Phenomenological models of dielectric functions and screened Coulomb potential

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The evolution of static dielectric constants and polarization with doping are analyzed and discussed using established experimental results. The variation of screened Coulomb potential with doping is derived theoretically to justify the said evolutions. The latter justification arises due to the influence of ionization energy ($\xi$) on the static dielectric functions. The bare Coulomb potential and the Thomas-Fermi screened potential with finite carrier density were recovered when $\xi \rightarrow \infty$ and $\xi \rightarrow E_F^0$ respectively. Basically, these phenomenological models are associated with the ionization energy based Fermi-Dirac statistics (fFDS).

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1. INTRODUCTION

Analogous to ferro- and paramagnetic systems that deal with spin alignments, Ferroelectrics (FE) exhibit spontaneous polarization below the Curie temperature ($T_C$) whereas the unpolarized state exists above $T_C$. The simplest Ferroelectric (FE) crystal, SnTe with NaCl structure was reported by Riedl et al. back in 1965. The Ferroelectricity (FE) observed in SnTe is of displacive nature, identical with other Perovskite FE. Presently, the Perovskite structured (Ba,Sr)TiO$_4$ (BST) plays an enormous role for the development of technological applications due to its high spontaneous polarization, $\sim 10^{-2}$ Cm$^{-2}$ at $T_C \approx 290$ K $[2]$. Although substituting Nb into the BST system reduces the twin formation and $T_C$ significantly, its dielectric constant and spontaneous polarization was found to be increased sharply $[3]$. Basically, FE are highly insulating, which prohibits direct current transport measurements. Consequently, measurements on polarization and dielectric constant are of more relevant to characterize FE. Due to its dielectric effect, FE has been exploited in microwave devices such as tunable oscillators, phase shifters and varactors $[4, 5, 6, 7]$. Moreover, FE also have the potential applications for detectors and devices based on the energy conversion principle namely, mechanical$\leftrightarrow$thermal$\leftrightarrow$electrical energies $[8]$. Yet another technological advancement of FE is its functionality as a gate insulator in Field-Effect Transistor (FET) as reported extensively by de Boer et al. $[9]$ and Podzorov et al. $[10]$ using organic molecules namely, Tetracene, Pentacene and Rubrene. One of their interesting observation is the dielectric constant’s inverse dependence on carrier mobility. Furthermore, developments of the dielectric gate that consists of La, Al and Oxygen to substitute the common SiO$_2$ has been successfully produced and even patented $[11]$. Perovskite FE with Ferromagnetic properties such as (Tb,Y,Bi)MnO$_3$ have been investigated experimentally $[2, 12, 13, 14]$ due to its possible technological impact on magneto-electric media, including the Dynamic Random Access Memory (DRAM) devices. BST related oxides are studied in the thin film form, usually grown by pulsed-laser deposition technique. Parallel to this, there are reports on the influence of the film’s thickness with FE. In this respect, a generalized Ginzburg-Devonshire theory was employed to evaluate the behavior of the FE thin film coated with two metallic electrodes $[15]$. Zheng et al. $[15]$ found that imperfect surface produces non-uniform polarization distribution and subsequently gives rise to the phase transition temperature or $T_C$. Apart from oxides, liquid crystal is one of the well known soft matter that works on the principle of molecular polarization $[16]$. By applying an intense alternating electric field during Triglycine Sulphate (TGS) crystal growth, Arunmozhi et al. $[17]$ concluded that this procedure leads to a longer relaxation time, which in turn reduces the dielectric constant and the spontaneous polarization. On the theoretical aspect, a thermodynamical model has been proposed to explain the $T$ and $E$ dependence of polarization and susceptibility of TGS by Otolinska et al. $[18]$. Moreover, non-oxide alloy, TlInS$_2$ was reported theoretically $[19]$ to explain the peculiarities in the dielectric susceptibility, which is connected with the assumption that there exists coexistence of proper and improper FE, somewhat mimicking the TbMnO$_3$, which also demonstrates the said coexistence $[2]$. Simple non-Fermi gas system and strongly correlated matter are known to exhibit remarkable electronic properties with minuscule substitutional doping. Handling such systems theoretically with the ionization energy ($\xi_T$) based Fermi-Dirac statistics (fFDS) has been shown to be precise. For example, simple systems such as the diluted magnetic semiconductors, Mn$_{0.02}$Ge$_{0.98}$ $[20]$ and Ga$_{1-x}$Mn$_x$As $[21, 22]$ as well as for complex crystals namely, Cuprate high-$T_c$ superconductors, YBa$_2$Cu$_3$O$_7$ $[23, 24, 25, 26, 27, 28]$ and Manganite ferromagnets, La$_{1-x}$Ca$_x$MnO$_3$ $[21, 22]$ have been shown...
quantitatively to be within the scope of iFDS. Therefore, iFDS is further applied here to scrutinize theoretically the evolution of polarization, static dielectric constant and the screened Coulomb potential with doping in FE BST and its derivatives. The reasons to revivify the dielectric functions and the screened Coulomb potential with iFDS is two-fold. The first one is as stated above, while the second reason being, to further our evaluation on the actual role of phonon in the Cupriconductors and also to justify why hole compensation effect is unnecessarily invoked in the First-Principles approach for the ferromagnetic semiconductors, both of which will not be addressed here. It is well known that for free-electrons, the Thomas-Fermi screening length determines the screened Coulomb potential while the bare Coulomb potential is recovered when the electrons density is literally zero. However, it is highlighted here that the bare Coulomb potential can still be recovered in the presence of finite electrons density, provided that the Coulomb potential can still be recovered in the presence of zero. However, it is highlighted here that the bare Coulomb potential while the bare Coulomb potential is recovered when the electrons density is literally zero. However, it is highlighted here that the bare Coulomb potential can still be recovered in the presence of finite electrons density, provided that the Coulomb potential approaches infinity. In addition to the theoretical justifications, experimental results from Pauling, Jaswal et al. and Bell et al. will be used to further reinforce the accuracy of iFDS. Unfortunately, the theory presented here is not yet suitable to predict the $T$ dependence of dielectric constant and polarizability, rather the substitutional doping dependence of the mentioned parameters will be accentuated and analyzed in detail.

