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ON THE MOTT TRANSITION AND THE NEW METAL-INSULATOR TRANSITIONS IN DOPED COVALENT AND POLAR CRYSTALS

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Abstract

The Mott transition and new metal-insulator transitions (MIT's) and their distinctive features in doped covalent semiconductors and polar compounds are studied within the continuum model of extrinsic carrier self-trapping, the Hubbard impurity band model (with on-site Coulomb repulsion and screening effects) and the extrinsic (bi)polaronic band model (with short- and long-range carrier-impurity, impurity-phonon and carrier-phonon interactions and intercarrier correlation) using the appropriate tight-binding approximations and variational methods. We have shown the formation possibility of large-radius localized one- and two-carrier impurity (or defect) states and narrow impurity bands in the band gap and charge transfer gap of these carrier-doped systems. The extrinsic Mott-Hubbard and (bi)polaronic insulating gaps are calculated exactly. The proper criterions for Mott transition, extrinsic excitonic and (bi)polaronic MIT's are obtained. We have demonstrated that the Mott transition occurs in doped covalent simiconductors (i.e. Si and Ge) and some insulators with weak carrier-phonon coupling near the large-radius dopants. While, in doped polar compounds (e.g. oxide high-T_c superconductors (HTSC) and related materials) the MIT's are new extrinsic (or intrinsic) (bi)polaronic MIT's. We have found that the anisotropy of the dielectric (or (bi)polaronic) properties of doped cuprate HTSC is responsible for smooth (or continuous) MIT's, stripe formation and suppression of high-T_c superconductivity. Various experimental results on in-gap states, bands and MIT's in doped covalent semiconductors, oxide HTSC and related materials are in good agreement with the developed theory of Mott transition and new (bi)polaronic MIT's.

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1 Introduction

The doped semiconductors and insulators possess exceptional electronic properties [1-13]. At some doping level they show the metallic behaviour. The origin and the nature of the metal-insulator transitions (MIT's) in doped systems is still poorly understood, although the MIT's in doped semiconductors and insulators were expreimentally and theoretically studied during the last decades. The conventional Wilson band formalism [1,3,4,11], Mott-Hubbard model [1-5,10,11] and the Anderson localization model [1-5,12,14] have been widely used for decades in describing the MIT's both in undoped and in doped systems. Apparently, the MIT's in doped compounds are quite different from those in undoped systems [13,15-19]. Experiments on doped oxide high-T_c superconductors (HTSC) and other systems [6-8,10,20] have shown that the MIT's in these materials are not always correlation- and disorder-induced transitions. Therefore, the problem of MIT's in these doped systems is one of central issues in condensed matter physics. This problem is closely related to high-T_c supreconductivity in underdoped HTSC [11,13]. As these HTSC are well known to be close to a MIT. The insulating state of undoped covalent crystals, such as, Si and Ge is described by the Wilson (i.e. one-electron) band model, while the insulating state of undoped transition metal oxides (including also HTSC) with partially filled d-bands is described by the conventional Mott-Hubbard band model. According to the Mott-Hubbard band model the MIT occurs at $U \geq W$, where U is the Coulomb repulsive energy between the two electrons on the same lattice site, W is the overall electronic bandwidth. The Mott criterion for MIT (or critical density $n = n_c$ of the hydrogen-like atoms) is given by

$$n_c^{1/3} a_H \simeq 0.25, \tag{1}$$

where a_H is the Bohr radius of the hydrogen-like atoms. The Mott-Hubbard band model is also applicable for description of the splitting of the half-filled impurity band into the so-called lower and upper Hubbard bands in the energy gap of doped insulators and semiconductors. In particular, in case of n-type Si and Ge the critical doping value n_c determined from the Mott criterion (1) is close to the observed doping value for the MIT. However, in case of p-type semiconductors the n_c determined from (1) does not consistent very well with the observed doping level for the MIT (see [1]). The divergence of the Mott criterion (1) from the observed doping value for the MIT is especially noticeable in doped oxide HTSC. Indeed, the Mott criterion (1) predicts a critical doping value $x_c = n_c/n_0$ (where n_0 is the density of the host lattice atoms) which is much lower than the observed critical doping $x_c = 0.02$ for destruction of the long-range antiferromagnetic (AF) order in oxide HTSC [6,7,10,11]. While the MIT in these systems occurs at more higher doping level $x_c = 0.05 \div 0.07$ [6-8,10,11,21]. As is generally known the proper criterion for Anderson transition in terms of $n_c^{1/3} a_H$ is not obtained yet. Mott and Davis [1] have roughly derived the criterion of such a MIT in the form

$$n_c^{1/3} a_H \sim 0.1. \tag{2}$$

The serious difficulties appear in the quantitative description of the MIT and the so-called ε_2-conductivity in doped covalent semiconductors [2]. Althouth much theoretical effort has been devoted to examining these questions (see [1,2]), the situations are still unclear and the quantitative theory of Mott transition in doped systems is not elaborated yet in any complete form. In particular, the energy gap between lower and upper Hubbard impurity bands has not been determined yet properly [11]. Further, many experiments show [1] that in doped semiconductors the MIT occurs when $n = n_c$ at which the impurity band is separated by some energy gap from the conduction or valence band. This energy gap vanishes at more higher doping level. The quantity of such as energy gap should be also determined properly. So far, the (bi)polaronic effects characteristic for any polar compounds are not included in the above models of the MIT's (see also [11]). In principle, the carrier localization transitions due to coupling to the lattice degrees of freedom (intrinsic (bi)polaronic effects) are the new MIT's [18]. The second issue is the extrinsic (bi)polaronic effects [19] which are particularly important for doped HTSC and related materials. This issue deserves exploration in more detail. In this work, we study the possibility of the Mott transition and other new extrinic (bi)polaronic MIT's and their distinctive features in doped covalent and polar crystals. We begin with the continuum model of extrinic carrier self-trapping [22] taking into account the short- and long-range carrier-defect, carrier-phonon and defect-phonon interactions and the intercarrier correlation. We demonstrate that the extrinsic single particle and pair self-trapping of carriers lead to the formation of one- and two-carrier localized in-gap states in the doped systems. We focus on the formation possibility of large-radius hydrogen-like and non-hydrogen-like in-gap states in the absence and presence of the extrinsic (bi)polaronic effects, respectively. We present a physical motivation for the formation of in-gap Hubbard impurity bands and extrinsic (bi)polaronic bands. Our calculations of the ground state energies of one- and two-carrier impurity centers, the Mott-Hubbard gap and the extrinsic (bi)polaronic energy gaps are based on the variational methods, the adiabatic and tight-binding approximations. We propose proper criterions for Mott transition, excitonic and extrinsic (bi)polaronic MIT's in doped systems.

