, with the leads made of either Si or Ge crystals and the atoms in the channel region containing a mix of Si and Ge atoms. The AGF calculation applies periodic boundary conditions in the transverse direction, creating an infinite cross-section. The goal was to optimize the distribution of Si and Ge atoms to achieve a target (minimum or maximum) thermal conductivity. The AGF method is used to calculate the thermal conductivity for each candidate structure.

The BO process was employed to repeatedly optimize the structure, ultimately identifying configurations with the target conductance. Figure 1(b) shows the obtained optimal structures. For structures with maximum thermal conductivity,

the optimal configuration typically consisted of a Si–Si lead, with a continuous Si bridge connecting the leads, enabling coherent phonon transport. On the other hand, structures with minimal thermal conductivity were aperiodic layered structures that disrupted phonon transmission, in contrast to periodic layered structures, which generally have higher thermal conductance.

Two key findings emerged from the study (Ju et al., 2017): (1) the obtained optimal structure yielding the minimum thermal conductance was non-intuitive; (2) only  $\sim 1\%$  of all candidate structures needed to be calculated to identify the global optimum. The global optimal structure was verified by keeping the problem sufficiently small, allowing an exhaustive search for all candidates. This ensured the high efficiency of the BO-based MI optimization scheme for solving the nanostructure heat-conduction problem.

In addition to identifying optimal solutions, MI also provided new insights into material properties. By analyzing the optimal structure, researchers could perform “reverse science” to investigate the mechanisms behind the observed superior properties.

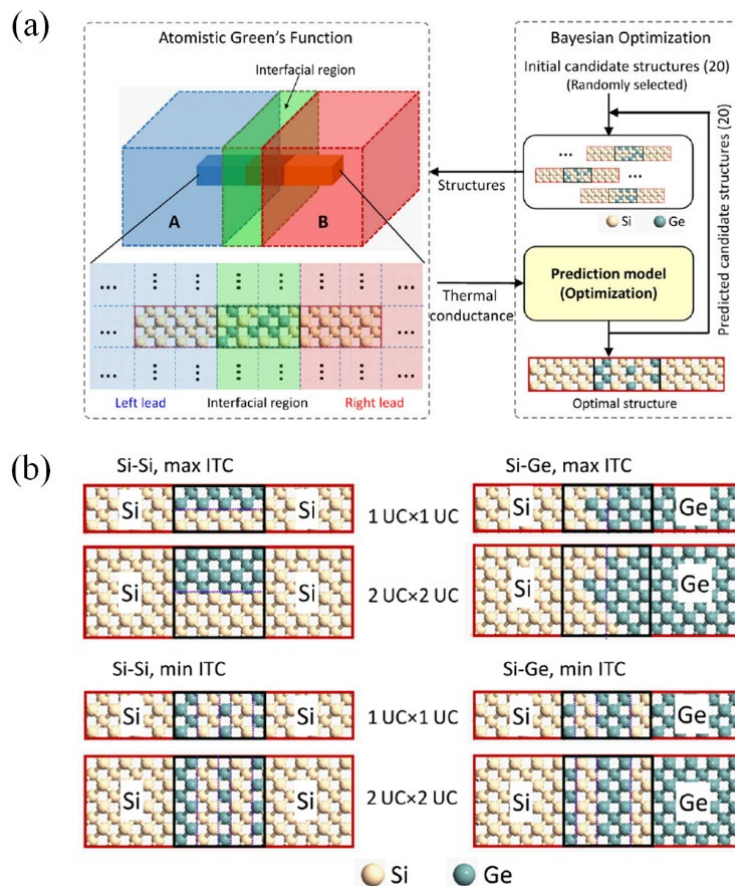


Fig. 1 (a) Optimization procedure for the Si/Ge interface nanostructures. (b) Optimized structures with the maximum and minimum interfacial thermal conductance (Ju et al., 2017).

We may explore this mechanism by considering the design of a Si/Ge superlattice (SL) structure. As shown in Fig. 2(a), unit layers (ULs) of either Si or Ge are connected to form a superlattice between the Si leads. A simple descriptor is adopted here to describe a specific structure, denoting Si and Ge with the binary digits “0” and “1”, respectively. For instance, for an optimization problem involving a 14-UL SL, an SL with two UL periodicity is described as “11001100110011.” This binary digit descriptor is simple and intuitive and was initially chosen for its simplicity. However, after trying more sophisticated descriptors, we empirically found that this method performs well in terms of optimization efficiency.

An example of an optimized structure with minimum thermal conductance is shown in Fig. 2(a) for an 8-UL SL. This structure is aperiodic and non-intuitive. Figure 2(b-d) shows various systematic analyses to understand why a specific

aperiodic SL achieves the minimum thermal conductance. Aperiodic SLs with varying unit lengths and atomic fractions were more effective at reducing thermal conductivity than their periodic counterparts. The analysis showed that the thermal conductance decreased with increasing layer thickness due to Fabry–Pérot oscillations. Additionally, phonon scattering increased with the number of interfaces, emphasizing the competitive relationship between these parameters in reducing thermal conductivity. The analysis shown in Fig. 2(e-f) explored the coherent and incoherent effects on phonon transmission by comparing the full AGF calculation with the cascade transmission model, which considers the system as a series of resistances at each interface. While the cascade model reflected only incoherent phonon transport, the full AGF calculation captured coherent phonon transport across multiple layers. The convergence of transmission in the full AGF calculation suggests that constructive and destructive interferences were balanced in periodic SLs, highlighting the potential for further reduction in thermal conductance by adjusting these interferences. In the case of the optimal aperiodic SL, the structure effectively suppressed constructive phonon interference, leading to minimal thermal conductance.

