Density functional theory for superconductors and its application to layered nitride superconductors

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Recently, Gross *et al.* formulated a new scheme based on density functional theory for superconductors (SCDFT) [1]. There, by solving the gap equation derived from the Kohn-Sham Bogoliubov-de Gennes equation, we can estimate the superconducting transition temperature (T_c) without introducing any adjustable parameters. It has been shown that SCDFT reproduces successfully the experimental T_c of various conventional superconductors, such as simple metals[1], MgB_2[2], and CaC_6[3].

In this talk, I will first review SCDFT and discuss how the retardation effect and the mass renormalization effect in the standard Migdal-Eliashberg (ME) theory are taken into account. Since SCDFT gives essentially the same result as that of the ME theory, we can use SCDFT to determine whether the pairing mechanism is the conventional ME type or not. In the second part of my talk, I will introduce our recent SCDFT study for nitride superconductors [4], and demonstrate how SCDFT can be used for this purpose.

In late 90's, Yamanaka *et al.* discovered high T_c superconductivity in layered nitrides β-MNCl (M=Zr, Hf) [5]. The parent compound is a band insulator with a band gap of a few eV, and it becomes a superconductor upon doping electrons. The maximum T_c is ~26K for the HfNCl-based system, which had been the second highest record among transition-metal compounds until the recent discovery of superconductivity in the iron-based superconductors. Although the pairing mechanism of the nitride superconductors is of great interest, it is yet to be fully understood. While several experiments suggest that the pairing gap function is a fully-gapped s-wave, there are also many experimental indications suggesting unconventional pairing mechanism.

In this talk, I will show that T_c estimated by SCDFT is at maximum half of the experimental T_c and its doping dependence is opposite to the experiments. These results suggest that we need to go beyond the ME theory to clarify the pairing mechanism of β-MNCl [4].

References:
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