2 The extrinsic single particle and pair self-trapping of carriers

In insulators and semiconductors upon doping with donor or acceptor impurities, the additional carriers with effective mass m^* appear in the conduction or valence band. Later on these carriers can be trapped by impurity (or defect) potential. We calculate the ground state energies of interacting one carrier-impurity-phonon and two carrier-impurity-phonon systems within the continuum model of extrinsic carrier self-trapping [22] in covalent and polar crystals depending on the character of the carrier-impurity, impurity-phonon and carrier-phonon interactions and intercarrier correlation. In covalent compounds, such as, Si and Ge the short-range impurity-phonon and carrier-phonon interactions are present. While in polar crystals both short- and long-range impurity-phonon and carrier-phonon interactions coexist. In this respect, the polar compounds can be considered as a more general case.Then the total energies of one- and two-carrier impurity centers in the continuum model and adiabatic approximation will be given by functionals depending on the lattice deformation described by the elastic dilation $\Delta(r)$, the lattice polarization described by the electrostatic potential $\phi(r)$, and the one- and two-electron wave functions. In particular, the total energy of the one-carrier impurity center is given by [21].

$$E_1(\psi,\Delta,\phi)=\int\psi(r)\left[\frac{-\hbar^2}{2m^*}\nabla^2+V_{sD}\delta(r)-\frac{Ze}{\varepsilon_\infty r}\right]\psi(r)d^3r+$$
$$+\int\left[E_d\psi^2(r)+E_{dD}\delta(r)\right]\Delta(r)d^3r+\int\left[(-e)\psi^2(r)+Ze\delta(r)\right]\phi(r)d^3(r)+$$
$$+\frac{K}{2}\int\Delta^2(r)d^3r+\frac{\tilde{\varepsilon}}{8\pi}\int(\nabla\phi(r))^2d^3r, \qquad (3)$$

where $\psi(r)$ is the one-electron wave function, V_{sD} is the short-range defect potential, Ze is the charge of a defect, ε_∞ is the high frequency dielectric constant, E_d and E_{dD} are the deformation potentials of a carrier and a defect, respectively, K is an elastic constant, $\tilde{\varepsilon}^{-1}=\varepsilon_\infty^{-1}-\varepsilon_0^{-1}$, ε_0 is the static dielectric constant.

The total energies of the two-carrier impurity center can be calculated with and without inclusion of the intercarrier correlation in the continuum theory of extrinsic carrier self-trapping. In order to obtain general expressions for this energy amenable to analytic analysis, first we ignore the effect of such a correlation on the carrier-lattice interactions, the kinetic energies of carriers and the intercarrier Coulombic repulsion. Then the total energy of the two-carrier impurity center $E_2(\Psi,\Delta,\phi)$ (where $\Psi(r_1,r_2)=\psi(r_1)\psi(r_2)$) is given by simply doubling the terms with $\psi(r)^2$ in Eq.(1) and adding the intercarrier Coulomb repulsion energy in the form:

$$\int\int\psi^2(r_1)\frac{e^2}{\varepsilon_\infty|r_1-r_2|}\psi^2(r_2)d^3r_1d^3r_2 \qquad (4)$$

The functionals $E_1(\psi,\Delta,\phi)$ and $E_2(\Psi,\Delta,\phi)$ after minimizing first with respect to Δ and ϕ and then with respect to a trial wave function choosen in the simple form [21] $\psi(r)=(\alpha\sqrt{2}/a_0)^{3/2}exp\left[-\pi(\alpha r/a_0)^2\right]$ have the forms

$$E_1(\alpha)=B[\alpha^2-g_s\alpha^3-g_l\alpha] \qquad (5)$$

and

$$E_2(\alpha)=2B[\alpha^2-G_s\alpha^3-G_l\alpha], \qquad (6)$$

respectively, where $B=3\pi\hbar^2/2m^*a_0^2$, $g_s=g_{sL}(1+b_s)$, $g_l=g_{lL}(1-\eta+\eta b_l)$, $G_s=g_{sL}(2+b_s)$, $G_l=g_{lL}(1-2\eta+\eta b_l)$, $g_{sL}=E_d^2/2Ka_0^2B$, $g_{lL}=e^2/\varepsilon_\infty a_0B$, $b_s=2^{5/2}[(E_{dD}/E_d)-(KV_{sD}/E_d^2)]$, $b_l=2^{3/2}Z$, $\eta=\varepsilon_\infty/\varepsilon_0$, α is the variational parameter characterizing the localization degree of a carrier, a_0 is the lattice constant.

When $g_l<2-3g_s$, $3g_sg_l<1$ and $G_l<2-3G_s$, $3G_sG_l<1$, the functionals (5) and (6) have the minimums at $\alpha_D=[1-\sqrt{1-3g_sg_l}]/3g_s$ and $\alpha_D=[1-\sqrt{1-3G_sG_l}]/3G_s$, respectively.

These minimums of the functionals $E_1(\alpha)$ and $E_2(\alpha)$ corresponding to the formation of large-radius $a_D > a_0$ delocalized (D) (shallow or nearly deep) impurity states are determined from the relations [23,24]

$$E_1(\alpha_D) = \frac{B}{27g_s^2}[2 - 9y_1 - 2(1 - 3y_1)^{3/2}] \tag{7}$$

and

$$E_2(\alpha_D) = \frac{2B}{27G_s^2}[2 - 9y_2 - 2(1 - 3y_2)^{3/2}] \tag{8}$$

respectively, where $y_1 = g_s g_l$ and $y_2 = G_s G_l$.

When $g_l > 2 - 3g_s$ and $G_l > 2 - 3G_s$, the functionals (3) and (4) have other minimums at $\alpha = \alpha_L \simeq 1$ corresponding to the formation of nearly small-radius localized (L) impurity states. Such minimums of the functionals $E_1(\alpha)$ and $E_2(\alpha)$ can be also determined roughly by the continuum model.

