

First-principles calculations of the coherence length and magnetic penetration depth based on superconducting density functional theory

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Predicting superconducting length scales from microscopic theory has remained a long-standing challenge despite major progress in first-principles calculations of superconducting transition temperatures. We present a unified framework within superconducting density functional theory that incorporates finite-momentum Cooper pairs [1] and enables parameter-free calculations of the coherence length and magnetic penetration depth. Applications to elemental superconductors, V₃Si, and high-pressure H₃S show good agreement with experiments. The approach allows the Uemura plot to be reproduced entirely from first principles, providing a microscopic interpretation of the empirical T_c –Fermi temperature correlation and establishing a predictive link between electronic structure and superconducting electrodynamics [2].

	Al	Nb	Sn	In	Ta	Pb	V ₃ Si	H ₃ S
Exp. T_c [K]	1.14	9.5	3.72	3.4	4.48	7.19	17	184
Calc. T_c [K]	1.6	8.1	4.0	3.1	4.4	5.3	21	181
Exp. ξ [nm]	1600	38~40	230	260	93	90	4	2.0
Calc. ξ [nm]	636	34	132	254	80	104	2.2	3
Exp. λ [nm]	16	27~39	34	30	52	37	90	20-37
Calc. λ [nm]	21	34	43	28	33	22	97	19

Fig. 1: Comparison of the calculated T_c , coherence length, and magnetic penetration depth with experimental values. V₃Si, H₃S and Nb are type-II superconductors, whereas the others are type-I superconductors.

[1] N. Witt, Y. Nomura, S. Brener, R. Arita, A.I. Lichtenstein, T.O. Wehling, “Bypassing the lattice BCS-BEC crossover in strongly correlated superconductors through multiorbital physics”, npj Quantum Materials volume **9**, 100 (2024)

[2] M. Kawamura, T. Nomoto, N. Witt, R. Arita, “First-principles calculation of coherence length and penetration depth based on density functional theory for superconductors”, arXiv:2603.05123, to appear in Phys. Rev. Lett.