2. THEORETICAL DETAILS

2.1. Polarizability and optical dielectric function

The electronic polarization, $P$, of a particular crystal can be defined as

$$ P = C \sum_j \alpha_j(n_j) \mathbf{E}^{\text{local}}_j. \quad (1) $$

$C$, $\alpha_j(n_j)$ and $\mathbf{E}^{\text{local}}_j$ denote the atoms concentration, polarizability at atom $j$, which is proportional to electrons number in atom $j$, and the local electric field at atom site $j$ respectively. The local electric field for individual ions can be written as $\mathbf{E}^{\text{local}}_i = \mathbf{E} + \frac{1}{\sigma_{\text{ion}}} \mathbf{P}$ by assuming a spherical geometry for individual ions and the crystals are purely ionic. $\mathbf{E}$ is the macroscopic electric field while $\frac{1}{\sigma_{\text{ion}}}$ is the Lorentz factor. In order to understand the evolution of $P$ with $n$ as a result of doping, another equation that relates doping with $n$ is required. To this end, iFDS is utilized that eventually gives

$$ n = \int \frac{E}{f_e(E)N_e(E)} dE, $$

where

$$ = \frac{1}{2\pi^2} \left( \frac{2m_e}{\hbar^2} \right)^{3/2} e^{\lambda(E_p^0 - E_i)} \int_0^\infty E^{1/2} \exp(-\lambda E) dE $$

$$ = 2 \left( \frac{m_e}{2\pi \lambda \hbar^2} \right)^{3/2} \exp \left( \lambda(E_p^0 - E_i) \right). \quad (2) $$