Now using the two-electron trial wave function $\Psi(r_1, r_2) = N[1+\beta(\sigma r_{12})^2]exp\{-\sigma^2(r_1^2+r_2^2)\}$ with electron correlation ($\beta \neq 0$), we obtain the following functional for the total energy of the two-carrier impurity center

$$E_2(\alpha, \beta) = 2B\frac{c_1(\beta)}{c_2(\beta)}[\alpha^2 - G_s(\beta)\alpha^3 - G_l(\beta)\alpha] \tag{9}$$

where $N = (\sqrt{2}\alpha/a_0)^{3/2}/\sqrt{c_2(\beta)}$, $\sigma = \sqrt{\pi}\alpha/a_0$, r_{12} is the relative distance between the carriers having the coordinates r_1 and r_2,

$$G_s(\beta) = g_{SL}[\frac{2c_3(\beta)}{c_1(\beta)c_2(\beta)} + \frac{c_4(\beta)b_s}{c_1(\beta)}],\ G_l(\beta) = g_{lL}[\frac{c_5(\beta)}{c_1(\beta)c_2(\beta)} + \frac{c_6(\beta)b_l}{eta/c_1(\beta)} - \frac{c_7(\beta)2eta}{c_1(\beta)c_2(\beta)}],$$

$c_1(\beta) = 1 + 2\beta + 13\beta^2/4$, $c_2(\beta) = 1 + 3\beta + 15\beta^2/4$, $c_3(\beta) = 1 + 9\beta/2 + 309\beta^2/32 + 1395\beta^3/128 + 23754\beta^4/4096$, $c_4(\beta) = 1+3\beta/2+15\beta^2/16$, $c_5(\beta) = 1+6\beta+261\beta^2/16+1437\beta^3/64+28185\beta^4/2048$, $c_6(\beta) = 1 + 5\beta + 35\beta^2/4$, $c_7(\beta) = 1 + 11\beta/2 + 449\beta^2/32 + 2302\beta^3/128 + 43545\beta^4/4096$.

The conditions for the formation of the stable D and metastable L or stable L and metastable D states of one- and two-carrier impurity centers are defined as $E_1(\alpha_D) < E_1(\alpha_L)$, $E_2(\alpha_D) < E_2(\alpha_L)$ or $E_1(\alpha_D) > E_1(\alpha_L)$, $E_2(\alpha_D) > E_2(\alpha_L)$. Our calculations show that the value of α_D in $E_2(\alpha_D)$ at $\beta \neq 0$ is larger than the value of α_D in $E_2(\alpha_D)$ at $\beta = 0$. While the value of α_L in $E_2(\alpha_L)$ with electron correlation is smaller than the value of $\alpha_L \simeq 1$ in $E_2(\alpha_L)$ without electron correlation. The formation of large-radius D states of one- and two-carrier impurity centers is of primary interest for MIT's in doped systems. Therefore, in the following sections we consider only the formation possibility of such impurity states and bands in doped covalent semiconductors and oxide HTSC. Three types of one- and two-carrier impurity states can be formed depending on the strength of carrier-lattice coupling. In particular, at a weak carrier-lattice coupling (near the defect) the one-carrier ground state and the two-carrier excited state of large-radius impurity centers with $E_1(\alpha_D) < E_2(\alpha_D)$ are formed. These large-radius impurity centers involve negligible lattice deformations extending over many lattice sites and the polaronic effects around the impurities are almost absent. While at a strong carrier-lattice coupling (near the impurity) either the extrinsic polaronic ground state with $E_1(\alpha_D) < E_2(\alpha_D)$ or the extrinsic bipolaronic ground state with $E_2(\alpha_D) < 2E_1(\alpha_D)$ are formed.

3 Extrinsic Hubbard bands and correlation-induced metal-insulator transition in doped covalent semiconductors

We now determine the formation possibility of large-radius D states of one- and two-carrier impurity centers in a given doped system. First we consider the covalent semiconductors in which there is only the short-range component of the carrier-lattice interaction. We sequentially study the formation of large-radius in-gap impurity states, extrinsic Hubbard bands, extrinsic Mott- Hubbard gap and correlation-induced MIT in these systems. To determine the short-range carrier-lattice coupling constant g_s, we estimate the deformation potential E_d as $E_d = (2/3)E_F$, where E_F is the Fermi energy. For Si, the dielectric constant $\varepsilon = \varepsilon_0 = 11.7$ [25], $E_F = 12.5eV$ [26], $K = 0.988 \cdot 10^{22} dyn/cm^2$ [25] and $a_0 = 5.43A$ [4]. The effective electron mass m_e^* can be determined as the mean value of the effective masses of electrons $m^* \simeq 0.19m_e$ and $m_3^* = 0.98m_e$ observed in Si [25]. Then we find $m_e^* = \sqrt{m_1^* m_3^*} \simeq 0.43m_e$, $B = 2.83eV$, $g_s \simeq 0.124(1+b_s)$, $g_l \simeq 0.226$ (when $Z=1$), $G_s = 0.124(2+b_s)$, $G_l = 0.146$, $y_1 = 0.028(1+b_s)$ and $y_2 = 0.181(2+b_s)$. While in p-type Si the effective hole mass m_h^* is very close to $0.6m_e$ [27]. In this case we have $B = 1.833eV$, $g_s \simeq 0.192(1+b_s)$, $g_l = 0.336$ (when $Z=1$), $G_s = 0.192(2+b_s)$, $G_l = 0.217$, $y_1 \simeq 0.0645(1+b_s)$ and $y_2 = 0,0416(2+b_s)$. For Ge, $\varepsilon = \varepsilon_0 = 15.8$ [25], $E_F = 11.5eV$ [26], $K = 0.772 \cdot 10^{12} dyn/cm^2$ [25] and $a_0 = 5.65A$ [4], $m_e^* = 0.22m_e$ [27], $B \simeq 5.1eV$, $g_s = 0.067(1+b_s)$, $g_l = 0.088$, $G_s = 0.067(2+b_s)$, $G_l \simeq 0.0567$, $y_1 = 0.0059(1+b_s)$ and $y_2 = 0.0038(2+b_s)$. The ionization energies of the one-carrier impurity centers $E_I = |E_1(\alpha_D)|$ in Si and Ge are calculated for $-1 \leq b_s \leq 2$ by using the relation (5). The values of E_I are 0.036-0.040 eV and 0.052-0.060 eV for n- and p-type Si, respectively. While the values of E_I are 0.010-0.012 eV for n-type Ge. The energies of the two-carrier impurity states $E_2(\alpha_D)$ determined from the relation (6) for n- and p-type Si are equal to $|E_2(\alpha_D)| \simeq (0.02 \div 0.03)eV < |E_1(\alpha_D)|$ and $|E_2(\alpha_D)| \simeq (0.03 \div 0.04)eV < |E_1(\alpha_D)|$, respectively. These results are indicative of the absence of any polaronic effects in Si and Ge. Therefore, at $E_1(\alpha_D) < E_2(\alpha_D)$ using a rigid lattice model for description of the shallow impurity states in doped systems is well justified. In this case the hydrogen-like impurity centers are formed. Indeed, the values of E_I determined from (5) as discussed above are very close to the values of E_I determined from the simple hydrogen-like model of impurity centers.