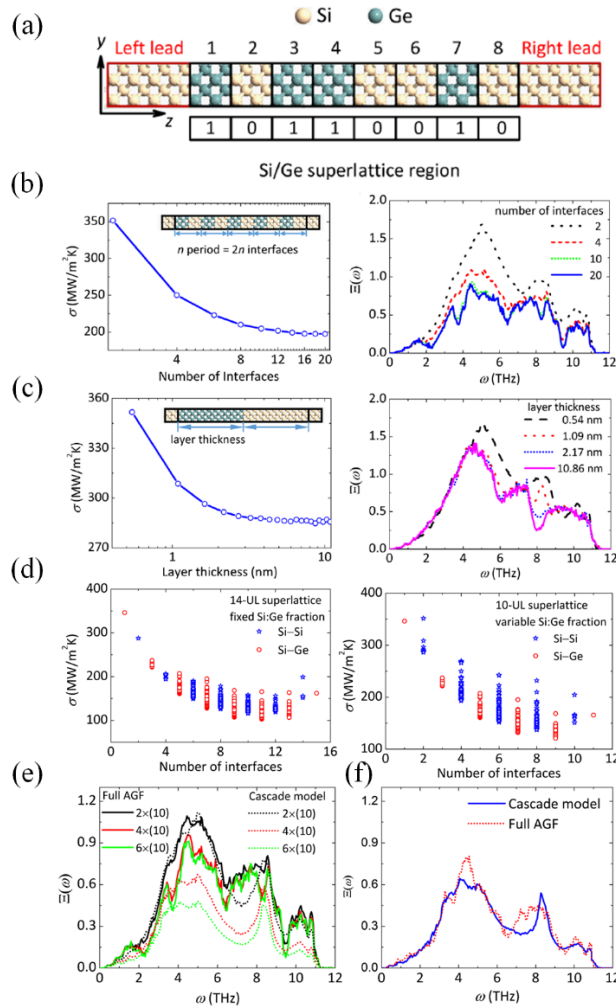


Fig. 2 (a) Schematic of the 8-unit-layer (UL) SL with an equal fraction of Si and Ge atoms at the Si–Si interface, illustrating the descriptor. (b) Thermal conductance and phonon transmission as a function of layer thickness. (c) Thermal conductance and phonon transmission as a function of the number of interfaces. (d) Thermal conductance as a function of the number of interfaces for a 14-UL SL with equal Si/Ge fraction and 10-UL with variable Si/Ge fractions. Comparison of phonon transmission obtained from the cascade model and full AGF calculation: (e) periodic superlattices with different number of periods, where one period consists of a Si UL and Ge UL denoted as “10.” (f) Optimal aperiodic superlattice structure with a total thickness of 10 UL (Ju et al., 2017).

Given the practical difficulty of realizing the SiGe SL, we next applied the MI design methodology to the GaAs/AlAs SL structure, which can be fabricated by molecular beam epitaxy (MBE) with molecular-scale interface smoothness. The goal was to predict and experimentally verify the optimal structure with minimal thermal conductivity. To ensure the accuracy of the AGF calculation for phonon transport, we extracted interatomic force constants (IFCs) using first principles, including those at the GaAs/AlAs interfaces. We also accounted for monolayer roughness, which is inevitable in the MBE process. By integrating the mass matrices and IFCs, the dynamical matrix was obtained, which was then used in the AGF method to calculate phonon transmission and thermal conductivity. The overall flow chart of the optimization process is shown in Fig. 3(a)—the BO optimization process with AGF calculations identified the minimum thermal conductivity structure. This structure was fabricated by MBE, and its thermal conductivity was measured using time-domain thermoreflectance (TDTR). As shown in Fig. 3(b), the experimental results closely matched the calculation results, validating the MI design approach.

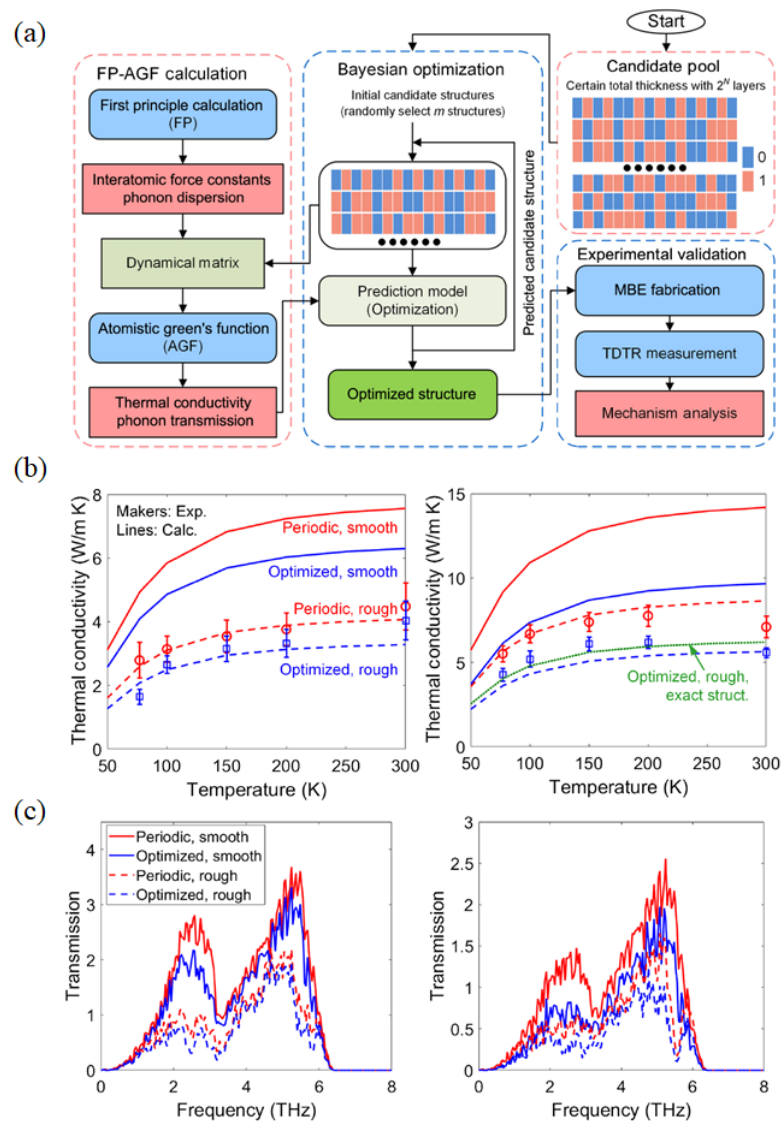


Fig. 3 (a) Flowchart illustrating the optimal control of thermal conduction in GaAs/AlAs interface SL nanostructures. (b) Experimental and calculated thermal conductivities of the 16-UL (left) and 48-UL (right) optimized aperiodic and periodic SL nanostructures. (c) Corresponding phonon transmission functions for the 16-UL and 48-UL structures (Hu et al., 2020).

