The Mechanism of the Intramolecular Diamagnetic Supercurrents and Its Application to the Realization of Room Temperature Superconductivity

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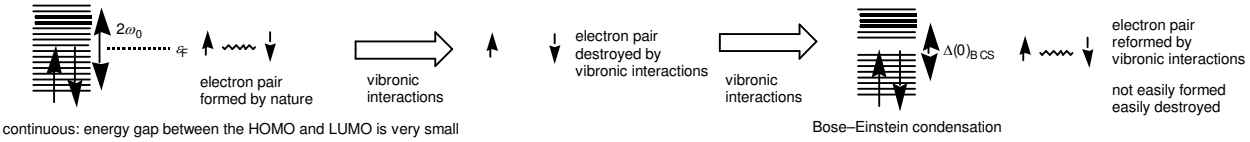
We suggest more general theory than the BCS theory in order to elucidate the relationships between the intramolecular diamagnetic supercurrents at 298 K in microscopic sized π-conjugated hydrocarbons such as benzene and polyacenes and the conventional superconductivity at low temperatures in bulk systems [1], which have not been elucidated for about 100 years. According to our calculations, intramolecular diamagnetic supercurrents in microscopic sized π-conjugated hydrocarbons are induced by electron pairing as a consequence of Coulomb interactions (electron–phonon interactions can be neglected). The estimated critical supercurrent temperatures (T_c) for microscopic sized π-conjugated hydrocarbons are much larger (10^4~10^5 K) than those for the macroscopic sized conventional superconductivity (10^0~10^2 K). This is because the stabilization energy ($\Delta(0)_{BCS}$) as a consequence the electron–phonon interactions are very small (10^0~10^2 K) in the conventional superconductivity (Figure), on the other hand, the HOMO–LUMO gaps, the physical meaning of which is similar to that of $\Delta(0)_{BCS}$ in the conventional superconductivity, are very large (10^4~10^5 K) in microscopic sized π-conjugated hydrocarbons. However, the HOMO–LUMO gap decreases with an increase in molecular size and thus the electron–phonon interactions cannot be neglected in macroscopic sized π-conjugated hydrocarbons. Therefore, the T_c values for the macroscopic sized π-conjugated hydrocarbons would be very low (10^0~10^2 K). However, we can expect that the bulk materials, the energy gaps between the occupied and unoccupied orbitals of which are very large (i.e., more than 4 eV), such as very pure diamonds with no impurities, have a possibility to exhibit room temperature macroscopic supercurrents [1(d)].

The role of the electron–phonon interactions in the conventional superconductivity



[1] (a) T. Kato, *Chemical Physics Research Journal* (Nova Science Publishers Inc., New York, 2007); (b) T. Kato and T. Yamabe, Synth. Met. 157 (2007) 793; (c) T. Kato and T. Yamabe, J. Phys. Chem. A 111 (2007) 8731; (d) T. Kato, Chem. Phys. 345 (2008) 1; (e) T. Kato, J. Phys. Chem. C 113 (2009) 402.