Theoretical Study and Evaluation of Charge Transfer Rate At Zn Metal Contact with SnO₂ Semiconductor Devices

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Abstract

In this paper, the tin oxide SnO₂ has been used in Zn/ SnO₂ junction devices structure to investigate the electric characteristic and charge transfer rate stability. The Zn/ SnO₂ Hetrojunction structures have been utilized to investigated the charge transfer rate using the quantum transition theory . The charge transfer rate properties of Zn/ SnO₂ devices with the orientation energy of configuration has been studied by quantum analysis of electronic transfer between donor and acceptor materials with MATLAP simulation program . It has been estimated and investigated using the work function of Zn metal and electronic affinity of SnO₂ adding interface junction, which consists of higher doped SnO₂ with the variation of energy absorption parameters of Zn metal ,it influenced the electric properties of Zn/ SnO₂ devices due to limited transfer of charge .The orientation energy is effected with dielectric and refractive indices for metal and semiconductor . The orientation energy effected on the electric properties behavior in Zn/ SnO₂ devices due to results of charge rate. The charge transfer rate is increased with increased the overlapping strength coupling and reach to maximum at coupling 1.60 × 10⁻¹¹eV² for all energy of system. From the calculation result of charge transfer rate , the rate is best at 2.119eV and has been achieved for Zn/ SnO₂ devices with orientation energy 0.06267eV .

Key Word: Charge Transfer Rate, SnO₂ Semiconductor.

1. Introduction. The charge transfer reaction is one of the best process in different science such that; physics, biophysics, chemistry and more electronic devices. It's involved the electrons are transfer between donor–acceptor electronic state from one to other in variety system such that metal, molecule and semiconductor applied devices system [1]. The charge transfer at hetrostructure devices such that; metal–semiconductor interface, molecule–metal and molecule–semiconductor are become very promise field in technology devices [2]. In recently, the hetero material devices are used in solar cells, optical devices materials; photonic devices and photo catalysis–structures [3]. The metal/semiconductor was very an important interest in more electronics fields such that; organic photovoltaic, solar cell and organic light emitting diodes [4]. Marcus R., Dogonadeze L and Gerischer were developed
the concept of charge transfer for contact solid with materials [5]. Hadi et al. show that orientation energy and alignment energy levels are the most important parameters for electron transfer processes in variety materials devices [6]. The transfer of electrons in hetrostructure materials are occurs from energy level in donor to energy level in acceptor material when alignment energy levels to each other and closed materials [7]. The electron transfer occurs at metal contact with semiconductor when the energy levels of metal and semiconductor were alignment with each other. The potential at interface limited by the work function for metal electronic affinity of semiconductor [8]. The barrier height is the main important parameter for the transfer resistance at interface, its depended on the alignment energy level of semiconductor and metal [9]. The energy levels of metal contact with semiconductor is illustrated in figure (1) [9].

![Figure (1).](image)

In the metal-semiconductor devices, the interface is very important for electronic properties through limited the charge transfer due to potential creation at interface [10]. In this work, we have studied and discussion of the electron transfer rate at devices constructed by the heterojunctions with Zn metals and SnO\textsubscript{2} semiconductor oxides. Further, the electron transfer mechanisms for Zn/SnO\textsubscript{2} has been explained according to quantum transition theory. The coefficients of electronic transfer of Zn contact with SnO\textsubscript{2} cross potential at interface of Zn-SnO\textsubscript{2} devices are calculated theoretically using MATLAB program.