In doped systems with $E_1(\alpha_D) < E_2(\alpha_D)$ the MIT can be described by the Mott-Hubbard impurity band model. The Hubbard Hamiltotian is written as

$$H = \sum_{ij\sigma} T_{ij} c_{i\sigma} c_{j\sigma} + U \sum_i n_{i\sigma} n_{i,-\sigma}, \tag{10}$$

where $E_0 = T_{ii}$ is the site energy which is necessary in order to bind a carrier in the isolated impurity center, $t = T_{ij}$ is the transfer energy between nearest-neighbor $< ij >$ sites on the impurity superlattice, U is the on-site Coulomb repulsion, $n_{i\sigma} = c^{+}_{i\sigma} c_{i\sigma}$ is the number operator, $c^{+}_{i\sigma}(c_{i\sigma})$ is the creation (annihilation) operator of a carrier at site i with spin σ.

According to the Hubbard model there are two energy levels E_0 and $E_0 + U$ on each site of the impurity superlattice. In order to determine the energy gap between the lower and upper extrinsic Hubbard bands, we calculate the Coulomb repulsive energy U between two carriers with antiparallel spins on the same impurity centers using the direct variational method. The screening effects due to the presence of two carriers on the same impurity lead to the decreasing of the total charge Z of this impurity. So, we assume that such an impurity has any effective or incomplete charge Z^*. The Hamiltonian of a two-carrier hydrogenic impurity center is given by

$$H = -\frac{\hbar^2}{2m_1^*}\nabla_1^2 - \frac{\hbar^2}{2m_2^*}\nabla_2^2 - \frac{Z^* e^2}{\varepsilon_0}\left(\frac{1}{r_1} + \frac{1}{r_2}\right) + \frac{e^2}{\varepsilon r_{12}}, \tag{11}$$

where the first and second terms are the kinetic energy of two carriers, the third term is the potential energies of these carriers in the Coulomb field of nuclei and the fourth term is the carrier-carrier Coulomb repulsive energy.

The ground state energy of such a two-carrier impurity center is determined from the functional

$$E(Z^*) = \int\int \Psi^* H \Psi d^3 r_1 d^3 r_2, \tag{12}$$

After substituting the trial variational wave function choosen in the simple form

$$\Psi = \psi_{1s}(r_1)\psi_{1s}(r_2) = \frac{1}{\pi}\left(\frac{Z^*}{a_H}\right)^3 exp\left[-\frac{Z^*(r_1 + r_2)}{a_H}\right] \tag{13}$$

in (12), we obtain the following expression for $E(Z^*)$:

$$E(Z^*) = Z^*\left(Z^* - 2Z + \frac{5}{8}\right)\frac{e^2}{\varepsilon a_H}, \tag{14}$$

where $a_H = \hbar^2\varepsilon/m^* e^2$, $m^* = m_1^* = m_2^*$.

Minimizing $E(Z^*)$ with respect to Z^* gives the relation

$$Z^* = Z - \frac{5}{16}. \tag{15}$$

Then the Mott-Hubbard gap is given by

$$U = \int\int \psi_{1s}^2(r_1)\frac{e^2}{\varepsilon r_1 2}\psi_{1s}^2(r_2)d^3 r_1 d^3 r_2 = \frac{10}{8}Z^* E_I, \tag{16}$$

where $E_I = e^2/2\varepsilon a_H$ is the ionization energy of the isolated impurity center.

At $Z = 1$ we obtain $U \simeq 0.86 E_I$. The proper criterion for Mott transition should be determined from the relation

$$W = U \simeq 0.86 E_I, \tag{17}$$

where $W = 2f(z)J$, $f(z)$ is any function which can be approximated as $f(z) = z$, z is the number of nearest neighbors (for cubic impurity superlattice $z = 6$), $J = \hbar^2/2m^* a_I^2$ is the transfer energy of tight-binding theory, a_I is the lattice constant of the impurity superlattice.

When $n = 1/a_I^3$ and $f(z) = z$ the criterion for MIT determined from (17) has the form

$$n_c^{1/3} a_H \simeq \sqrt{0.43/z}, \tag{18}$$

from which at $z = 6$ we obtain

$$n_c^{1/3} a_H \simeq 0.27. \tag{19}$$

The same criterion was also obtained in [5] within the another approach.

Now we compare the above results with the experimental findings in Si and Ge. At low doping density the activation energy of the so-called ε_2-conductivity in these semiconductors tends to the value $\simeq 0.86E_I$. As the energy state for the second carrier with the binding energy $E_I - 0.86E_I \simeq 0.14E_I$ exists in the neutral impurity center. Indeed, in Ge the so-called D^--state of the donor with the binding energy $\simeq 0.1E_I$ is observed (see [2]). So, the D^- -band in covalent semiconductors is the upper Hubbard impurity band. With increasing of the doping level, the upper Hubbard band due to the overlapping of the wave functions of localized impurity states is shifted torwards both the conduction (or valence) band and the lower Hubbard band. As a result, the activation energy of the ε_2-conductivity is decreased. Since in this case the energy gap between the lower and upper Hubbard bands becomes $U - W$ which is decreased with increasing W. Apparently, the activation energy of the ε_2-conductivity $\simeq 0.33E_I$ observed in Ge [2] is caused by this circumstance. Further, at $W = U$ the upper and lower (singly-occupied) Hubbard bands would merge and they form the doubly-occupied half-filled ordinary impurity band with half-bandwidth $W/2 = 0.43E_I$. Then the energy gap between the half-filled impurity band and the conduction (or valence) band is equal to $E_I - W/2 \simeq 0.57E_I$ when $n = n_c$. As discussed above many experimental results [1] speak well for the existence of such an energy gap between the impurity band and the conduction (or valence) band which would merge at higher doping level than $n = n_c$ in covalent semiconductors.

