Density Functional Theory for Plasmon-Assisted Superconductivity: Development and Its Applications

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One of the most fascinating goals in the studies of superconductivity is the predictive calculation of superconducting transition temperatures ($T_c$). For a conventional phonon-induced superconducting mechanism, a predictive first-principles scheme is established by the recent progress in the density functional theory for superconductors (SCDFT) (Lueders et al., PRB 2005); the current SCDFT-based scheme systematically reproduces $T_c$ observed by experiments in the conventional systems such as niobium and MgB$_2$, with discrepancies no more than a few kelvin. However, further extensions to include other mechanisms are imperative to treat more general materials.

Recently, there has been substantial progress in this issue. Gross and coauthors have developed an extended scheme to incorporate the pairing mediated by spin fluctuations (Essenberger et al., PRB 2014). On the other hand, we have addressed the plasmon mechanism of superconductivity (Akashi and Arita, PRL 2013). This mechanism is expected to be relevant in a wide range of systems because it can cooperate with the conventional phonon mechanism. Our extended scheme enables us to evaluate the effects on $T_c$ of the plasmon and phonon mechanisms on equal footing.

In the presentation, we introduce its formulation and recent applications to Li and sulfur hydride under pressure.