Here, $\mu = -\lambda E_p^0$ whereas $E_i$ represents the electronion Coulomb attraction, which is also an accurate representation of doping-parameter. The derivation of iFDS, $f(E) = \exp(-\mu - \lambda(E_{\text{initial state}} \pm E_i))$ by employing the restrictive conditions, $\sum E_{\text{initial state}} \pm E_i = n$ and $\sum E_{\text{initial state}} \pm E_i = E$ can be found in the Refs. The $E_{\text{initial state}}$ denotes the energy at certain initial state and the Lagrange multipliers, $\mu_e + \lambda E_i = -\ln \left( \frac{(n_e/V)(2\pi \lambda \hbar^2/m_e)^{3/2}}{\lambda} \right)$ and $\mu_h - \lambda E_i = -\ln \left( \frac{(p/V)(2\pi \lambda \hbar^2/m_h)^{3/2}}{\lambda} \right)$. $V$ is the volume in $k$-space and $E_p^0$ is the Fermi level at $T = 0$ K. $m_e,h$ is the electrons or holes mass, $h = \hbar/2\pi$, is the Planck constant, while $n$ and $p$ are the electrons and holes number. In the previous work, $\lambda = 1/k_B T$ since the variation of $n$ with respect to the variation of $T$. Contrary to the previous objective, $\lambda$ in this case can be connected with the binding energy of an electron in a Hydrogen atom, which is given by $E_n = (m/2\hbar^2)(e^2/4\pi\epsilon_0)^2(1/n^2)$. Here, $n$ denotes the principal quantum number. The reason is to calculate the variation of $n$ due to electrostatic potential, of which the $n$ as given in Eq. is actually the induced electrons density, $n_{\text{ind}}$ arises as a result of both external and induced electrostatic potential. To obtain such a result, one has to make use of the two restrictive conditions introduced in iFDS as stated above that respectively give

$$ n = \frac{V}{2\pi^2} e^{\mu - \lambda E_i} \int_0^\infty k^2 \exp \left( -\lambda \frac{\hbar^2 k^2}{2m} \right) dk,$$

$$ E = \frac{V \hbar^2}{4m \pi^2} e^{\mu - \lambda E_i} \int_0^\infty k^4 \exp \left( -\lambda \frac{\hbar^2 k^2}{2m} \right) dk.$$

Solving the above integrals, one can arrive at $E = 3n/2\lambda = E_B$, hence $\lambda = (12\pi\epsilon_0/e^2)^2n^2R_B$, after taking $n = 1$. $R_B$ represents the Bohr radius. Notice the essential factor, $e^{\lambda(E_p^0 - E_i)}$ in Eq. that will be used together with $\lambda$ to define the carrier density above $E_p^0$ as a result of the external and induced electrostatic field and finally to explicitly derive the static dielectric function and the screened Coulomb potential for the strongly correlated (non-Fermi gas) systems. The dielectric function ($\epsilon(\omega,k)$) for an isotropic polarization can be defined as

$$ \lim_{k \to 0} \epsilon(\omega) = \frac{1}{E} \left[ E + \frac{C}{\epsilon_0} \sum_j \alpha_j(n_j) \mathbf{E}^{\text{local}}_j \right]. $$
\[ \epsilon(\omega, 0) = 1 + \frac{C}{E_{0}} \sum_{j} \alpha_{j}(n_{j}) E_{j}^{\text{local}}. \] (3)

\[ \epsilon(\omega = 0) \text{ and } \epsilon(\omega = \infty) \text{ are the static and optical dielectric constants respectively, while } \omega \text{ is the frequency.} \]

2.2. Static dielectric function

If the positive ions in the background are allowed to have a sinusoidal variation that leads to the positive charge density, \( \rho^+(x) = n_0^{\text{+}} e + \rho_{\text{ext}}(k) \sin(kx) \) in the \( x \) direction, then the response of the electrons charge density is \( \rho^-(x) = -n_0^{\text{e}} \rho + \rho_{\text{ind}}(k) \sin(kx) \). The term, \( \rho_{\text{ext}}(k) \sin(kx) \) defines the external electrostatic field that acts on the electrons. In other words, the electrons will be deformed as a result of \( \varphi_{\text{ext}}(k) \) and \( \varphi_{\text{ind}}(k) \). The latter being the induced electrostatic potential. One can employ the Poisson equation, \( \nabla^2 \varphi = -\frac{\rho}{\epsilon_0} \), \( \varphi(k) = \varphi_{\text{ext}}(k) + \varphi_{\text{ind}}(k) \) and \( \rho(k) = \rho_{\text{ext}}(k) + \rho_{\text{ind}}(k) \) in order to arrive at

\[ \varphi(k) = \frac{\rho(k)}{k^2 \epsilon_0}. \] (4)