We further performed “reverse science” by analyzing the phonon transmission in the optimal aperiodic and periodic



SL structures obtained by the AGF calculations. The phonon transmission was consistently lower in the optimized aperiodic structures across nearly the entire spectrum, particularly in the acoustic phonon range (Fig. 4(a-f)). The analysis revealed that the enhanced phonon localization in the optimal structure contributed to the reduced thermal conductivity. This localization is linked to the constructive aperiodicity of the structure, which effectively inhibits phonon transport.

To further explore the physical mechanisms underlying the phonon localization, the inverse participation ratio (IPR) and local density of states (LDOS) were analyzed (Fig. 4(g-h)). The results showed that the optimal aperiodic structure exhibited stronger phonon localization than the periodic structure, particularly above the optical phonon frequency. Weighted IPR and LDOS analyses indicated that the reduced thermal conductivity in the optimal structure resulted from enhanced phonon localization within the acoustic phonon range.

The study also identified specific local structures within the optimized SL that were crucial for reducing phonon transmission across different frequency ranges. By analyzing the phonon patterns, researchers identified several key local structures that maximize the inhibition of phonon transmission, leading to the lowest thermal conductivity. The optimal SL possessed all these local structures, which contributed to its superior thermal performance.

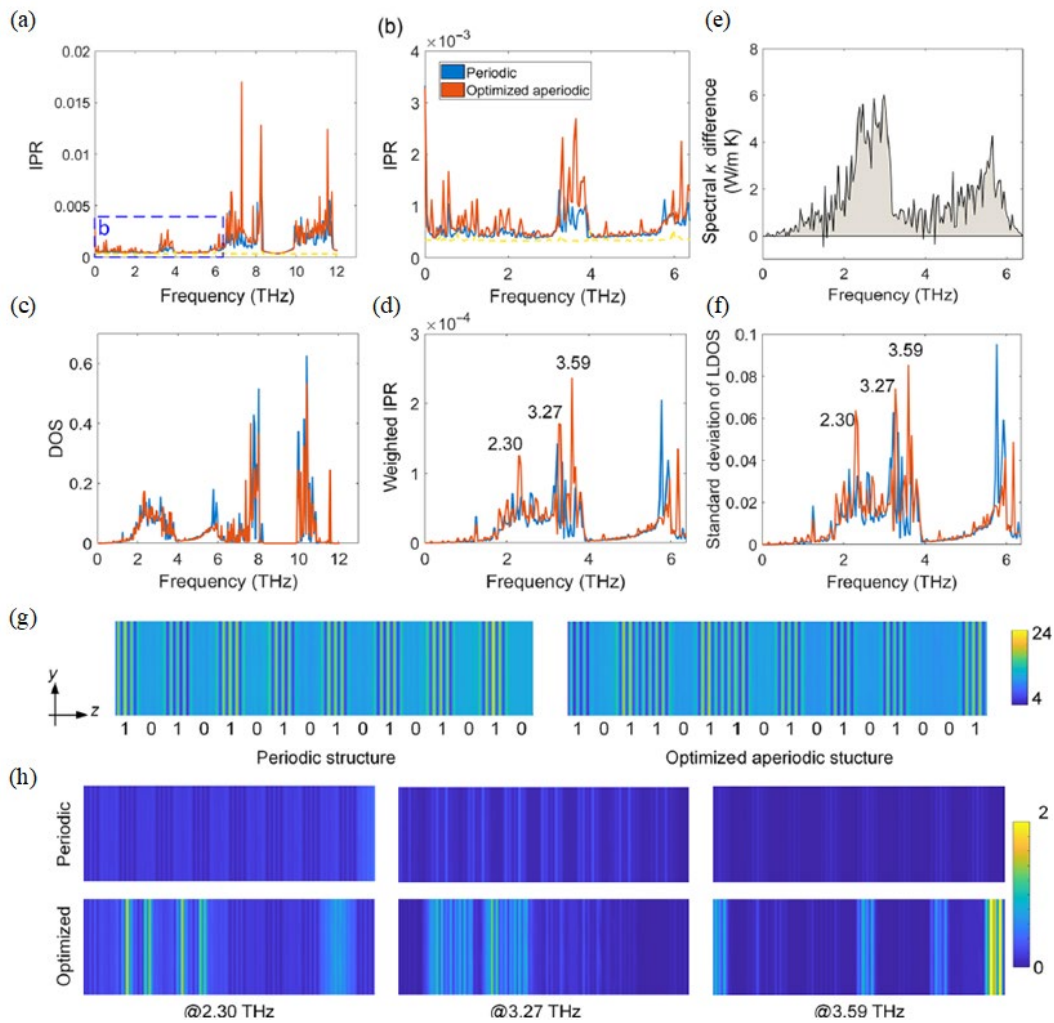


Fig. 4 Comparison of the frequency-dependent IPR  $I(\omega)$  of the two structures in the (a) full and (b) acoustic phonon frequency ranges. Blue-dashed square in (a) denotes the acoustic phonon range and is magnified in (b). Yellow dashed lines denote the small and uniform IPR for pure GaAs crystals. (c) Spectral DOS of the two structures in the full phonon frequency range. (d) Spectral weighted IPR in the acoustic phonon frequency range. (e) Spectral thermal conductivity difference between the periodic structure and optimized aperiodic structure. (f) Spectral standard deviation of the LDOS for the two structures in the acoustic phonon frequency range. (g) Projected LDOS distribution in the y-z plane for acoustic phonons in periodic and optimized aperiodic structures. (h) Projected LDOS in the y-z plane for the two structures at 2.30, 3.27, and 3.59 THz (Hu et al., 2020).

### 3. Optimizing the trade-off between thermal and electrical transport

Many real-world applications involve the optimization of multiple, sometimes conflicting targets. This is a critical issue for thermoelectric materials that exhibit high electrical and low thermal conductivities. To address this issue, we demonstrated the feasibility of the MI design approach for multi-objective optimization by predicting the optimal thermoelectric structure of graphene nanoribbons (GNRs) (Yamawaki et al., 2018). Short-period nanostructured GNRs were analyzed, where hexagonal lattices with removed carbon atoms are denoted as 0 and complete hexagonal lattices as 1. The study focused on optimizing both the power factor (electrical conductivity multiplied by the Seebeck coefficient) and thermal resistance.

