Materials informatics using effective Hamiltonians

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Research Area : Advanced Materials Informatics through Comprehensive Integration among Theoretical, Experimental, Computational and Data-Centric Sciences（PO：Shinji Tsuneyuki）

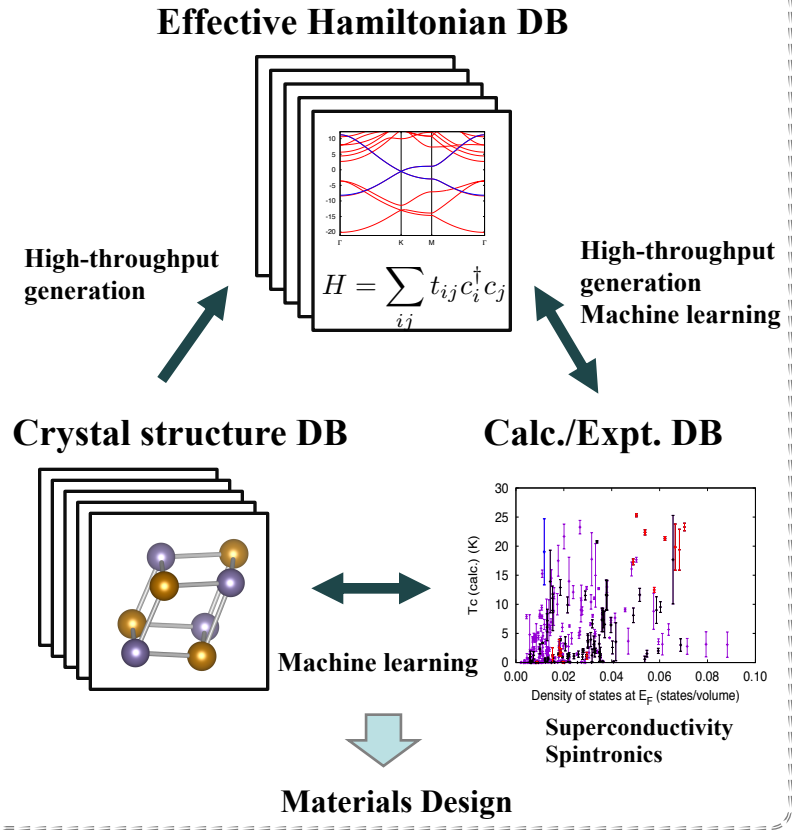
Brief overview

To study the physical properties of materials, effective Hamiltonian approach has been often employed. Using effective Hamiltonians, calculations become easier and it is possible to discuss the physical properties of several materials systematically. Recently, it has become possible to create the effective Hamiltonians quantitatively by first-principles calculations. On the other hand, to utilize the data science approach, several crystal structure databases and electronic structure databases have been developed. Therefore, to combine the conventional effective Hamiltonian approach and the data science approach and to establish a new route to design functional materials, we create an effective Hamiltonian database from the first-principles calculations.

Achievement

First, we develop a high-throughput method to calculate a tight-binding Hamiltonian from first-principles calculations. A part of the implementation is included in the latest Wannier90 code[1]. We also implement a high-throughput method to obtain the electron-phonon couplings to discuss superconductivity[2].

For magnetic materials, we obtain a spin current formula to calculate the Dzyaloshinkii-Moriya interaction[3,4] and apply the method to the database of tight-binding Hamiltonians. The relation between these databases of effective Hamiltonians and calculated physical quantities are discussed using machine-learning techniques. These findings will play a key role for future materials design.



Reference/Link

[1] http://www.wannier.org
[2] T. Koretsune and R. Arita, Comp. Phys. Comm. **220C** 239 (2017)
[3] T. Kikuchi, T. Koretsune, R. Arita, G. Tatara, Phys. Rev. Lett **116** 247201 (2016)
[4] T. Koretsune, T. Kikuchi and R. Arita, J. Phys. Soc. Jpn. **87** 041011 (2018)