The FE here concerns with the displacement of charge \( (D(k)) \), thus \( \epsilon(0,k) \) can be defined \[ 32 \] as \( D(k) = \epsilon(0,k) E(k) \). Using, \( \nabla \cdot D = \nabla \cdot E = \rho_{\text{ext}}/\epsilon_0 \), \( \nabla \cdot E = \rho/\epsilon_0 \) and the Poisson equation, one can also show that \[ 32 \]

\[ \epsilon(0,k) = \frac{\int_{-\infty}^{\infty} \rho_{\text{ext}}(k) e^{ik \cdot r} dk}{\int_{-\infty}^{\infty} \rho(k) e^{ik \cdot r} dk} = \frac{\int_{-\infty}^{\infty} \varphi_{\text{ext}}(k) e^{ik \cdot r} dk}{\int_{-\infty}^{\infty} \varphi(k) e^{ik \cdot r} dk}. \] (5)

Now, at absolute zero (0 K), the Fermi level is given by \( E_{F}^{0} = \frac{\hbar^2}{2m_e} (3\pi^2 n_0)^{2/3} \). However, in the presence of \( \varphi_{\text{ext}}(x) \) and \( \varphi_{\text{ind}}(x) \), \( E_{F}(x) = \frac{\hbar^2}{2m_e} [3\pi^2 n(x)]^{2/3} \). Using the Thomas-Fermi (TF) approximation, one can write \( E_{F}(x) - E_{F}^{0} = \epsilon [\varphi_{\text{ext}}(x) + \varphi_{\text{ind}}(x)] = \epsilon \varphi(x) \). As a consequence, linearization can be carried out to estimate the induced carrier density, \( n(x) - n_0 \) at certain point \( x \), in which \( E_{F}^{0}(n_0) \) can be linearized as \( L(n_0) \) at \( n_0 = n(x) \) to give

\[ L(n_0) = E_{F}(x) + \frac{dE_{F}^{0}}{dn_0} [n_0 - n(x)]. \] (6)

Since the standard linear approximation gives \( L(n_0) \approx E_{F}^{0} \), and \( dE_{F}^{0}/dn_0 = 2E_{F}^{0}/3n_0 \), one can rewrite Eq. (6) as below

\[ \frac{dE_{F}^{0}}{dn_0} [n(x) - n_0] \approx E_{F}(x) - E_{F}^{0} \approx \epsilon \varphi(x). \]

\[ n(x) - n_0 \approx \frac{3n_0}{2E_{F}^{0}} \epsilon \varphi(x). \] (7)

Utilizing iFDS or Eq. (23) specifically, such that \( n = n_{\text{ind}} = n(x) - n_0 \), then Eq. (7) can be expressed as

\[ n = n(x) - n_0 \approx \frac{3n_0}{2E_{F}^{0}} \epsilon \varphi(x) \exp \left[ \lambda \left( E_{F}^{0} - \xi_{F} \right) \right]. \] (8)

Consequently, using \( \lim_{\xi_{F} \to \infty} n(x) = n_0 \), one can surmise that it is rather impossible to induce a region of enhanced electron concentration. However, \( \lim_{\xi_{F} \to E_{F}^{0}} n(x) = n_0 \left[ 1 + (3/2E_{F}^{0}) \epsilon \varphi(x) \right] \) supports the free-electron or Boltzmann-particle systems, which also satisfies the original TF approximation. It is worth noting that, for the latter limit, the electrons with its total energy, \( TE > E_{F}^{0} \), are literally free, forming the Fermi gas. In contrast, Eq. (8) denies such scenario, as long as \( E_{F}^{0} < TE < \xi_{F} \). To see this effect clearly, the screened Coulomb potential is derived and discussed in the subsequent section. Employing Eq. (11) and \( \rho_{\text{ind}}(x) = -[n^{-}(x) - n_{0}] e \) (as introduced earlier), the Fourier components of Eq. (8) can be written as

