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Reduction of superconducting transition temperature by spin fluctuations in elemental transition metals: first-principles study KEN-TARO TSUTSUMI, Dept. of Phys., Univ. of Tokyo, MITSUAKI KAWAMURA, ISSP, RYOSUKE AKASHI, Dept. of Phys., Univ. of Tokyo, SHINJI TSUNEYUKI, Dept. of Phys., Univ. of Tokyo and ISSP — Effects of spin fluctuations(SF) in superconductors are mainly discussed in the context of the origin of a possible pairing interaction in unconventional superconductors. However, the SF effect is also crucial in conventional phonon-driven superconductors. Ferromagnetic fluctuations driven by the exchange effect are relevant in many metals in which electrons are nearly homogeneous and they can suppress the singlet pairing. So far, there are some efforts to include this SF effect in the Eliashberg theory in case of transition metals, e.g. Nb and V(H. Rietschel and H. Winter, Phys. Rev. Lett. 43, 1256(1979)). On the other hand, non-empirical calculations on this effect are lacking. We used the recently developed extended version of density functional theory for superconductors(M. Lueders et al., Phys. Rev. B 72, 024545 (2005)) including the SF effect(F. Essenberger et al., Phys. Rev. B 90, 214504 (2014)) and explored the SF effect on T_c of V, Nb and Al from first-principles. We show that the SF effect commonly reduces the T_c of transition metals and the amount of its reduction is correlated with the magnitude of electronic localization.

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