2. Theory. The rate of charge transfer reaction due to Landau-Zener rule with the total density for electrons \( F(\epsilon, \epsilon_F) \) is [11].

\[
J_{ET} = \frac{2\pi}{\hbar} \int_{-\infty}^{\infty} F(\epsilon, \epsilon_F) |U_{mS}(\epsilon)|^2 \text{WFC} \, d\epsilon \quad \text{(1)}
\]

Where \( \hbar \) is the Dirac constant, \( U_{mS}(\epsilon) \) is strength coupling and WFC is the weight Franck Condon probability. The Franck Condon probability is written as [12].

\[
\text{WFC} = \sqrt{\frac{1}{4\pi T_{mS}k_B T}} e^{-\frac{(T_{mS} + \Delta V^0)^2}{4T_{mS}k_B T}} \quad \text{(2)}
\]

Where \( T_{mS} \) is reorientation energy, \( \Delta V^0 \) is driving energy, \( k_B \) is the Boltzman constant and \( T \) is the temperature. Substituting Eq. (2) in Eq. (1) with electronic state \( \rho(E) \) of metal to results.

\[
J_{ET} = \frac{2\pi}{\hbar} \int_{-\infty}^{\infty} F(\epsilon, \epsilon_F) \rho(E) \frac{1}{\sqrt{4\pi T_{mS}k_B T}} |U_{mS}(\epsilon)|^2 e^{-\frac{(T_{mS} + \Delta V^0)^2}{4T_{mS}k_B T}} \, d\epsilon \quad \text{(3)}
\]
The density function $F(\epsilon, \epsilon_F)$ [13] is reduced for $E_{CB} - E_F >> k_B T$ to
\[
F(\epsilon, \epsilon_F) = \frac{1}{(\epsilon - \epsilon_F)^{\frac{1}{k_B T}}} e^{-\frac{-(\epsilon - \epsilon_F)}{k_B T}} \quad \text{(4)}
\]

where $\epsilon_{CB}$ is the conduction band energy and $\epsilon_F$ is the Fermi energy. The drive energy $\Delta V^0$ is relative to occupied energy $E$ by [14].
\[
\Delta V^0 = \Delta V - \epsilon \quad \text{..................................(5)}
\]

Inserting Eq.(4) and Eq.(5) in Eq.(3) to obtained.
\[
J_{ET} = \frac{2\pi}{\hbar} \int_{-\infty}^{\infty} e^{-\frac{(\epsilon_{CB} - \epsilon)\gamma}{k_B T}} \rho(E) \sqrt{\frac{1}{4\pi T m_3 k_B T}} |U_{ms}(\epsilon)|^2 e^{-\frac{(T_{ms} + \Delta V^0 - \epsilon)^2}{4T m_3 k_B T}} \, d\epsilon \quad \text{......(6)}
\]

The exponent function in Eq.(6) can be expand to.
\[
e^{-\frac{(T_{ms} + \Delta V^0 - \epsilon)^2}{4T m_3 k_B T}} = e^{-\frac{(T_{ms} + \Delta V^0)^2}{4T m_3 k_B T}} e^{\frac{(T_{ms} + \Delta V^0)\gamma}{k_B T}} e^{-\frac{\gamma^2}{4T m_3 k_B T}} \rho(E) \, d\epsilon \quad \text{......(7)}
\]

The first term remove out of integral and the second term in right hand side is finished and Eq.(7) reduce with $E_{CB} - E_F >> k_B T$ to.
\[
J_{ET} = \frac{2\pi}{\hbar} \int_{-\infty}^{\infty} e^{-\frac{(T_{ms} + \Delta V^0)^2}{4T m_3 k_B T}} e^{\frac{(T_{ms} + \Delta V^0)\gamma}{k_B T}} \int_{-\infty}^{\infty} |U_{ms}(\epsilon)|^2 e^{-\frac{\gamma^2}{4T m_3 k_B T}} e^{-\frac{(\epsilon - \epsilon_F)\gamma}{k_B T}} \rho(E) \, d\epsilon \quad \text{......(8)}
\]

The high potential is given by.
\[
U(eV)) = \frac{(T_{ms} + \Delta V^0)^2}{4T m_5} \approx W_m - \chi \quad \text{...............(9)}
\]