\[ \int_{-\infty}^{\infty} \rho_{\text{ind}}(k) e^{i k \cdot r} dk = -\frac{3n_0}{2E_{F}^{0}} e^{2} \exp \left[ \lambda \left( E_{F}^{0} - \xi_{F} \right) \right] \int_{-\infty}^{\infty} \varphi(k) e^{i k \cdot r} dk \]

\[ = -\frac{3n_0 e^{2}}{\epsilon_0 2E_{F}^{0}} \exp \left[ \lambda \left( E_{F}^{0} - \xi_{F} \right) \right] \int_{-\infty}^{\infty} \frac{\rho(k)}{k^2} e^{i k \cdot r} dk. \] (9)

Using Eq. (10) with term by term division, the Fourier component of the static dielectric function at zero frequency, \( \epsilon(0,k) \) can be derived from Eq. (14) as given below

\[ \epsilon(0,k) = 1 + \frac{\xi_{F}^{2}}{k^2} \exp \left[ \lambda \left( E_{F}^{0} - \xi_{F} \right) \right]. \] (10)

Firstly, notice that both \( \epsilon(0,k) \) and \( \epsilon(\omega, 0) \) are proportional to the factor of \( \exp \left[ \lambda \left( E_{F}^{0} - \xi_{F} \right) \right] \) and \( \epsilon(0,k) \neq \epsilon(\omega,0) \). Secondy, the TF screening parameter remains the same, \( \xi_{F}^{2} = 3n_0/2\epsilon_0 E_{F}^{0} e^{2} \). Considering the Fermigas system with \( E_{F}^{0} = \xi_{F} \), then one can arrive at the original TF dielectric function, \( \epsilon(0,k) = 1 + \xi_{F}^{2}/k^2 \). If however, \( \xi_{F} \to \infty \), then \( \epsilon(0,k) \to \text{constant} \).
Imagine a test charge $e$ is placed at certain energy level ($> E_F^0$) in the background of a sinusoidal variation of the positive ions, then the Fourier transformed electrostatic potential for the unscreened Coulomb potential, $\varphi_q(k)$ can be shown to be $q/k^2\epsilon_0$ using Eq. (4). The Fourier inversion of $\varphi_q(k)$ is $\varphi_q(r) = \left[1/(2\pi)^3\right]\int_{-\infty}^{\infty} 2\pi k^2(q/\epsilon_0 k^2)e^{ikr}dk = \left[q/4\pi^2\epsilon_0\right]\int_{-1}^{1} e^{ikr} \cos \theta d(\cos \theta) = q/4\pi\epsilon_0 r$ as it should be. Subsequently, one can derive the screened Coulomb potential, $\varphi(r)$ using Eq. (5), in which $\epsilon(0,k) = \varphi_q(k)/\varphi(k)$. As such, $\varphi(k) = (q/\epsilon_0 k^2)\left[k^2/(k^2 + K^2_{s,t})\right]$. Notice the parameterization, $K^2_{s,t} = K^2_{s,t} \exp \left[\lambda(E_F^0 - E_x)\right]$ that has been used for simplicity. Finally, the Fourier inversion of $\varphi(k)$ is $\varphi(r)$ that can be derived as

$$\varphi(r) = \frac{1}{(2\pi)^3} \int_{-\infty}^{\infty} \frac{\pi k^2 q}{\epsilon_0(k^2 + K^2_{s,t})} dk \times \exp(\frac{iq}{2\pi\epsilon_0 r}) \int_{0}^{\infty} \frac{\cos \theta}{k^2 + K^2_{s,t}} \sin(kr) d(\cos \theta) = \frac{q}{4\pi\epsilon_0 r} \exp \left[-K_{s,t}r/2\lambda(E_F^0 - E_x)\right].$$