As shown in Fig. 5, the optimized structure had vacancies distributed throughout the GNR area, except along the edges, which enhanced thermoelectric performance due to the strong flattening of the electronic bands and the zigzag structure in the middle area, leading to increased phonon scattering. The labyrinthine shape of the optimized structure enhanced phonon localization, thereby reducing thermal conductivity.

A new simulation model featuring an antidot nanostructured region connected to semi-infinite pristine GNRs was constructed. This structure consists of pristine and antidot sections, with the optimal configuration significantly improving the thermoelectric FOM ( $ZT$ ) by 11 times compared with the pristine structure. The aperiodic distribution of antidots effectively enhanced both thermal and electrical properties, demonstrating the power of MI in optimizing complex, multi-objective material designs.

We further analyzed the phonon and electron transport properties to understand the underlying mechanisms of the enhanced thermoelectric performance. We found that aperiodic structures provided greater freedom for structural regulation, further reducing thermal conductivity. Furthermore, the optimal antidot distribution inhibited electron transmission in the resonant state, thereby enhancing thermoelectric performance.

Analysis of the local density of states (LDOS) distribution confirmed that state localization in the optimal structure suppressed electron transport, contributing to the overall efficiency of the thermoelectric material.

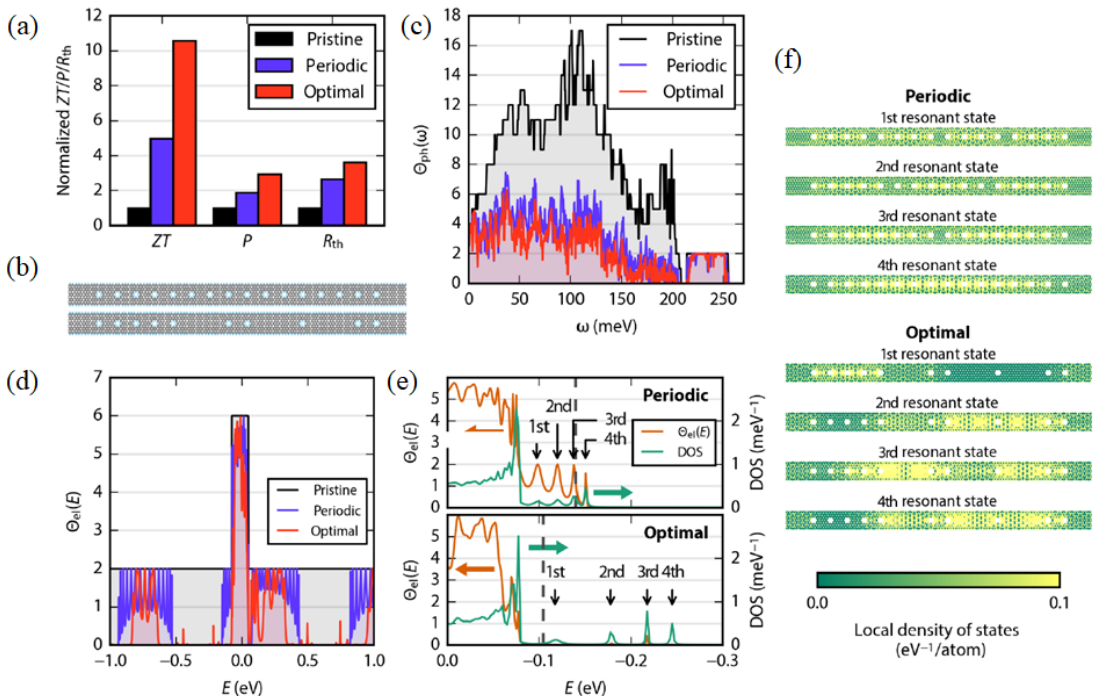


Fig. 5 (a) Comparison of thermoelectric properties of pristine, periodic, and optimal structures. (b) Periodic and optimal aperiodic antidot GNRs. (c) and (d) Phonon and electron transmission functions. (e) Transmission and DOS in the nanostructured region, with edge states represented by dashed lines. (f) LDOS distribution of resonant states in periodic and optimal structures (Yamawaki et al., 2018).

The work shows that a specific structure can break the trade-off between thermal and electrical transport. We have recently conducted further investigations into how the interface structure between grains in polycrystalline materials influences this trade-off. In the example introduced herein, we consider silicon grain boundaries as a case study owing to their importance in thermoelectric applications (Lortaraprasert and Shiomi, 2022). We employed machine learning with structural descriptors to study the relationship between the Si grain boundary structure and its thermal and electrical properties. We constructed a robust machine learning prediction model for thermal conductance at crystalline–crystalline and crystalline–amorphous interfaces using disorder descriptors and atomic density, along with high-throughput calculations based on Green’s function methods. We also constructed high-accuracy machine learning models for predicting both thermal and electrical conductance, as well as their ratio, using only small amounts of crystalline grain boundaries. While this is not an optimization problem, as in previous examples, it follows the same black-box modeling to relate the structure and thermoelectric properties. Figure 6 shows that modeling can be performed with extremely high accuracy. Notably, the black-box machine learning model was extremely robust, simultaneously predicting transport through both crystalline and amorphous structures. Furthermore, machine learning identified structures that increased the electrical-to-thermal conductance ratio, thereby breaking the trade-off. We found that variations in the interatomic angle and distance at the grain boundaries were the most predictive descriptors of thermal and electrical conductance, respectively. This suggests that populating materials with grain boundaries that have large angular variations and small distance variations could improve thermoelectric performance. This insight for decoupling thermal and electrical conductance should prove useful as the controllability of material structure continues to advance.

