マテリアルズ・インフォマティクスによる伝熱機能材料の設計

Designing Thermal Functional Materials via Materials Informatics

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With the advances in materials and integration of electronics and thermoelectrics, the demand for novel crystalline materials with ultimate high/low thermal conductivity is increasing. However, search for optimal thermal materials is challenge due to the tremendous degrees of freedom in the composition and structure of crystal compounds and nanostructures, and thus empirical search would be exhausting. Materials informatics, which combines the simulation/experiment with machine learning, is now gaining great attention as a tool to accelerate the search of novel thermal materials.

In this work, we introduced our recent progresses (Fig. 1) in developing materials informatics method for designing thermal functional materials: the database screening and the nanostructure designing. For the database screening, we explored crystals with high thermal conductivity via feature-based screening and transfer learning, and we found novel crystals that have not been explored before in the sense of thermal conductivity, for example the carbon crystals with mixed phases of diamond and lonsdaleite, BC_2N, which have potential as alternative to diamond. For the nanostructure designing, we realized high efficiency nanostructure designing for high/low thermal conductance using the Bayesian optimization [1-2] and Monte Carlo tree search [3]. Those successful applications show that the materials informatics method are highly useful for designing thermal functional materials.

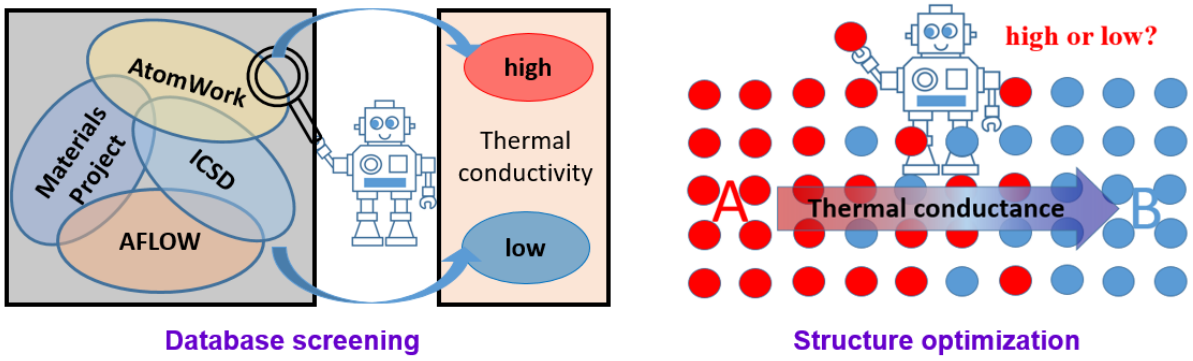

Fig. 1. Application of materials informatics on designing thermal functional materials: (a) database screening and (b) structure optimization.

References

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