$\pi k^2$ denotes the area in k-space. The screened Coulomb potential in this case is a function of doping parameter, $E_F$ and one can enumerate the evolution of $\varphi(r)$ with doping for non-Fermi gas systems. The $E_F$ that originates from iFDS can be used to justify that an electron to occupy a higher state $N$ from the initial state $M$ is more probable than from the initial state $L$ if the condition $E_F(L) < E_F(L)$ at certain $T$ is satisfied. As for a hole to occupy a lower state $M$ from the initial state $N$ is more probable than to occupy the state $L$ if the same condition above is satisfied. $E_F(initial state) is the energy of a particle in a given system at a certain initial state and ranges from $+\infty$ to 0 for the electrons and 0 to $-\infty$ for the holes. Simply put, the magnitude of $\varphi(r)_{M+e-N}$ due to the polarization initiated excitation of an electron (hole) from the initial state $M (N)$ to $N (M)$ is quantitatively smaller than $\varphi(r)_{M-e-N}$. This effect can be non-trivially verified from the Eq. (11). On the contrary however, placing a test charge with its $TE > E_F^0$ and $E_F^0 = E_F$ imply Fermi gas that eventually gives rise to the TF screening potential $\frac{q}{4\pi\epsilon_0 r} e^{-K_{s,t}r}$. Add to that, Eq. (11) also reduces to the unscreened Coulomb potential even at finite $n_0$ provided that $E_F \to \infty$. The limit, $E_F \to \infty$ conceptually means that the electrons in the presence of the sinusoidal potential of positive ions are infinitely rigid with zilch polarization and eventually can be thought of as a sphere of a net charge $q$, as seen by the previously placed test charge $e$. Therefore, the potential is indeed a bare Coulomb potential, $q/4\pi\epsilon_0 r$. Refer to Fig. 11 to clearly observe the transition of the TF screened potential (●) to the Coulomb bare potential (■) as a result of iFDS, at finite carrier density ($n_0 \neq 0$). The solid lines, ▲ ($E_F \to E_F^0$) and ■ ($E_F \to \infty$) are obtained from Eq. (11) with its appropriate limits.

3. DISCUSSION

Having derived all the required functions, now it is possible to venture into the experimental data reported by various researchers starting from the 1920s. Notice that the above derivations strictly requires substitutional doping that significantly maintains a single phase or solid solution. Obviously, doping with a purpose of creating a second phase or multi-phases are not applicable with iFDS based theory. The Clausius-Mossotti relation in the optical range is given by

$$\frac{\varepsilon - 1}{\varepsilon + 2} = \frac{N^2 - 1}{N^2 + 2} = \frac{C}{3\epsilon_0} \sum_j \alpha_j(n_j).$$

$N$ represents the refractive index. Using this relation, the electronic polarizability of atom $j$, which is a function of electron number in atom $j (\alpha_j(n_j))$ for a wide variety of ions [29, 30] were calculated and tabulated in the Ref. 32. The magnitude of $\sum_j \alpha_j(n_j)$ can be assumed to be accurate since those ions (plasma) easily satisfy the Lorentz factor [29, 33] for spherical ions or atoms. Figure 2(a)-d depict the relation between $\alpha_j(n_j)$ and $E_F$ for $1+ \rightarrow 4+$ ions respectively. Those experimental data points [21, 22] were fitted in Fig. 2(a)-d with $\sum_j \alpha_j(n_j) = \lambda \exp(\gamma)$, which is in accordance with the principle of Eqs. (11), (12) and (13). Here, the fitting parameters, $\lambda = constant$ of proportionality while $\gamma = \lambda(E_F^0 - E_F)$. Both values ($\lambda$ and $\gamma$), obtained from the fittings are given in the Fig. 2(a)-d itself. In accordance with iFDS, polarizing a 4+ ion, say Ce$^{4+}$ needs to overcome an energy proportional to 6325 kJmol$^{-1}$ (the 5th ionization energy), while La$^{3+}$, Ba$^{2+}$ and Cs$^+$ need to overcome the energies proportional to 4819 kJmol$^{-1}$ (the 4th ionization energy), 3600 kJmol$^{-1}$ (the 3rd ionization energy) and 2234.3 kJmol$^{-1}$ (the 2nd ionization energy) respectively. The absolute values are actually equal to the energy needed to ionize an atom or ion such that the electron is excited to a distance $r$. However, the ionization energies stated above are for taking that particular electron to $r \to \infty$. Considering this scenario, one can surmise that both $\lambda$ and $\gamma$ are predicted to reduce with increasing valence state. As anticipated, the decreasing magnitudes of both $\lambda$ and $\gamma$ with increasing valence
states have been calculated so as to fit the experimental data points. Furthermore, one can also understand the exponential decrease of \( \alpha_j(n_j) \) with \( 1+ \) (Fig. 2)), 2+ (Fig. 4)), 3+ (Fig. 5)) and 4+ (Fig. 6)) ions, which are as a result of increased \( \varepsilon_f \). Simply put, the exponential reduction of \( \alpha_j(n_j) \) for \( \text{Cs}^+ \rightarrow \text{Li}^+ \), \( \text{Ba}^{2+} \rightarrow \text{Be}^{2+} \), \( \text{La}^{3+} \rightarrow \text{B}^{3+} \) and \( \text{Ce}^{4+} \rightarrow \text{C}^{4+} \) are due to increased \( \varepsilon_I \). Similarly, the reduction of both \( X \) and \( Y \) is also due to reduced \( \alpha_j(n_j) \) for high valence state ions (4+) as compared with 1+ ions. It is important to realize that \( Y \propto \lambda \), which implies that \( Y \) increases with increasing ionic size since \( \lambda \propto n^2/2r_B \) as defined earlier.

