# First-principles study of the Mott transition and superconductivity in $A_3C_{60}$

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Doped fullerides $A_3C_{60}$ (A=alkali metal), which turn superconducting with a maximum transition temperature ($T_c$) of $\sim$ 40K, have attracted increasing attention. As for the pairing mechanism, the validity of the standard Migdal-Eliashberg theory has been questioned[1]. In *ab initio* calculation based on superconducting density functional theory[2], which works successfully for conventional superconductors, $T_c$s are estimated less than half of the experimental value[3].

In 2002, the emergence of phonon-driven superconductivity close to the Mott transition [strongly correlated superconductivity (SCS)] was proposed[4]. The key of this proposal is the presence of a weak phonon-driven attraction in the form of an inverted Hund's rule coupling, which is not renormalized by the strong short-range repulsion. However, the interacting parameters in the Hamiltonian are yet to be evaluated from first principles.

Recently, we developed an *ab initio* downfolding scheme, which we call "constrained density-functional perturbation theory" [5], to derive the electron-phonon coupled effective Hamiltonian. We applied this method to $C_{60}$ superconductors, and found that the magnitude of the phonon-mediated exchange interaction $J_{\rm ph}$ is $\sim$ 0.05 eV. By the constrained random phase approximation[6], we also estimated the electron-electron interactions such as Hubbard $U$, distant Coulomb repulsions $V$, and the Hund's coupling $J_{\rm H}$[7]. We find that $J_{\rm H}$ is $\sim$ 0.035 eV ($< J_{\rm ph}$), which suggests that SCS is indeed realized in doped $C_{60}$ superconductors.

By means of extended dynamical mean field theory[8], we then solved the resulting effective low energy model, where we consider the anomalous Green's function. We calculated $T_c$ as a function of the volume of the unit cell. We also determined the phase boundary between the metallic phase and the Mott insulating phase. We show that the obtained phase diagram agrees well with the experiment quantitatively[9].

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