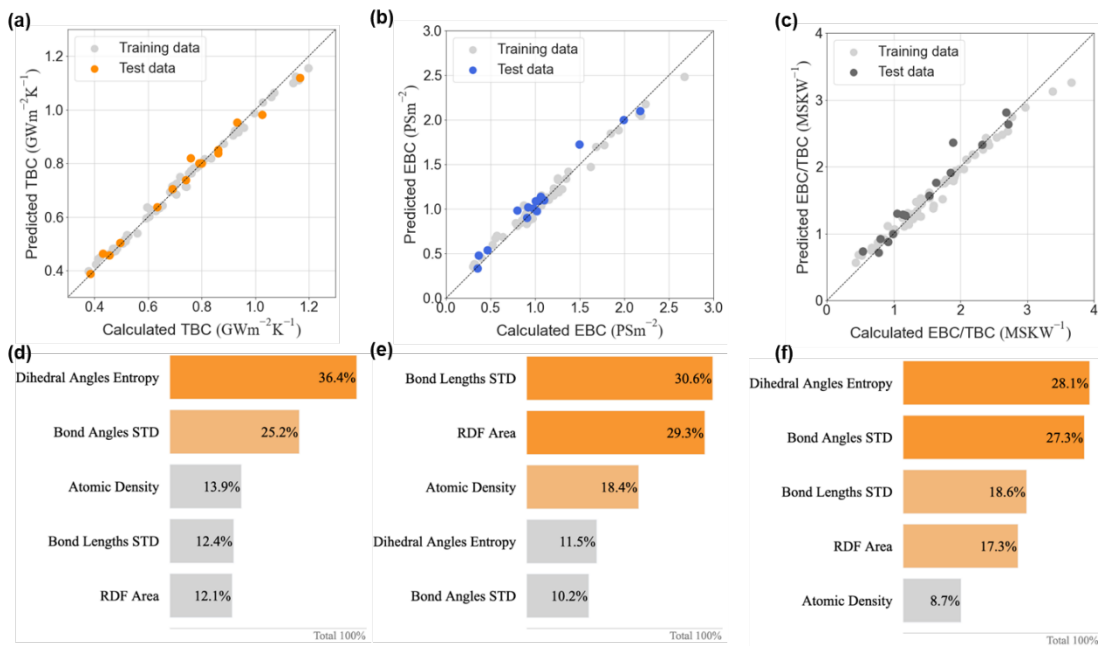


Fig. 6 (a) Machine learning prediction results for 75 crystalline–crystalline grain boundaries. (b) and (c) Parity plots between calculated and ensemble-predicted values. (e) and (f) Importance for thermal boundary conductance (TBC), electrical boundary conductance (EBC), and EBC/TBC, respectively (Lortaraprasert and Shiomi, 2022)



#### 4. Structure design of selective thermal radiation

Radiative cooling technology, which cools objects by thermal radiation, has shown significant potential for applications in thermal management and energy saving for various objects such as buildings, machines, and even humans. The goal is to tailor the surface structure or material to achieve a target emission spectrum, which depends on the specific application. Two representative types are commonly considered. One is a narrowband wavelength-selective thermal emitter, where only photons with specific wavelengths are emitted, resulting in an emission spectrum with a sharp peak at the target wavelength. Performance is typically evaluated in terms of the Q factor, which quantifies the narrowness of the peak. Narrowband wavelength-selective thermal emitters are used in incandescent light sources, microbolometers, and infrared heaters. The second type is the sky radiator, which radiates heat to space through the atmospheric-transparent window at wavelengths ranging from 8  $\mu\text{m}$  to 13  $\mu\text{m}$ . To maximize the radiative heat flow through the atmospheric window while minimizing the absorption of thermal radiation from the atmosphere, the surface material or structure should have high emissivity within the atmospheric transparent window and low emissivity outside. In both cases, the complexity of optimizing the structural design of photonic crystals makes them ideal candidates for MI optimization.

One of our early studies on thermal radiation involved directly applying our MI design methodology with BO, developed for the heat conduction problem, to design a narrowband wavelength-selective thermal emitter (Fig. 7(a-b)) (Sakurai et al., 2019). While considering various structure types, such as multilayers, photonic crystals, and metal–insulator–metal metamaterials, we chose multilayers due to their relative simplicity of fabrication and scalability. The target structure consisted of 18 unit layers, each composed of Ge, Si, or  $\text{SiO}_2$ . The goal was to achieve high emissivity at a target wavelength ( $\lambda_t$ ) with a narrow bandwidth while suppressing emissivity at other wavelengths to minimize radiative heat loss. Emission spectra were obtained using the transfer matrix method (TMM). The TMM calculation is computationally efficient, enabling optimization with a large degree of freedom. With three types of materials, 18 unit layers, and some degrees of freedom to vary the thickness of the unit layer, the total number of candidate structures exceeded 8 billion, which required more than 10 million calculations, even with a highly efficient MI method capable of identifying the global optimal solution with structure-property data of only  $\sim 1\%$  of the total candidates. Optimization was performed to minimize the FOM and difference between the emission spectrum of the structure and target spectrum.

The optimal structures for  $\lambda_t = 6.0, 5.0$ , and  $7.0 \mu\text{m}$ , shown in Fig. 7(c), were found to consist of aperiodic multilayered configurations. The spectral directional emissivity of these structures, as shown in Fig. 7(d), demonstrates the desired sharp and high-emissivity peaks at the target wavelengths without redundant peaks elsewhere.

These optimized structures were experimentally fabricated, and tailored emissive peaks were observed, albeit with a slight redshift and reduced peak emissivity due to deviations in layer thickness during fabrication. Nonetheless, the key features were successfully replicated, confirming the validity of the optimization process.