Where $W_m$ and $\chi$ are the work function and electron affinity of semiconductor. The Fermi energy level depends on the applied potential $U_{app}$ [15].
\[
\epsilon_F = eU_{app} + \epsilon_F^0 \quad \text{....................(10)}
\]

Then Eq.(8) with Eq.(9) and Eq.(10) reduced to
\[
J_{ET} = \frac{2\pi}{\hbar} \int_{-\infty}^{\infty} e^{-\frac{(W_m - \chi)}{k_B T} - \frac{eU_{app}}{k_B T}} e^{\frac{(T_{ms} + \Delta V^0)\gamma}{k_B T}} \int_{-\infty}^{\infty} |U_{ms}(\epsilon)|^2 e^{-\frac{\gamma^2}{4T m_3 k_B T}} \rho(E) \, d\epsilon \quad \text{..............(11)}
\]

The density of concentration is [16-17].
\[
n_{eq} = N_e e^{-\frac{-(\epsilon - \epsilon_F^0)}{k_B T}} \int_{-\infty}^{\infty} \rho(E) f(E) \, d\epsilon \quad \text{.................(12)}
\]

We reformed Eq.(13) and inserting in Eq.(12) to given .Inserting Eq.(12) in Eq.(11) to results.
Then the expectation value of strength coupling is given by

\[ \langle \hat{\mathcal{U}}_{\text{ms}}(\epsilon)^2 \rangle = \int_{-\infty}^{\infty} f(\epsilon) \rho(\epsilon) |\mathcal{U}_{\text{ms}}(\epsilon)|^2 \, d\epsilon \approx \langle |\mathcal{U}_{\text{ms}}(0)|^2 \rangle \ldots \ldots \ldots \ldots (14) \]

Inserting Eq.(14) in Eq.(13) and integrate over space to obtained,

\[ J_{\text{ET}} = \frac{2\pi}{h} \frac{1}{4\pi T_{\text{ms}} k_{\text{B}} T} e^{\frac{W_{\text{m}} - \mathcal{X}}{k_{\text{B}} T}} \sqrt{n_{\text{eq}}} \int_{-\infty}^{\mathcal{X}} e^{-\frac{\epsilon^2}{4T_{\text{ms}} k_{\text{B}} T}} \langle |\mathcal{U}_{\text{ms}}(0)|^2 \rangle \, d\epsilon \ldots \ldots (15) \]

The solution of integral in Eq.(15) for the first approximation is obtained

\[ J_{\text{ET}} = \frac{2\pi}{h} \frac{1}{4\pi T_{\text{ms}} k_{\text{B}} T} e^{\frac{W_{\text{m}} - \mathcal{X}}{k_{\text{B}} T}} \sqrt{n_{\text{eq}}} \langle |\mathcal{U}_{\text{ms}}(0)|^2 \rangle \left( \frac{\pi}{4T_{\text{ms}} k_{\text{B}} T} \right) \ldots \ldots (16) \]

The effective orientation energy \( T_{\text{ms}}(eV) \) for electron transfer is [18].

\[
T_{\text{ms}}(eV) = \frac{e^2}{4\pi \epsilon_0} \left[ \frac{1}{2d_s} \left( \frac{1}{n_m^2} - \frac{1}{\epsilon_m} \right) + \frac{1}{2d_m} \left( \frac{1}{n_m^2} - \frac{1}{\epsilon_m} \right) - \frac{1}{4d_s} \left( \frac{n_m^2 - n_m^2}{n_m^2 + n_m^2} \right) \right] - \frac{1}{4d_m} \left( \frac{n_m^2 - n_m^2}{n_m^2 + n_m^2} \right) \ldots \ldots (17)
\]

where \( e \) is the charge of electrons, \( \epsilon_0 \) is the permittivity \( a_s \), and \( a_m \) were radii for semiconductor and metal respectively , \( ds \) and \( dm \) were the distance between semiconductor, metal and interface alternatively , \( R_m-s \) was the distance between semiconductor and metal, \( \epsilon_s \) and \( \epsilon_m \) were the statistical and optical dielectric constant.

