First-principles calculation of superconducting properties: T_c and H_c

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Superconductivity, in which the electrical resistance of metals vanishes at extremely low temperatures, is an interesting phenomenon in which quantum effects appear on a macroscopic scale and has unique applications, such as in quantum computers, superconducting magnets, and magnetic sensors. First-principles calculation will be helpful to design new superconducting materials, by predicting superconducting properties such as transition temperature (T_c) and critical magnetic field (H_c), above which superconductivity disappears.

Density functional theory for superconductors (SCDFT) is an extension of conventional DFT by including superconducting singlet order parameter as a "density," which can treat electron-phonon interaction, Coulomb repulsion, and spin-fluctuation fully non-empirically. We developed an open-source program superconducting-toolkit (SCTK) based on SCDFT and applied it to all elemental materials[1], quartanary hydride superconductors[2]. We recently formulated a first-principles method to compute the superconducting coherence length ξ_0 related to the upper critical field H_{c2} as

$$H_{c2} = \frac{\Phi_0}{2\pi\xi_0^2},$$

where Φ_0 is the quantized flux unit $h/(2e)$. We performed a benchmark calculation of this method for elements and compound systems, as shown in the table below. We expect that the overestimation (underestimation) of ξ_0 comes from the underestimation (overestimation) of the T_c.

	Al	Nb	Sn	In	Ta	Pb	V_3Si
Exp. T_c [K]	1.18	9.1	3.7	3.4	4.5	7.2	17
Calc. T_c [K]	1.9	8.2	4.2	3.3	4.6	5.6	21
Exp. ξ_0 [nm]	1300~1600	38~40	94~230	275~440	93	51~90	3
Calc. ξ_0 [nm]	523	31	122	227	76	102	2.1

References

1. Kawamura, M; Hizume, Y; Ozaki, T, Phys. Rev. B, **2020**, 101, 134511.
2. Koshoji, R, Fukuda, M, Kawamura, M; Ozaki, T, Phys. Rev. Materials, **2022**, 6, 114802.