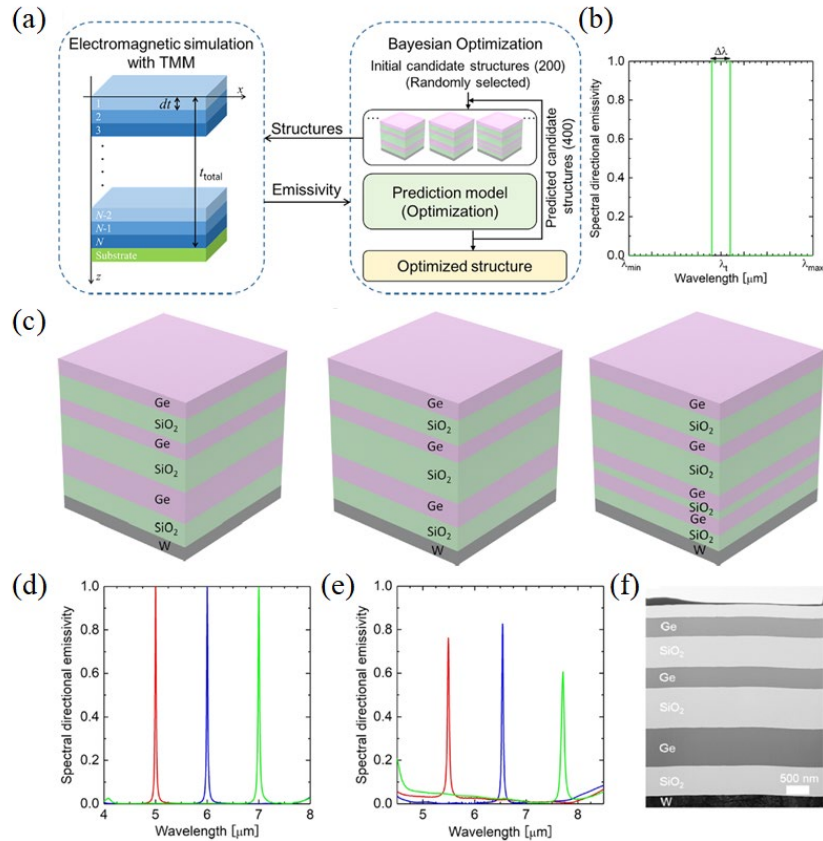


Fig. 7 (a) Schematic of the optimization method combining TMM and BO algorithm. (b) Schematic of the ideal optical property of a narrow-band thermal radiator. (c) Optimal structures of narrow-band thermal radiators at target wavelengths of 6.0, 5.0, and 7.0  $\mu\text{m}$ , respectively. (d) Calculated spectral directional emissivity of the optimal structure. (e) Measured spectral directional emissivity of the fabricated structure. (f) Cross-sectional TEM images of the fabricated sample at  $\lambda_t = 6.0 \mu\text{m}$  (Sakurai et al., 2019).

Further investigation of the optical properties of the optimized structures revealed that the enhanced emissivity originated from the localized modes within the Ge or SiO<sub>2</sub> layers, similar to the defect modes in photonic crystals. These localized modes are responsible for the sharp emissivity peaks and the suppression of higher-order harmonics, as shown in Fig. 8(a-c). The power dissipation analysis, depicted in Figs. 8(d-f), indicated that most thermal energy dissipation occurred in the metallic substrate, primarily due to optical losses, further validating the effectiveness of the optimized structures.

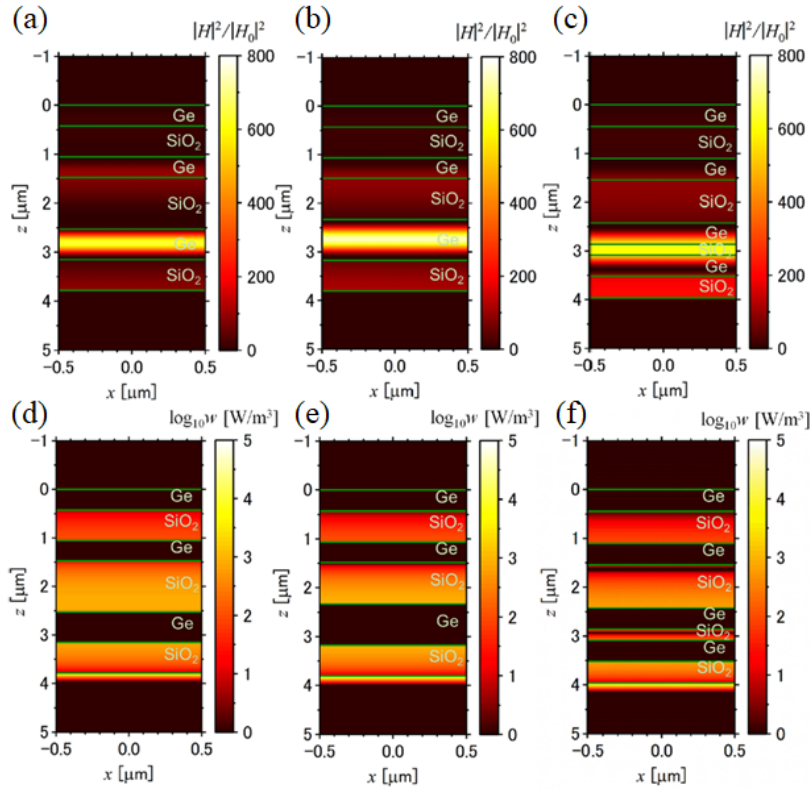


Fig. 8 Contour plots of the normalized magnetic field intensity (a–c) and power dissipation density (d–f) for target wavelengths of (a, d) 5.0  $\mu\text{m}$ , (b, e) 6.0  $\mu\text{m}$ , and (c, f) 7.0  $\mu\text{m}$  (Sakurai et al., 2019).

For sky radiators, we have applied MI design to complex structures using the rigorous coupled wave analysis (RCWA) method. Figure 9(a) shows the optimization of the material type and geometry of the grating structure (Guo et al., 2020). The optimal structure is shown in Fig. 9(b). The emissivity peaks of the optimal structure aligned well with the atmospheric transparent window, and its high emissivity remained robust against changes in the incident angle, as shown in Fig. 9(c). This enhancement in absorption was attributed to the excitation of the magnetic polariton resonance.

The dependence of the emissivity on the polar angle for p- and s-polarized incident waves is shown in Figs. 9(d) and 9(e). The p-polarized incident wave shows a significant increase in emissivity within the 8–11  $\mu\text{m}$  range, highlighting the role of the top grating structure in exciting phonon polaritons. Further analysis of the magnetic resonance shown in Fig. 9(f–i) reveals that strong magnetic dipoles appear at wavelengths corresponding to the emissivity peaks. As emissivity decreases, these magnetic dipoles become less concentrated, confirming that the absorption enhancement is related to magnetic polariton resonance.

