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Density functional theory for plasmon-assisted superconductivity RYOSUKE AKASHI, Department of Applied Physics, University of Tokyo, RY-OTARO ARITA, Department of Applied Physics, University of Tokyo; PRESTO — The predictive calculation of superconducting transition temperatures (Tc) is a fascinating but extremely difficult problem in the field of superconductivity. For a conventional phonon-induced superconducting mechanism, an accurate predictive scheme to calculate Tc is established by the recent progress in the density functional theory for superconductors (SCDFT) [Lueders et al., PRB 72, 024545 (2005); Marques et al., PRB 72, 024546 (2005)]; the current SCDFT-based scheme systematically reproduces Tc observed by experiments in the conventional systems such as niobium and MgB2, with discrepancies no more than a few kelvin. However, further extensions including other mechanisms are essential to treat more general materials. Recently, we extended the SCDFT-based scheme to include a plasmon mechanism of superconductivity [Akashi and Arita, PRL 111, 057006 (2013)]. The plasmon mechanism, which has been considered solely in rather dilute electron systems, is also expected to be relevant in a wider range of materials because it can cooperate with the conventional phonon mechanism. Our extended scheme enables us to evaluate the effects on Tc of the plasmon and phonon mechanisms on equal footing. In the talk, we present recent applications to elemental metals.

> Ryosuke Akashi Department of Applied Physics, University of Tokyo

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