The refractive index \( n_m \) of metal can by calculated using [19].

\[ |n_m| = n_m, n_m^* = \sqrt{N^2 + k^2} \ldots \ldots \ldots (18) \]

Where \( N \) is refraction coefficient and \( k \) is extinction coefficient,

\[ n_m = N + ik \] and conjugate \( n_m^* = N - ik \).

The dielectric constant \( \epsilon \) of metal can by calculated using [19].

\[ |\epsilon| = \epsilon \epsilon^* = \sqrt{\epsilon_1^2 + \epsilon_2^2} \ldots \ldots \ldots \ldots (19) \]

Where \( \epsilon_1 \) and \( \epsilon_2 \) are dielectric parameters , \( \epsilon_1 = N^2 - k^2 \) and \( \epsilon_2 = 2Nk \).

The radii of the material is [20].

\[ a_l = \left( \frac{3M}{4\pi N D} \right)^{\frac{1}{3}} \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots (20) \]

where \( M \) is the molecular weight, \( D \) is the mass density and \( N \) is Avogadro’s number.

3. Results. The main purpose of this work is to calculate and investigate the charge transfer possibility in \( \text{Zn/ SnO}_2 \) devices structure by using quantum transition theory that can introduce good tools to understanding the electric characteristic of this materials .The reorientation energy is influenced strongly on the electric characteristic through limited the
charge transfer cross interface. It influence the structure effect, dielectric effect and optical effect. The radii of Zn and SnO$_2$ are calculated using Eq.(20) with taking the molecular weight and mass density from table(1) for Zn and table (2) for SnO$_2$ with Avogadro's constant $6.02 \times 10^{23} \frac{\text{Molecule}}{\text{mol}}$, results of radii are summarized in both tables (1) and (2) for Zn and SnO$_2$.

**Table (1). The main properties of Zn metal.**

| Properties                     | Quantity          |
|--------------------------------|-------------------|
| Atomic Weight (g/mol)          | 65.39[19]         |
| Density (g/cm$^3$)             | 7.14 [19]         |
| Crystal structure              | Hexagonal [19]    |
| Energy gap (eV) at 300K        | 3.3 [21]          |
| Lattice constant(Å)            | a=b=c=4.52[21]    |
| Melting point (°C)             | 4195°C[19]        |
| Radius calculated (Å)          | 1.537             |
| Work function or Electron affinity (eV) | 4.33[22]         |

The SnO$_2$ semiconductor is best common transparent conductive oxide and extremely complicated refractive indices with optical absorption. The main characteristic of typical sample of SnO$_2$ is listed in table(2).

**Table (2). The main properties of SnO$_2$.**

| Properties       | SnO$_2$       |
|------------------|---------------|
| Atomic weight    | 150.69 [23]   |
| Crystal structure| Wurtzite [24] |
| Density (g/cm$^3$)| 6.95 [23]    |
| Refractive index | 1.94 [24]     |
| Dielectric constant | 4.175 [24]  |
It is clear that Eq.(17) show the calculation of orientation energy of system as a function of refractive index and dielectric constant of Zn metal and SnO$_2$ semiconductor. The refractive index and dielectric constant of Zn metal can carried by using refraction coefficient $N$ and the extinction coefficient $k$ that tabulated in table(3).