We now estimate the critical doping density at which the Mott transition occurs in Si and Ge. By taking $m_e^* \simeq 0.43m_e$ for n-type Si, we find $a_H \simeq 0.53(m_e\varepsilon/m_e^*)A \simeq 15A$. Then the value of n_c calculated from the relation (19) is equal to $n_c \simeq 5 \cdot 10^{18} cm^{-3}$ which is well consistent with the experimental data $n_c = (3.5 - 5.0)10^{18} cm^{-3}$ [1,28]. If we assume $m_h^* = 0.55m_e$ [27] for p-type Si, we obtain $a_H \simeq 12A$ and $n_c \simeq 10^{19} cm^{-3}$. For n-type Ge assiming $m_e^* = 0.22m_e$ [27], we find $a_H = 38A$ and $n_c \simeq 3 \cdot 10^{17} cm^{-3}$ which is also close to the experimental value $n_c \simeq 1.7 \cdot 10^{17} cm^{-3}$ [1,2]. Thus, the MIT in doped Si and Ge is the extrinsic Mott transition.

4 Extrinsic excitonic metal-insulator transition

In doped compounds the extrinsic excitonic states can be formed. Such an exciton is bound to an impurity atom or ion with binding energy

$$E_b^{ex} = \frac{\mu e^4}{2\hbar^2 \varepsilon_0^2}, \tag{20}$$

where $\mu = m_e^* m_h^*/(m_e^* + m_h^*)$ is the reduced mass of an exciton.

In particular, the transition of a carrier from the singly-occupied impurity center to the nearest-neighbor impurity centers (e.g. excitation of a carrier from the lower to upper Hubbard impurity band) leads also to the creation of such a bound exciton. As a consequence, the Mott transition takes place if the condition (17) is satisfied together with the condition

$$E_b^{ex} \leq U. \tag{21}$$

Otherwise the vanishing of the Mott-Hubbard gap at $W = U$ or $n_c \simeq (0.27)^3/a_H^3$ is not accompanied by the MIT which can occur at the overlapping of the doubly-occupied half-filled impurity band with the conduction or valence band. Then the criterion for the new excitonic MIT (at $\mu \sim m_e^*$ or $\sim m_h^*$) determined from the condition $W/2 = f(z)J = E_I \sim E_b^{ex}$ has the form

$$n_c^{1/3} a_H \simeq 0.41. \tag{22}$$

The excitonic mechanism for the MIT is realized at $m_e^*/m_h^* > 6$ or $m_h^*/m_e^* > 6$ which is satisfied (e.g., in polar solids, in alkali iodides [29]) and in the absence of the strong (bi)polaronic effects. However, simultaneous fulfilment of these conditions is unlikely. Apparently, the excitonic MIT can be realized in some semiconductors and insulators at modest ε_0. In particular, the MIT is observed in CsI under the hydrostatic pressure ($\sim 50 kbar$) (see[29]). The extrinsic excitonic MIT can occur also in this compound with donor impurities.

5 Extrinsic (bi)polaronic metal-insulator transitions in doped polar systems

The d-electron systems, mostly oxides and cuprate HTSC are assumed to be typical Mott insulators with AF order. In HTSC the Cu^{2+} ion is in a d^9 state with a half-filled $d_{x^2-y^2}$ orbital. However, in heavy transition-metal oxides, such as, cuprate HTSC the oxygen $2p_\sigma$ band becomes close to that of the half-filled copper $3d$ band. In this case, the character of the minimum charge excitation gap changes from the Mott-Hubbard type gap between the two 3d Hubbard bands to the charge-transfer (CT) type gap between the fully occupied oxygen 2p band and the copper 3d upper Hubbard band [11]. Such insulators is now called CT insulators as contrasted to the Mott-Hubbard insulators. In the p-type CT insulators an added hole mainly occupies the oxygen $2p_\sigma$ band, which is higher than the lower 3d Hubbard band. At low doping level, the doped carriers are trapped by the impurity (or defect) potential with the formation of a shollow (at $b_s < 0$) or a deep (at $b_s > 0$) state in the CT gap of the cuprate HTSC . In particular, in $La_{2-x}Sr_xCuO_4$ (LSCO) the situation $b_s < 0$ is realized [18]. In this case the short-range defect potential is repulsive and it can be considered like a hard core (see also [22]). The carrier-phonon interactions around the impurity ion (i.e. Sr^{2+} in LSCO) or defect (e.g., oxygen vacancy in other HTSC) in a rigid lattice are thus suppressed by the short-range repulsive defect potential. Therefore, at $b_s \leq 0$ a rigid lattice model is a good approximation and the impurity states can be described properly by the hydrogen-like model [10,18]. In this case the ionization energy E_I of the hydrogen -like impurity center well consistent with the observed value of E_I should be determined by using any effective dielectric constant ε_{eff} (see [1]). Some combination (or mean value) of ε_∞ and ε_0 can be used for ε_{eff}. We believe that the simple approximation $\varepsilon_{eff} = \sqrt{\varepsilon_\infty \varepsilon_0}$ is suitable for doped cuprates with $\eta = \varepsilon_\infty/\varepsilon_0 \ll 1$ (e.g. $\varepsilon_\infty = 2-7$ [9,10,30] and $\varepsilon_0 = 22 - 105$ [10,30-32]). For LSCO we can use $\varepsilon_\infty = 4$ or 5 and $\varepsilon_0 > 100$. Then the relation $\varepsilon_{eff} \simeq 5\varepsilon_\infty$, seems to be reasonable approximation. Indeed, by taking $\varepsilon_\infty = 5$ and $m_h^* \simeq 1.5m_e$ [33], we obtain $E_I = 13.6(m_h^*/m_e)\varepsilon_{eff}^{-2}eV \simeq 0.033eV$ which is close to the observed values of $E_I \simeq 0.02-0.035eV$ in HTSC [10]. While the value of $x_c = n_c/n_0 = V_0/V_I \simeq 0.015$ calculated by using the relation $f(z)J = E_I$ (see also below) of the tight-binding model and the approximation $f(z) = z$ is also close to the observed doping value $x_c = 0.02$ [6,7,10,11] for destruction of the AF order in LSCO, where $V_0 = 137A^3$ is the volume per CuO_2 unit in the orthothombic LSCO, $V_I = a_I^3 = 9261A^3$. However, the critical doping value x_c in LSCO calculated from the Mott criterion (1) is equal to $x_c = 0.0015$ [18] which is much lower than the value $x_c = 0.02$. Besides the MIT in doped oxide HTSC occurs at more higher doping level $x_c = 0.05 \div 0.07$ [6-8,10,11,21]. It means that the MIT in doped cuprates is not Mott transition. It is now believed [18] that at $b_s < 0$ the MIT in doped polar compounds is intrinsic (bi)polaronic MIT. Here we demonstrate that the MIT in doped polar materials is not Mott transition in the another case $b_s > 0$. Such a MIT is called by us as the extrinsic (bi)polaronic MIT. In the case $b_s > 0$, the formation of large D or even small L (bi)polarons bound to impurities or defects becomes possible in some doped HTSC (e.g. $La_{2-x}Ca_xCuO_4$, $La_{2-x}Na_xCuO_{4-\delta}$, $La_{2-x-y}Th_yBa_xCuO_4$, $Ba_{1-x}K_xBiO_3$ and $(Y_xCa_{1-x}Ba_2Cu_4O_8)$ with small-radius impurities (Ca^{2+},Th^{4+},Na^+,K^+) and these extrinsic (bi)polaronic effects are the driving forces for the new MIT's in such HTSC. The conditions for the formation of non-hydrogen-like impurity (or defect) centers in polar materials with trapped large polarons and bipolarons can be written in the forms