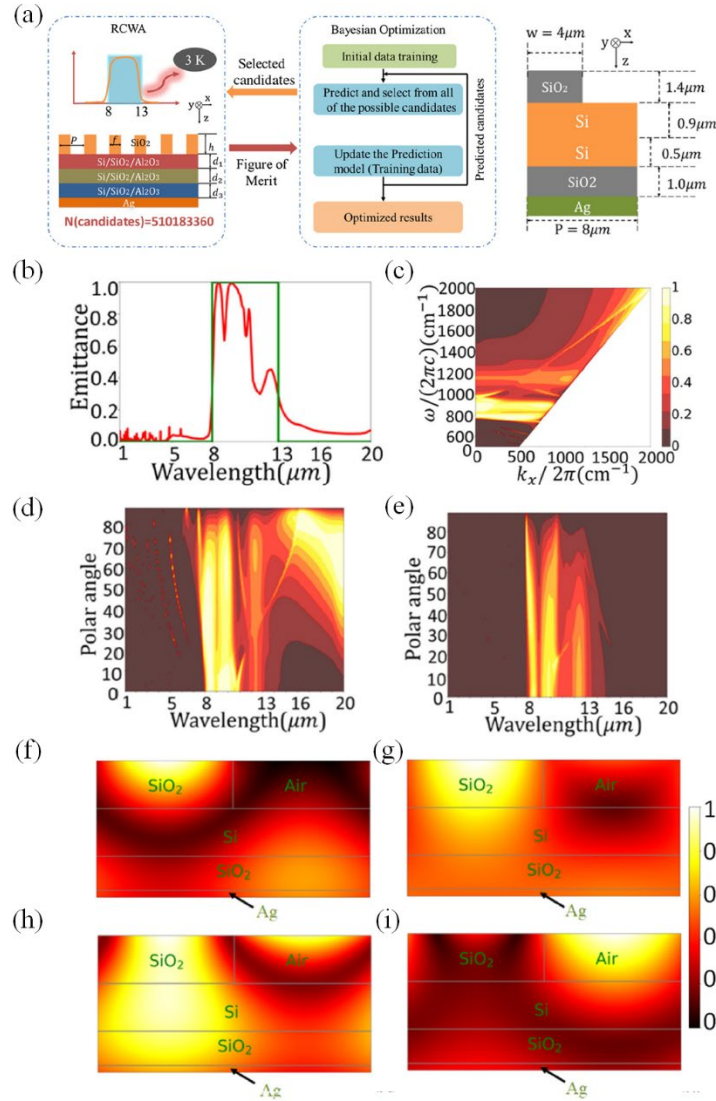


Fig. 9 (a) Schematic of the MI method based on RCWA coupled with the BO method. (b) Radiative properties of the optimal structure. (c) Emissivity dispersion of the optimal structure under  $p$ -polarized incident waves. Polar angle dependence of emissivity for  $p$ -polarized (d) and  $s$ -polarized (e) waves. Contour plot of normalized magnetic field for incident wavelengths of (f) 8.93  $\mu\text{m}$ , (g) 9.46  $\mu\text{m}$ , (h) 10.58  $\mu\text{m}$ , and (i) 10.82  $\mu\text{m}$ , respectively (Guo et al., 2020).

We also designed a two-dimensional structure, but as the degrees of freedom increased, we sought a more efficient means of optimizing through quantum annealers. By using quantum fluctuations, a quantum annealer enables an efficient optimization process to find the global minimum of a given objective function over a set of candidate solutions. However, the current implementation of QA machines involves solving combinatorial optimization problems represented in the quadratic unconstrained binary optimization (QUBO) format, making them unsuitable for surrogate-type optimization. Therefore, we developed a method that utilizes a factorization machine to convert the surrogate model into the QUBO format. This method, called factorization machine for quantum annealing (FMQA), can handle optimization problems with a large number of candidates (Kitai et al., 2020). A flowchart of the FMQA process is shown in Fig. 10(a).

The structure to be optimized was a block-stacking metamaterial (Fig. 10(b)) composed of SiO<sub>2</sub> and SiC wires embedded in poly(methyl methacrylate) (PMMA) arranged with a periodic boundary condition along the  $y$ -axis. The  $x$ - $z$  plane was divided into uniform units, each consisting of SiO<sub>2</sub>, SiC, or PMMA. The structure was encoded into binary sequences.

The FMQA algorithm efficiently optimized the FOM of the structure. As shown in Fig. 10(b), FMQA outperformed random search in finding a structure with a higher FOM after fewer iterations. Moreover, the efficiency of FMQA in terms of computing time is demonstrated in Fig. 10(c), where it outperformed exhaustive search methods, particularly

for larger structures, indicating its potential to overcome computational barriers in MI.

The optimization process revealed that structures with SiO<sub>2</sub> located at the top and bottom and SiC in the middle consistently exhibited high FOM. The effectiveness of this configuration was further analyzed by evaluating the electric power dissipation density, as shown in Fig. 10(f). The results indicated that SiO<sub>2</sub> layers dominate absorption in the lower wavelength band (8–11 μm), while the SiC layer absorbs most energy in the higher wavelength band (11–13 μm). Strong magnetic field confinement in the optimal structure correlates with high emissivity, confirming that the magnetic polariton resonance drives high emissivity in these structures.