### Table 3. The index of refraction $n$ and the extinction coefficient $k$ [19].

| Energy $E$(eV) | Refractive index (N) | extinction coefficient(K) | Energy $E$(eV) | refractive index (N) | extinction coefficient(K) |
|---------------|---------------------|----------------------------|---------------|---------------------|--------------------------|
| 1.033         | 1.288               | 5.400                      | 2.066         | 2.080               | 4.723                    |
| 1.078         | 1.309               | 4.902                      | 2.094         | 1.708               | 4.792                    |
| 0.952         | 1.316               | 6.221                      | 2.119         | 1.332               | 4.475                    |
| 0.866         | 1.362               | 6.688                      | 2.275         | 0.972               | 4.287                    |
| 0.992         | 1.383               | 5.891                      | 2.255         | 0.756               | 3.762                    |
| 0.751         | 1.446               | 7.415                      | 2.666         | 0.547               | 3.427                    |
| 0.827         | 1.474               | 6.968                      | 2.917         | 0.477               | 3.047                    |
| 1.127         | 1.689               | 4.406                      | 3.220         | 0.391               | 2.746                    |
| 1.181         | 1.970               | 4.017                      | 3.594         | 0.314               | 2.304                    |
| 1.240         | 2.871               | 3.287                      | 4.06          | 0.301               | 2.007                    |

The refractive index is estimation using Eq.(18) with refraction index $N$ and the extinction coefficient $k$ from table(3), results are shown in table (4).

### Table 4. The calculated refractive index $n$ for Zn metal.

| $E$(eV) | $N$[19] | $K$[19] | $n = N + ik$ | $n_m$ |
|---------|---------|---------|--------------|-------|
| 1.033   | 1.288   | 5.400   | 1.288+5.400i | 5.551 |
| 1.078   | 1.309   | 4.902   | 1.309+4.902i | 5.074 |
| 0.952   | 1.316   | 6.221   | 1.316+6.221i | 6.358 |
| 0.866   | 1.36    | 6.688   | 1.362+6.688i | 6.826 |
Furthermore, the dielectric constant was computed by using Eq. (19), results are listed in Table (5).

| | \(N\) | \(K\) | \(\varepsilon_1 = N^2 - k^2\) | \(\varepsilon_2 = 2Nk\) | \(\varepsilon = \varepsilon_1 + i\varepsilon_2\) | \(|\varepsilon|\) |
|---|---|---|---|---|---|---|
| 0.992 | 1.38 | 5.891 | 1.383+5.891i | 6.051 |
| 0.751 | 1.44 | 7.415 | 1.446+7.415i | 7.555 |
| 0.827 | 1.47 | 6.968 | 1.474+6.968i | 7.123 |
| 1.127 | 1.68 | 4.406 | 1.689+4.406i | 4.719 |
| 1.181 | 1.97 | 4.017 | 1.970+4.017i | 4.474 |
| 1.240 | 2.87 | 3.287 | 2.871+3.287i | 4.364 |
| 2.066 | 2.08 | 4.723 | 2.080+4.723i | 5.160 |
| 2.094 | 1.70 | 4.792 | 1.708+4.792i | 5.087 |
| 2.119 | 1.33 | 4.475 | 1.332+4.475i | 4.669 |
| 2.275 | 0.97 | 4.287 | 0.972+4.287i | 4.396 |
| 2.255 | 0.75 | 3.762 | 0.756+3.762i | 3.838 |
| 2.666 | 0.54 | 3.427 | 0.547+3.427i | 3.471 |
| 2.917 | 0.47 | 3.047 | 0.477+3.047i | 3.084 |
| 3.220 | 0.39 | 2.746 | 0.391+2.746i | 2.774 |
| 3.594 | 0.31 | 2.304 | 0.314+2.304i | 2.325 |
| 4.06 | 0.30 | 2.007 | 0.301+2.007i | 2.030 |
| 1.0 | 6.22 | 1 | | |
| 1.0 | 1.288 | 5.40 | -27.499 | 13.920 | -27.499+13.920i | 30.8 |
| 1.309 | 4.90 | -22.319 | 12.839 | -22.319+12.839i | 25.7 |
| 0.9 | 1.316 | 6.22 | -36.970 | 16.380 | -36.970+16.380i | 40.4 |

Table 5. Results of the dielectric constant of Zn metal.
Upon the results of dielectric constant and refractive index of Zn metal in tables(4) and (5) and taken refractive and dielectric indices of SnO$_2$ from table(2) with radii for metal $= 1.537\,\text{Å}$ and semiconductor $= 2.048\,\text{Å}$ and using Eq.(17) to calculate the orientation energy $T$ for Zn/SnO$_2$ with MATLAB and taken the distances $d_s$ and $d_m$ for semiconductor and metal $= 3.048\,\text{Å}$, $= 2.537$ and interface $ms = 3.585$ with taken $\frac{A_2}{\tau} = 14.4$. Results are listed in tables (6) for Zn/ SnO$_2$.

