Designing Nanostructures for Phonon Transport via Materials Informatics

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As the length scales of materials are reduced to nanoscale, it becomes possible to tune heat transport by manipulating the nanostructures. However, it is rather difficult to identify the detail optimal structure for heat conduction due to the various and coupled factors. The key next-generation technology here can be materials informatics, which is a new interdisciplinary research to provide efficient tools to accelerate the material discovery and design.

In this work, we developed a framework by combining the atomistic Green's function, Bayesian optimization and Monte Carlo tree search method to design nanostructures for phonon transport. The Bayesian optimization, which is good at dealing cases with limited number of candidates, was performed to design the Si/Ge interfacial structures that minimize/maximize the interfacial thermal conductance across Si-Si and Si-Ge interfaces, and the result indicates that the optimal structures were obtained by calculating only a few percent of the total candidates, considerably saving the computational resources. The Monte Carlo tree search, which can be applied to cases with huge or unlimited number of candidates, was performed to design Si/Ge rough interface and pillar structure to effectively enhancing and inhibiting phonon transport.

The present work has shown the effectiveness and advantage of materials informatics in designing nanostructures to control phonon transport, which can be extended to other nanostructures and properties.

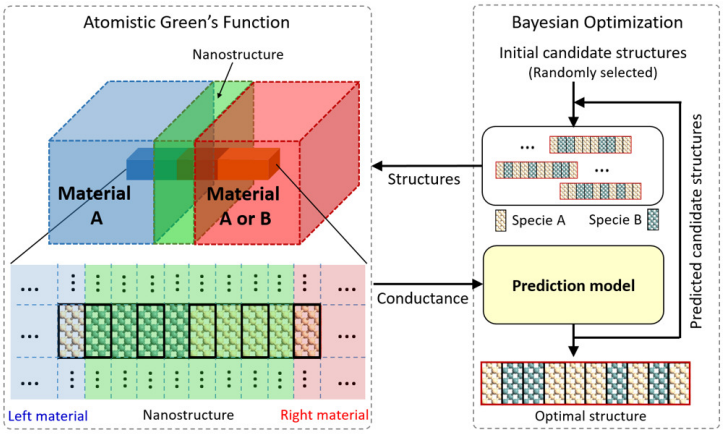

Fig. 1: Schematics of materials informatics method combing Atomistic Green's function and Bayesian optimization.

[1] S. Ju, T. Shiga, L. Feng, Z. Hou, K. Tsuda, and J. Shiomi, *Phys. Rev. X* **7**, 021024 (2017).