Out of naivety, one should not assume that \( Y \) is supposed to increase from \( \text{Li}^+ \rightarrow \text{Be}^{2+} \rightarrow \text{B}^{3+} \rightarrow \text{C}^{4+} \) since the ionic size is increasing. This is because, different elements have different ionic properties due to different number of positive charge protons, which determines the Coulomb interactions. Actually, \( Y \) will increase from \{C, Si, Ti, Zr, Ce\} \( 4+ \rightarrow \{C, Si, Ti, Zr, Ce\}^3+ \) and so on for the respective ions. The average \( \varepsilon_I \) has been determined with \( \varepsilon_I[(X+n)] = \sum z_j \varepsilon f \), where \( z \) is the valence state. Prior to averaging, the initial, \( \text{Bi}^{3+}, \text{B}^{2+}, \text{Sr}^{2+} \) and \( \text{Ca}^{2+} \) ionization energies for all the elements mentioned above were taken from Ref. [34]. In summary, the proportionality, \( \alpha_j(n_j) \propto e^{A(E_f^0-E_f)} \) is indeed valid. On the other hand, the static dielectric constant, \( \epsilon(0, k) \) must also satisfy Eq. [10]. To this end, \( \text{BaTiO}_3 (\bullet) \), \( \text{SrTiO}_3 (\square) \), \( \text{CaTiO}_3 (\bigtriangleup) \) and \( \text{Ba}_{0.5}\text{Sr}_{0.5}\text{TiO}_3 (\diamondsuit) \) samples obtained from Ref. [31] are plotted in Fig. 4 as a function of average \( \varepsilon_I \) at \( T = T_C + 200 \text{ K} \). The average \( \varepsilon_I s \) for \( \text{Ba}^{2+} \), \( \text{Sr}^{2+} \) and \( \text{Ca}^{2+} \) are given by 734, 807, and 867 kJ mol\(^{-1}\) respectively. After applying iFDS, one can predict that \( \epsilon(0, k) \) should decrease from \( \text{BaTiO}_3 \rightarrow \text{SrTiO}_3 \rightarrow \text{CaTiO}_3 \) while the magnitude of \( \epsilon(0, k) \) for \( \text{Ba}_{0.5}\text{Sr}_{0.5}\text{TiO}_3 \) is expected to be between \( \text{BaTiO}_3 \) and \( \text{SrTiO}_3 \). All these predictions are remarkably in accordance with Eq. [10]. In fact, those experimental data [31] have been reproduced with significant accuracy using Eq. [10] as indicated with a solid line. Equation [10] has been rewritten as \( \epsilon(0, k) = X \exp[Y] \) in which the fitted values for \( X \) and \( Y \) are given in Fig. 3 itself. Equation [10] has been rewritten in the stated form because \( \epsilon(0, k) \gg 1 \) or \( K^2 \exp[\lambda(E_f^0-\varepsilon_f)] 

