物性研究所セミナー

標題：Benchmark of density functional theory for superconductors
日時：2020 年 6 月 9 日(火)　午後 4 時～午後 5 時
場所：ZOOM 開催
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要旨：

The first-principle calculation of the superconducting properties, such as the transition temperature (Tc) is of great interest to explore new materials as well as to understand the mechanism of known superconductor. Density functional theory for superconductors (SCDFT) is one of the frameworks for such calculations; this method enables us to perform fully non-empirical simulation in the superconducting phase within reasonable computational cost. In this method, we can treat the electron-phonon interaction, the electron-electron repulsion, and the spin-fluctuation (SF) mediated interaction in a first-principles manner. However, the accuracy of the current approximated functional of SCDFT has not been verified systematically, although such verification is highly desirable before we apply this method to the wide range of materials.

For this purpose, we performed systematic benchmark calculations for elemental bulks [1]. We developed a method to treat the spin-orbit interaction (SOI) together with SF and examined their effect on Tc. We found the following results: (1) The calculations, including SOI and SF, reproduce the experimental Tc quantitatively. (2) The effect by SOI is small excepting a few elements such as Pb, Tl, and Re. (3) SF reduces Tcs, especially for the transition metals, while this reduction is too weak to reproduce the Tcs of Zn and Cd. (4) We reproduced the absence of superconductivity for alkaline (earth) and noble metals. These calculations confirm that our method can be applied to a wide range of materials and implies a direction for the further improvement of the methodology.

[1] M. Kawamura, Y. Hizume, and T. Ozaki, Phys. Rev. B 101, 134511 (2020).