$$E_2(\alpha_D) - 2E_1(\alpha_D) > 0 \tag{23}$$

and

$$E_2(\alpha_D) - 2E_1(\alpha_D) < 0, \tag{24}$$

respectively. In the case $E_2(\alpha_D) < 2E_1(\alpha_D)$ a large extrinsic D bipolaron can exist and be energetically stable with respect to two well-separated large extrinsic D polarons. If $E_2(\alpha_D) > 2E_1(\alpha_D)$ a large extrinsic D bipolaron is energetically unstable with respect to decomposition into two separate large extrinsic D polarons. In this case the overlapping of the extrinsic polaronic band with the valence (oxygen 2p) or conduction (copper 3d upper Hubbard) band

Table 1: The calculated values of the parameters of extrinsic D polarons and bipolarons in doped cuprates without electron correlation ($\eta = 0$)

b_s	$E_1(\alpha_D)eV$	$E_2(\alpha_D)eV$	E_{bU}	R_{bU}
0.5	-0.09105	-0.18965	0.00754	0.04140
1.0	-0.09284	-0.19407	0.00838	0.04514
1.5	-0.09482	-0.19910	0.00945	0.04986
2.0	-0.09955	-0.20496	0.01089	0.005609

leads to the MIT. While, in the case $E_2(\alpha_D) < 2E_1(\alpha_D)$ first the dissociation of a large extrinsic D bipolaron (or a large-radius negative U-center) takes place and then the overlapping of the extrinsic polaronic band with valence or conduction band leads to the MIT. According to (24) the condition for the formation of the negative U-center in the D-state without electron correlation has the form

$$2(b_s+2)^2[1-3y(b_s+1)C_1(\eta,Z)]^{3/2} - 2(b_s+1)[1-3y(b_s+2)C_2(\eta,Z)]^{3/2} + \\ +9y(2+3b_s+b_s^2)C_3(\eta,Z) < 6+4b_s, \qquad (25)$$

where $y = g_{SL}\cdot g_{lL}$, $C_1(\eta,Z) = 1+\eta(b_l-1)$, $C_2(\eta,Z) = 1+\eta(b_l-2)$, $C_3(\eta,Z) = 1+\eta(b_s+b_l)$. The condition for the formation of the large-radius negative U-center in the D-state with electron correlation is also determined from (24).

We now make numerical estimations of the formation possibility of large-radius extrinsic D polarons and bipolarons in doped HTSC for $Z = 1$ and different $b_s > 0$. In particular, in La_2CuO_4 the volume of the unit cell is equal to $V = a_0^3 \sim 190A^3$. So, we can take $a_0 \sim 6A$. Further, by taking $m_h^* \simeq 1.5m_e$ [33], $\varepsilon_\infty \simeq 5$ [10], $E_F \sim 7eV$ [34-36], $E_d = (2/3)E_F \simeq 4.66eV$ and $K \sim 1.4\cdot10^{12}dyn/cm^2$ [37] we obtain $B = 0.66eV$, $g_s \sim 0.0865(1+b_s)$, $g_l \sim 0.72(1+1.82\eta)$, $G_s = 0.0865(2+b_s)$ and $G_l = g_l(1-\eta)$. The values of η characteristic for doped cuprates are $\eta \sim 0.02-0.10$. It is obvious that the binding energies of extrinsic D polarons and bipolarons are defined as $E_{bI} = |E_1(\alpha_D)|$ and $E_{bU} = |E_2(\alpha_D) - 2E_1(\alpha_D)|$, respectively. Another characteristic parameter of an extrinsic D bipolaron is the ratio $R_{bU} = E_{bU}/2E_{bI}$. Our calculations show that the formation of a large-radius negative U-center (or extrinsic D bipolaron) without electron correlation is possible only for $\eta = 0$ (see Table 1) and the binding energy of such a bipolaron is about $E_{bU} \sim 0.01$eV. While the formation of a large-radius extrinsic D bipolaron with electron correlation is possible for $\eta \leq 0.1$ (see Table 2). In this case the value of E_{bU} is decreased with increasing η. The characteristic energies of extrinsic D polarons and bipolarons $E_1(\alpha_D)$, $E_2(\alpha_D)$ and E_{bU} should be manifested in the optical absorption spectra of doped HTSC. Indeed, the calculated values of E_{bU} are in good agreement with the absorption peaks of the far-infrared transmission spectra of the YBaCuO superconductor at $\simeq 0.013 - 0.039eV$ [38].