4. CONCLUSIONS

In conclusion, the evolution of polarizability, polarization, optical-static dielectric constants and the screened Coulomb potential has been derived for non-Fermi gas system using iFDS. These functions are able to explain the doping effect as well as reproduces the experimental doping trend with high accuracy in the well known BST and its related Perovskites namely, \( \text{BaTiO}_3 \), \( \text{Ba}_{0.5}\text{Sr}_{0.5}\text{TiO}_3 \), \( \text{SrTiO}_3 \) and \( \text{CaTiO}_3 \). The relationship between polarizability and iFDS is also found to be highly precise as compared with Pauling’s experimental data on 1+, 2+, 3+ and 4+ ions, which in turn justifies the applicability of iFDS.

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FIG. 1: The screened electrostatic potential with iFDS effect has been calculated against \( r \) with Eq. [11]. The solid lines are from Eq. [11]. In the limits, \( \varepsilon_I \rightarrow E_f^0 \) and \( \varepsilon_I \rightarrow \infty \), one can recover the TF screened potential \((1/r-e^{-K_z r})\) and bare Coulomb potential \((1/r)\) respectively. Notice that \((1/r-e^{-K_z r})\) and \(1/r\) are represented with filled circle and filled square respectively.

FIG. 2: Polarizability as a function of electrons number, \( \alpha_j(n_j) \) are calculated (solid lines) against \( \varepsilon_I \) in order to fit the experimental data points for a) 1+, b) 2+, c) 3+ and d) 4+ ions using \( \sum_j \alpha_j(n_j) = X \exp[Y] \), which is in accordance with the principle of Eq. [3]. The fitting parameters, \( X \) and \( Y \) are a constant of proportionality and \( \lambda(E_f^0-\varepsilon_f) \) respectively. All the experimental data points given in a), b), c) and d) were obtained from Pauling, [24] and Jaswal-Sharma, [31].
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\begin{equation}
\phi(r) = \frac{1}{r} \exp \left[ - \kappa_s r \right]
\end{equation}

\begin{equation}
\phi(r) = \frac{1}{r} \exp \left[ - \kappa_s r e^{\frac{1}{2} \lambda (E_F^0 - E_I)} \right]
\end{equation}
| Transition Metal | Exp. Data Points from |
|------------------|-----------------------|
| Li(+)            | Pauling [29]          |
| Na(+)            | Jaswal-Sharma (JS) [30]|
| K(+)             |                        |
| Rb(+)            |                        |
| Cs(+)            |                        |
| B(3+)            |                        |
| Al(3+)           |                        |
| Sc(3+)           |                        |
| Y(3+)            |                        |
| C(4+)            |                        |
| Si(4+)           |                        |
| Ti(4+)           |                        |
| Zr(4+)           |                        |
| Ce(4+)           |                        |
| Be(2+)           |                        |
| Mg(2+)           |                        |
| Ca(2+)           |                        |
| Sr(2+)           |                        |
| Ba(2+)           |                        |
| Li(+)            |                        |
| Na(+)            |                        |
| K(+)             |                        |
| Rb(+)            |                        |
| Cs(+)            |                        |
| B(3+)            |                        |
| Al(3+)           |                        |
| Sc(3+)           |                        |
| Y(3+)            |                        |
| C(4+)            |                        |
| Si(4+)           |                        |
| Ti(4+)           |                        |
| Zr(4+)           |                        |
| Ce(4+)           |                        |
| Be(2+)           |                        |
| Mg(2+)           |                        |
| Ca(2+)           |                        |
| Sr(2+)           |                        |
| Ba(2+)           |                        |

Calculated values:

- X: $4.0 \times 10^3$
- Y: 5.882

- X: $4.4 \times 10^2$
- Y: 1.563

- X: $2.6 \times 10^2$
- Y: 1.0

Graphical representation of the data points and calculated values for different transition metals.
Calculated

- BaTiO$_3$
- Ba(0.5)Sr(0.5)TiO$_3$
- SrTiO$_3$
- CaTiO$_3$

Measured at $T_1 = T_c + 200$ K by Ruprecht-Bell [31]

\[ x = 8.1 \times 10^4 \]

\[ y = 6.67 \times 10^{-3} \]