Mechanism of high Tc superconductivity in layered nitride superconductors: Insights from DFT for superconductors

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Since the seminal discovery of high T_c cuprates, superconductivity in layered transition-metal compounds have been a subject of extensive research. In late 90's, Yamanaka *et al.* discovered superconductivity in layered nitrides β-*M*NCl (*M*=Zr, Hf) by intercalating alkali-metal atoms.[1] The maximum superconducting transition temperature (T_c) is ~15 K for the ZrNCl-based system and ~26K for the HfNCl-based system. In fact, T_c for the latter had been the second highest among transition-metal compounds until the recent discovery of superconductivity in the iron-based superconductors.

The mother compound is composed of alternate stacking of honeycomb *M*N bilayer and Cl_2 block layer. This is a band insulator having a band gap of a few eV, and becomes a superconductor upon doping electrons. As for the pairing mechanism, it has been an issue of hot debates: 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.

Recently, density functional theory for superconductors (SCDFT) has been formulated and extensively applied to various conventional superconductors. While SCDFT contains no adjustable parameter such as μ*, it has been shown that it can reproduce experimental T_c very accurately.[2] Thus SCDFT can be used as a litmus paper to determine whether the pairing mechanism is conventional or unconventional.

In this talk, I will present the result of our recent SCDFT calculation for β-*M*NCl, which strongly suggests that the pairing mechanism is unconventional.

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References:

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