Our variational calculations show that, with inclusion of the correlations between the pairing carriers, the binding energy of the extrinsic D bipolarons are increased markedly. As can be seen from Table 2, the values of $E_1(\alpha_D) = -(0.10 - 0.12)eV$ and $E_2(\alpha_D) = -(0.23 - 0.25)eV$ are in

Table 2: The calculated values of the parameters of extrinsic D polarons and bipolarons in doped cuprates with electron correlation

η	b_s	$E_1(\alpha_D)eV$	$E_2(\alpha_D)$	E_{bU}	R_{bU}
0.00	0.5	-0.09105	-0.22749 (0.6)	0.04538	0.24921
	1.0	-0.09284	-0.23152 (0.6)	0.04584	0.24684
	1.5	-0.09282	-0.23598 (0.5)	0.04634	0.24434
	2.0	-0.09703	-0.24134 (0.5)	0.04728	0.24360
0.02	0.5	-0.09804	-0.23392 (0.6)	0.03785	0.19304
	1.0	-0.10006	-0.23815 (0.5)	0.03804	0.19010
	1.5	-0.10230	-0.24304 (0.5)	0.03844	0.18789
	2.0	-0.10482	-0.24870 (0.5)	0.03905	0.18628
0.04	0.5	-0.10529	-0.24046 (0.6)	0.02987	0.14184
	1.0	-0.10756	-0.24492 (0.5)	0.02980	0.13851
	1.5	-0.11010	-0.25022 (0.5)	0.03002	0.13636
	2.0	-0.11297	-0.25626 (0.4)	0.03032	0.13418
0.06	0.5	-0.11283	-0.24709 (0.6)	0.02143	0.09499
	1.0	-0.11537	-0.25196 (0.5)	0.02122	0.09195
	1.5	-0.11822	-0.25752 (0.5)	0.02108	0.08915
	2.0	-0.12148	-0.26418 (0.4)	0.02121	0.08730
0.08	0.5	-0.12064	-0.25387 (0.5)	0.01258	0.05215
	1.0	-0.12348	-0.25911 (0.5)	0.01215	0.04918
	1.5	-0.12668	-0.26496 (0.5)	0.01159	0.04575
	2.0	-0.13037	-0.27225 (0.4)	0.01151	0.04414
0.10	0.5	-0.12874	-0.26088 (0.5)	0.00340	0.01322
	1.0	-0.13190	-0.26637 (0.5)	0.00258	0.00977
	1.5	-0.13548	-0.27272 (0.4)	0.00175	0.00647
	2.0	-0.13958	-0.28049 (0.4)	0.00119	0.00427

Table 3: The critical doping concentrations for MIT's in cuprate HTSC as a function of the parameters η and b_s

η	b_s	$n_c, 10^{21}cm^{-3}$	x_c
0.02	0.5	0.79280	0,10860
	1.0	0.81742	0.11198
	1.5	0.84506	0.11576
	2.0	0.87654	0.12007
0.06	0.5	0.97886	0.13409
	1.0	1.0121 (E+22)	0.13864
	1.5	1.0499	0.14382
	2.0	1.0936	0.14981
0.10	0.5	1.1930	0.16343
	1.0	1.2372	0.16947
	1.5	1.2880	0.17644
	2.0	1.3479	0.18464

reasonable agreement with the energies of the in-gap states observed in the doped cuprate HTSC at $\sim 0.1-0.2eV$ [39-42]. While the in-gap bands observed in many HTSC at $\sim 0.5-0.8$ [9,10,43] (see also [44]) eV can be associated with the energy levels of the two-dimentional extrinsic (or intrinsic) D (bi)polarons. As the localized in-gap states of these (bi)polarons are expected to be much (nearly 4 times [45]) deeper than such states of the three-demontional D (bi)polarons. When the doping level is increased towards the optimal level, first the extrinsic D bipolaron will dissociate into two extrinsic single D polarons and then the MIT occurs at the overlapping of doubly-occupied half-filled extrinsic polaronic band with the valence or conduction band. In orther words, the MIT driven by the carrier localization takes place if the kinetic energy of extrinsic polarons smaller than their binding energy E_{bI}. So the criterion of the new extrinsic (bi)polaronic MIT is defined as

$$f(z)J = E_{bI} \text{ or } \frac{z\hbar^2}{2m^*_{Ip}a_I^2} = E_{bI} \tag{26}$$

from which at $z = 6$ we find the critical doping value

$$n_c = \frac{1}{V_I} = a_I^{-3} = \left(\frac{m^*_{Ip}E_{bI}}{3\hbar^2}\right)^{3/2}, \tag{27}$$

where m^*_{Ip} is the effective mass of an extrinsic polaron. In cuprate HTSC the polarons have effective mass $m_p = 2m_e$ [10]. We assume that the extrinsic D polarons have nearly the same effective mass. Then the calculated values of n_c and x_c by using the values of $n_0 = 7.3 \cdot 10^{21} cm^{-3}$, $m^*_{Ip} = 2m_e$ and E_{bI} for different η and b_s are presented in Table 3.

As can be seen from Table 3, the crystalline dielectric anisotropy and the anisotropy of (bi)polaronic effects are responsible for the smooth MIT and the stripe formation in the doping range 0.06-0.15. Now, using the WO_{3-x} data [46], we can assume $m^*_{Ip} \simeq 2m_e$ and $n_0 \simeq 10^{22}cm^{-3}$. Further, assuming just as in HTSC $E_{bI} \simeq 0.09eV$ for this compound, we find $n_c \simeq$

$6.76 \cdot 10^{20} cm^{-3}$ and $x_c = 0.093 \simeq 0.1$ which are also consistent with the experimental values of $n_c > 10^{20} cm^{-3}$ and $x_c \leq 0.1$ [46]. It is known that the $Ba_{1-x}K_xBiO_3$ and $BaPb_{1-x}Bi_xO_3$ systems have cubic perovskite structure (with small ε_∞ [47] and without anisotropic properties) and electronic structure (with the band mass $m^* = m_e$ [47] and gap $\simeq 2eV$ [48] and large electron bandwidth or E_F [40,48] similar to the Cu-based HTSC. Therefore, we assume that the values of E_F and K for these systems are close to those in cuprate HTSC. Further, by taking $m_h^* \simeq m_e$, $\varepsilon_\infty = 2.5$, $\eta = 0.04$ and $b_s = 0.5$ for $Ba_{1-x}K_xBiO_3$, we obtain $E_1(\alpha_D) \simeq -0.27eV$ and $E_2(\alpha_D) \simeq -0.53eV$ which are very close to the energies of the two in-gap states observed in the doped oxides $Ba_{1-x}K_xBiO_3$ and $BaP_{1-x}Bi_xO_3$ at $0.24eV$ [40] and $0.50eV$ [47]. While assuming $m_{Ip}^* \simeq 2m_e$, $E_{bI} = 0.27eV$ and $n_0 \simeq 10^{22} cm^{-3}$, we find $n_c \simeq 3.2 \cdot 10^{21} cm^{-3}$ and $x_c \simeq 0.38$ which is also close to the observed critical doping value $x_c = 0.35$ for the MIT in $Ba_{1-x}K_xBiO_3$ system [49].