Table 6. Results calculated of orientation energy $T_{ms}$ (eV) for Zn/ SnO$_2$.

| E(eV) | N  | K  | Orientation energy |
|-------|----|----|-------------------|
| 0.8   | 66 | 1.362 | 6.68 | -42.880 | 18.230 | -42.880+18.230 | 46.5 |
| 0.9   | 92 | 1.383 | 5.89 | -32.789 | 16.300 | -32.789+16.300 | 36.6 |
| 0.7   | 51 | 1.446 | 7.41 | -52.900 | 21.459 | -52.900+21.459 | 57.0 |
| 0.8   | 27 | 1.474 | 6.96 | -46.390 | 20.549 | -46.390+20.549 | 50.7 |
| 1.1   | 27 | 1.689 | 4.40 | -16.559 | 14.890 | -16.559+14.890 | 22.2 |
| 1.1   | 81 | 1.970 | 4.01 | -12.259 | 15.830 | -12.259+15.830 | 20.0 |
| 1.2   | 40 | 2.871 | 3.28 | -2.559 | 18.880 | -2.559+18.880 | 19.0 |
| 2.0   | 66 | 2.080 | 4.72 | -17.980 | 19.649 | -17.980+19.649 | 26.6 |
| 2.0   | 94 | 1.708 | 4.79 | -20.047 | 17.098 | -20.047+17.098 | 26.9 |
| 2.1   | 19 | 1.332 | 4.47 | -18.249 | 11.929 | -18.249+11.929 | 18.3 |
| 2.2   | 75 | 0.972 | 4.28 | -17.440 | 8.339 | -17.440+8.339 | 19.3 |
| 2.2   | 55 | 0.756 | 3.76 | -13.585 | 5.695 | -13.585+5.695 | 14.7 |
| 2.6   | 66 | 0.547 | 3.42 | -11.449 | 3.749 | -11.449+3.749 | 12.0 |
| 2.9   | 17 | 0.477 | 3.04 | -9.059 | 2.909 | -9.059+2.909 | 9.51 |
| 3.2   | 20 | 0.391 | 2.74 | -7.389 | 2.148 | -7.389+2.148 | 7.69 |
| 3.5   | 94 | 0.314 | 2.30 | -5.209 | 1.450 | -5.209+1.450 | 5.40 |
| 4.0   | 6  | 0.301 | 2.00 | -3.940 | 1.209 | -3.940+1.209 | 4.12 |
The barrier for Zn/SnO$_2$ interface is estimated using Eq.(9) to results 0.37eV. However, the charge transfer rate is calculated using Eq.(16) with the orientation energy, Work function of Zn metal =4.33eV, electronic affinity of SnO$_2$ semiconductor = 3.96eV, unit cell of SnO$_2$ is calculated using with lattice constant $a = 4.74$, $c=3.19$ for SnO$_2$ and results is