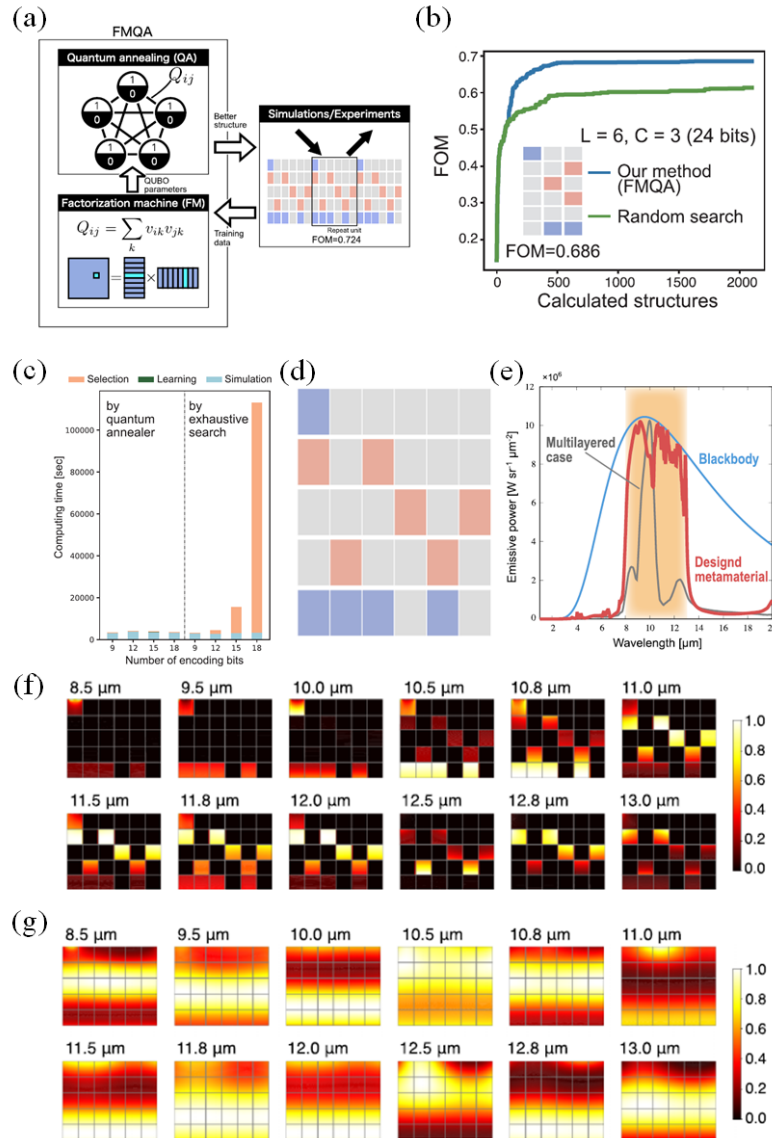


Fig. 10 (a) Schematics of the FMQA algorithm. (b) Best figure of merit as a function of the number of structures calculated (iterations) by FMQA using a quantum annealer and random search. (c) Comparison of computing time required to perform 500 iterations for automated materials discovery using exhaustive search and quantum annealer. (d) Optimal metamaterial structure, where blue, red, and gray squares denote SiO<sub>2</sub>, SiC, and PMMA, respectively. (e) Emissive power calculated by RCWA for the designed optimal structure, compared with the emissive power of a blackbody (blue line) and optimal structure with one column (gray line). Contour plots of (f) normalized electric power dissipation density and (g) normalized magnetic field for the optimal structure at selected wavelengths (Kitai et al., 2020).



## 5. Summary and perspectives

MI has emerged as a powerful tool for optimizing thermal materials with specific properties. Over the past several years, MI has been successfully applied to address a wide range of challenges in thermal management. However, several technical challenges remain to be overcome to advance this field further. They include issues related to scalability, computational complexity, the development of effective descriptors, and standardization and data integration, which were discussed in our previous review papers (Ju and Shiomi, 2019; Hu and Shiomi, 2021; Guo and Shiomi, 2024). Recently, we extended the MI approach to polymers, focusing on functionalizing them to enhance their thermal and dielectric properties. In polymer molding or compounding, the final properties are sensitive to processing parameters. Therefore, the above approach of sequentially connecting optimal design to experimental realization of materials is insufficient. To address this, we are developing a semi-automated MI system that integrates experimental fabrication and measurements directly into the optimization loop. This approach has enabled us to efficiently enhance the properties of polymer composites.

## Acknowledgement

I am deeply honored to receive the Nukiyama Memorial Award in 2022. I extend my sincere gratitude to the selection committee, my recommending professors, and the members of the Heat Transfer Society of Japan. The subject of the award is phonon engineering (the control of heat conduction using nanostructures and interfacial structures) using materials informatics. This award is not solely for me but also for the members of TEEL (past and present) and collaborators who have significantly contributed to this research.

The key elements of this research are ‘phonon engineering’ and ‘materials informatics,’ and I started working on the former in 2004. Phonon engineering involves controlling heat conduction by exploiting the quasi-ballistic or wave-like behavior of phonons on scales smaller than the mean free path or phase relaxation length. My journey began with analyzing quasi-ballistic heat conduction in relation to the kinetic theory of phonon particles during my tenure as a postdoctoral researcher and assistant professor in Prof. Shigeo Maruyama's laboratory. My early inspiration came from the advanced research on non-Fourier heat conduction by Prof. Nobuyuki Araki through heat propagation experiments and modeling as well as by Prof. Mitsuhiro Matsumoto through molecular dynamics simulations.

Initially, my focus was primarily on carbon nanotubes. However, during a sabbatical visit to Prof. Gang Chen's laboratory at MIT in 2010, my research expanded to thermoelectric materials and compound crystals. There, I was able to learn from Prof. Keivan Esfarjani (now a professor at the University of Virginia) the first-principles calculations, lattice dynamics and Green's function calculations. Around the same time, Prof. David Cahill at UIUC greatly influenced my work by teaching me nanoscale heat conduction measurement techniques.

Thanks to these experiences, I established TEEL in 2010, focusing on phonon engineering by integrating computational science, materials synthesis, and physical property measurements. This progress was made possible through the collaborative efforts of laboratory members such as Prof. Takuma Shiga (now at AIST), Prof. Takuma Hori (now at the University of Agriculture and Technology), Dr. Asuka Miura (now at Kyushu Institute of Technology), and others.

In 2015, Dr. Yibin Xu of NIMS invited me to participate in a project called the Materials and Information Integration Initiative (MI<sup>2</sup>I) of JST, which marked the beginning of my research on material informatics. Collaborations with researchers like Prof. Koji Tsuda at the University of Tokyo, Prof. Ryo Yoshida at the Institute of Statistical Mathematics, and other informatics researchers have since been pivotal in integrating thermal science with machine learning. I particularly recall the support of Professor Shenghong Ju (now at Shanghai Jiao Tong University) when we first began combining phonon computation and Bayesian optimization. Despite initial setbacks, including a referee dismissing our early work as meaningless, the methodology we proposed is now widely adopted.

This research has since expanded to include the development of design methodologies, experimental validations, exploration of other phenomena, industry–academia collaborations, and entrepreneurial ventures.

For these reasons, I (we) have been recognized with this award, and I sincerely thank everyone who has contributed to this journey.

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