Many double substitution experiments in La_2CuO_4 (i.e. Sr^{2+}, Ba^{2+}, Ca^{2+}, Nd^{3+}, Th^{4+} substitution for La^{3+}) are indicative of the structural and electronic transformations occuring at the "magic" doping $x = 1/8$ [8,50]. At $x \leq 1/8$ the formation of static stripes and the suppression of the superconductivity take place. These phenomena indicate the tendency towards localization of the mobile carriers (or dynamic stripes) [18]. We believe that the formation of the extrinsic (and intrinsic) D (bi)polarons is also accompanied by the structural transition and MIT. The above experiments in accordance with our predictions have demonstrated that the small-radius cations (i.e. Sr^{2+}, Ba^{2+}) with $E_{dD} < 0 (b_s < 0)$ are essentially important for the "1/8 anomaly". Indeed, LSCO exhibits only a weak suppression of the superconductivity at this particular doping level $x = 1/8$, and displays no transition to the tetragonal low temperature phase [50].

Another interesting question is the relationship between the AF excitations and the superconductivity in doped cuprates. As in these cuprate HTSC the superconducting (SC) state is next to the magnetic state as a function of doping. At present there is no consensus concerning the mechanizms of AF spin fluctuations and high-T_c superconductivity. The experimental probes of spin excitations show that the spin flictuations at Cu sites and O sites probed by nuclear magnetic relaxation rate result from the same fluctuations [51]. Hence the spin fluctuations and the existence of the so-called spin gap can be described properly by the extrinsic (and intrinsic) (bi)polaron formation leading to the appearance of the energy gap both for change excitations and for spin excitations. Indeed, recent experiments on cuprate HTSC speak well for the existence of a pseudogap which is not a spin gap only [52]. At the formation of large- and small-radius extrinsic bipolarons in $p-$ type cuprates, the localized holes decrease spin densities on Cu and O sites. As a consequence, the long-range AF order destroyed. Indeed, in most of the doped cuprates, the AF long-range order is reduced rapidly with doping and superconductivity appears only in the range of small or vanishing AF long-range order at $x \geq x_c$. Further, the spin glass phase exists in some doped cuprates (e.g. LSCO) at $T < 10K$ [6]. The origin of such a phase can be understood properly within the quasimolecular model of small-radius extrinsic (bi)polarons with local D_{2h} or D_{4h} symmetry [53,54]. As the small-radius extrinsic L (bi)polarons due to the lattice and vibronic anharmonicity (see [53]) may have double-well potential and such two-level systems form Bose or spin glass phase at low temperature. The formation of the stable small-radius L state of extrinsic (bi)polarons in doped three-dimensional cuprates is possible only for $b_s \gg 1$. While the large-radius Si^{2+} ion in LSCO has the negative b_s. In LSCO the formation of the small-radius intrinsic L (bi)polarons is possible only in the two-dimensional case (e.g. in the CuO_2 layer) due to the absence of the potential barrier separating large- and small-radius (bi)polaronic states. Therefore, the spin glass phase in LSCO seems to be associated with the presence of the immobile quasimolecular type L (bi)polarons in the CuO_2 layer together with the large-radius three-dimensional D (bi)polarons. For $T \ll T_c$ this spin glass phase should be insulating in the underdoped region. Indeed, such a situation is observed in LSCO at low and intermediate doping levels [6,10].

6 Conclusion

In this work we have tried to demonstrate the formation possibility of large-radius localized impurity (or defect) states and narrow impurity bands in the band gap and CT gap of carrier-doped covalent semiconductors and polar compounds. The formation of such extrinsic in-gap states and bands in various types of carrier-doped compounds is responsible for distinctive electronic properties of doped systems. In particular, the above described doping-induced changes play a key role in determining the mechanisms of MIT's and superconductivity in covalent and polar materials. We have determined the extrinsic Mott-Hubbard, excitonic and (bi)poaronic gaps and the proper criterions for Mott transition, extrinsic excitonic and (bi)polaronic MIT's in doped systems. We have found that the Mott transition can occur in doped covalent semiconductors (i.e. Si and Ge) and in some insulators doped with large-radius impurities for which the condition $U > E_b^{ex}$ is satisfied. Otherwise, in doped systems with strong carrier-phonon coupling the extrinsic (bi)polaronic MIT's are realized instead of Mott transition. So, in doped polar compounds (e.g. oxide HTSC and related materials) the MIT's are new phase transitions described adequately and consistently by the extrinsic (bi)polaronic band model. These MIT's are similar to the intrinsic (bi)polaronic or purely carrier-phonon-induced MIT's [18]. The MIT's in doped systems (without disorder) are basically Mott transition and extrinsic (or intrinsic) (bi)polaronic MIT's. The criterions for these MIT's obtained above are in good agreement with the experimental results on doped covalent semiconductors and oxide HTSC. While the possibility of the extrinsic excitonic MIT is restricted by the condition $m_h^*/m_e^* \gg 1$ (or $m_e^*/m_h^* \gg 1$). In doped systems, the disorder-induced Anderson transition is also possible at inhomogeneous distribution of impurities (or defects). The proper criterion for such a transition corresponding to the real experimental situations requires further investigations. The continuous MIT's driven by the anisotropy of the dielectric (or (bi)polaronic) properties of doped HTSC are responsible for the observed stripe formation and suppression of superconductivity in such systems. Our variational calculations show that the three-dimensional large-radius extrinsic D bipolarons is expected in doped cuprates and other oxide HTSC at $\eta \leq 0.1$. We stress that the formation of intrinsic (or lattice) bipolarons and extrinsic ones seems to be the main driving force not only for MIT's but also for high-T_c superconductivity in polar materials. In particular, the spin fluctuations in cuprate HTSC results from the real- and k-space pairing of extrinsic (and intrinsic) polarons [24]. Indeed, we have found that the calculated values of the extrinsic (bi)polaronic gaps are consistent with the observed two in-gap states (or bands) at $\sim 0.1 - 0.2eV$ and $\sim 0.5 - 0.8eV$ and with the obsorption peaks of the far-infrared spectra at $\sim 0.013 - 0.039eV$. While in non-polar compounds such as covalent semiconductors and metals due to the absence of the strong (bi)polaronic effects only the low-T_c superconductivity described by the phonon-mediated BCS pairing theory and by the superfluid condensation theory of Cooper pairs [55] is possible. As in the weak carrier-phonon coupling limit the SC transition temperature T_c is determined from the will-known BCS expression. Therefore, the value of T_c is expected to be very low. Indeed, the observed value of T_c in the first superconductor consisting of a $Si\ sp^3$ covalent network is about $4K$ [56].

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