| V | 1.033 | 1.288 | 5.400 | 30,822 | 5.551 | 0.061524927 |
|---|-------|-------|-------|--------|-------|---------------|
| V | 1.078 | 1.309 | 4.902 | 25,749 | 5.074 | 0.061673982 |
| V | 0.952 | 1.316 | 6.221 | 40,436 | 6.358 | 0.061369603 |
| V | 0.866 | 1.362 | 6.688 | 46,594 | 6.826 | 0.061313122 |
| V | 0.992 | 1.383 | 5.891 | 36,617 | 6.051 | 0.061418251 |
| V | 0.751 | 1.446 | 7.415 | 57,087 | 7.555 | 0.061253291 |
| V | 0.827 | 1.474 | 6.968 | 50,738 | 7.123 | 0.061285367 |
| V | 1.127 | 1.689 | 4.406 | 22,269 | 4.719 | 0.061829904 |
| V | 1.181 | 1.970 | 4.017 | 20,022 | 4.474 | 0.061968608 |
| V | 1.240 | 2.871 | 3.287 | 19,053 | 4.364 | 0.062041352 |
| V | 2.066 | 2.080 | 4.723 | 26,634 | 5.160 | 0.061642536 |
| V | 2.094 | 1.708 | 4.792 | 26,935 | 5.087 | 0.067919285 |
| V | 2.119 | 1.332 | 4.475 | 18,351 | 4.669 | 0.026707551 |
| V | 2.275 | 0.972 | 4.287 | 19,331 | 4.396 | 0.062019495 |
| V | 2.255 | 0.756 | 3.762 | 14,730 | 3.838 | 0.062515175 |
| V | 2.666 | 0.547 | 3.427 | 12,048 | 3.471 | 0.06302222 |
| V | 2.917 | 0.477 | 3.047 | 9.515 | 3.084 | 0.06380071 |
| V | 3.220 | 0.391 | 2.746 | 7.695 | 2.774 | 0.064702239 |
| V | 3.594 | 0.314 | 2.304 | 5.407 | 2.325 | 0.066662327 |
| V | 4.06 | 0.301 | 2.007 | 4.121 | 2.030 | 0.068564912 |
\[ V(\text{cm}^3) = 71.671 \times 10^{24}, \text{ the equilibrium density concentration } (2.22 \times 10^{24}), \text{ and taking the coupling } = (0.35 , 0.60, 0.85, 1.100 1.35 \text{ and } 1.60) \times 10^{-14}[28], \text{ results are listed in table(7).} \]

**Table 7. Results calculated of the charge transfer rate for Zn/ SnO\(_2\).**

| E(eV)   | Transition energy | \text{The charge Transfer Rate} \times 10^5 |
|---------|-------------------|------------------------------------------|
|         |                   | Electronic coupling                       |
|         |                   | 0.35  | 0.60  | 0.85  | 1.100 | 1.35  | 1.60  |
| 1.033   | 0.061524927       | 1.47  | 2.533 | 3.5   | 4.6   | 5.700 | 6.755 |
| 1.078   | 0.061673982       | 1.46  | 2.512 | 3.5   | 4.6   | 5.652 | 6.699 |
| 0.952   | 0.061369603       | 1.49  | 2.555 | 3.6   | 4.6   | 5.750 | 6.815 |
| 0.866   | 0.061313122       | 1.49  | 2.563 | 3.6   | 4.7   | 5.768 | 6.837 |
| 0.992   | 0.061418251       | 1.48  | 2.548 | 3.6   | 4.6   | 5.734 | 6.796 |
| 0.751   | 0.061253291       | 1.50  | 2.572 | 3.6   | 4.7   | 5.788 | 6.860 |
| 0.827   | 0.061285367       | 1.49  | 2.567 | 3.6   | 4.7   | 5.777 | 6.847 |
| 1.127   | 0.061829904       | 1.45  | 2.490 | 3.5   | 4.5   | 5.603 | 6.640 |
| 1.181   | 0.061968608       | 1.44  | 2.470 | 3.5   | 4.5   | 5.559 | 6.589 |
| 1.240   | 0.062041352       | 1.43  | 2.460 | 3.4   | 4.5   | 5.537 | 6.562 |
| 2.066   | 0.061642536       | 1.46  | 2.516 | 3.5   | 4.6   | 5.662 | 6.710 |
| 2.094   | 0.067919285       | 1.04  | 1.797 | 2.5   | 3.2   | 4.044 | 4.792 |
| 2.119   | 0.0626707551      | 2.69  | 4.612 | 6.5   | 8.4   | 10.37 | 12.30 |
| 2.275   | 0.062019495       | 1.43  | 2.463 | 3.4   | 4.5   | 5.543 | 6.570 |
4. Discussion. The orientation energy of Zn/SnO₂ has been varied from 0.0613 eV to 0.068 eV with different energy in range 0.866 eV to 4.06 eV, the optimum values of orientation energy is about 0.068 eV in maximum energy 4.06 eV approach. The dielectric constant Zn metal is varied from 4.121 to 57.087 corresponding to energy 4.06eV to 0.751eV whereas the refractive index parameters varied from 2.030 to 6.826 correspond to energy 4.06 to 0.866. On the other hand, the orientation energy difference with difference both refractive index and dielectric constant for Zn metal where the parameters of SnO₂ is constant. From the theoretical of charge transfer, it is clear that the variation of orientation energy strongly influenced on the transfer rate parameters. At 2.119 eV energy, the charge transfer rate is higher 2.690 x 10⁵ at orientation energy 0.062eV than energy 4.06 eV has lower transfer rate parameters 1.014 x 10⁵ at orientation energy 0.068eV. From table (6) the values of orientation energy remain same to 0.061eV until reach absorption energy 2.066 eV for Zn/SnO₂ with distances variation. Here Zn is acting as SnO₂, so after absorption of more than energy 2.094 eV, the orientation energy increased to the top values 0.0679eV. From the charge transfer rate, it is clear that the variation of orientation energy influence on the charge transfer rate parameters, the rate vitiated with variety of orientation energy. At increased the overlapping strength coupling, the charge rate is increased and reach to maximum at coupling 1.60 x 10⁻¹¹ eV² for all energy of system. The charge rate is higher at higher coupling than other values of coupling parameters. The values of charge transfer remain varies by same ratio except at energy 2.119 eV the system have large values of charge transfer comparing with other values of energy. Therefore, the high charge transfer rate in scale of 2.690, 4.612, 6.534, 8.457, 10.37 and 12.30 x 10⁵ have been achieved with performance orientation energy parameters 0.062eV by using absorption energy 2.119eV of Zn metal contact with SnO₂. This is because the orientation of Zn metal contact with SnO₂ is best in this energy comparing to other energies, the more energy has been added to charge energy to transfer through interface. However, the energy is around 4.06eV with orientation energy 0.0685eV, the system have been minimum charge transfer rate about 1.014, 1.739, 2.464, 3.188, 3.913 and 4.638 x 10⁵. In physical perspectives, the system at this energy need more energy to orientation structure to initial transfer and after orientation between Zn and SnO₂ system, the electrons should be need higher energy to transfer and this leads to facilitate minimum transfer rate.
5. Conclusion. The theoretical analysis of this work investigated the charge transfer rate based Zn/SnO2 devies with modified tin oxide Wurtzite structure. In this Zn/SnO2 devices, the orientation energy has been varied 0.0615 to 0.0685eV with the optimum charge transfer rate parameters have been found $1.014 \times 10^5$ to $2.690 \times 10^5$. The theoretical results have shown that the charge transfer rate enhanced by structure of material due to orientation energy. The charge transfer rate parameters increased with increased orientation energy and coupling overlapping of energy levels and reach maximum in range $2.690 \times 10^5$, $4.612 \times 10^5$, $6.534 \times 10^5$, $8.457 \times 10^5$, $10.37 \times 10^5$to reach top $12.30 \times 10^5$ with an increased orientation energy 0.0626 eV in absorption energy 2.119eV. Moreover, the charge transfer rate increases with the increase of operating overlapping coupling to reach maximum for all energies at strength coupling $1.60 \times 10^{-11}$ eV with room temperature, which also indicates the better transfer of charge cross interface of Zn/SnO2 devices.

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