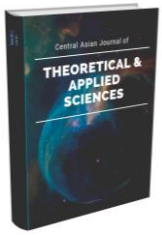

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Article

Theoretical Studies of Electronic Transition Characteristics of Zn-ZnO Interface

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Abstract: Electron transfer processes play a crucial role in chemical, physical, and electronic systems, particularly in metal-semiconductor interfaces used in devices like photovoltaics and LEDs. Among these, the Zn/ZnO interface is notable for its practical applicability, owing to ZnO's wide bandgap and semiconductor properties. Despite theoretical models, the detailed impact of material-specific optical constants on reorientation energy and electron transfer rate remains inadequately characterized. This study theoretically investigates the electronic transition characteristics at the Zn–ZnO interface by calculating the reorientation energy and electron transfer rate using quantum theory and MATLAB-based simulations. Findings demonstrate that electron transfer rate increases with decreased orientation energy, driven by enhanced energy level alignment. Maximum orientation energy (0.408 eV) was observed at 4.06 eV, with corresponding lowest transfer rate, whereas minimum orientation energy (0.334 eV) at 2.119 eV yielded higher transfer rates. The refractive index and dielectric constants derived from extinction and refraction coefficients significantly affect transition parameters. This work provides a detailed theoretical framework combining quantum transition models with empirical refractive and dielectric data to quantify energy alignment and transfer efficiency at a Zn/ZnO interface. The results offer a refined approach to predicting and optimizing electron transfer behavior in Zn/ZnO-based optoelectronic devices, informing future material design for enhanced energy conversion efficiency.

Keywords: theoretical studied, electronic transition, Zn–Zno interface

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1. Introduction

The electronic transfer processes are the basic processes in more chemistry, physical, biophysical system and different electronic devices. In a variety of metal, molecule, and semiconductor applied device systems, electrons must go from a donor electronic state to an acceptor electronic state [1]. In other areas of electronics, such as organic photovoltaics, solar cells, and organic light-emitting diodes, metal/semiconductor was of great interest[2]. The fundamental concept of electron transition in solid contact with materials are developing due to Marcus R., Gerischer and Dogonadeze L [3].Recently, the electron transfer theory become active area search in physical applied and electronic devices technology especially in molecule semiconductor , molecule -metal and metal – semiconductor interface[4]. The transfer mechanisms in various material systems when

the energy levels of the materials were aligned with one another were the subject of several theoretical introductions by Hadi et al. in the previous years [5]. It will be necessary for the electrons to go from one state in the donor material to the acceptor state in another material that has similar energy levels and is closed to the other materials[6]. The detailed information of energy levels alignment are limited the possible and quantity of electronic transfer at these contact, its crucial for the improved and developed of higher efficient applicable[7]. The potential barrier created at interface between metal and semiconductor and electrons are transition cross the forbidden potential energy due to gained the kinetic energy when an electrical voltage was applied between two materials [8]. In this contribution, the electron transfer occurs between Zn metal and with ZnO ,it most common II-VI semiconductor materials and widely has using in most electronic applications.It has energy-band gap around 3.4 eV [9].

The purpose of this work is studied and calculated the characteristics of electronic transition and rate for the electronic transfer interaction of Zn metal with ZnO semiconductor . The electronic transfer coefficients of Zn / ZnO interface is computed and analysis theoretically , and the electronic transfer rate is calculated using MATLAP program.

2. Materials and Methods

The electrons transfer process must be described using Landau-Zener rule and given by [10].

$$J_{ET} = \frac{2\pi}{\hbar}|U_{mS}(\epsilon)|^2\, WFC \tag{1}$$

where WFC is the weight Franck Condon probability, $U_{mS}(\epsilon)$ is the strength coupling, and $\hbar$ is the Dirac constant.The chance of Franck Condon is expressed as [11].

$$WFC = \sqrt{\frac{1}{4\pi T_{mS} k_B T}}\, e^{-\frac{(T_{mS}+\Delta \boldsymbol{V}^0)^2}{4T_{mS}k_B T}} \tag{2}$$

Where T_{mS} is reorientation energy , $\Delta \boldsymbol{V}^0$ is driving energy , k_B is the Boltzman constant and $T$is the temperature . Introduce the density of electronic state $\rho(E)$ for metal and inserting Eq.(2) in Eq.(1) to given.

$$J_{ET} = \frac{2\pi}{\hbar}\sqrt{\frac{1}{4\pi T_{mS} k_B T}}\,\rho(E)|U_{mS}(\epsilon)|^2\, e^{-\frac{\left(T_{mS}+\Delta V^0\right)^2}{4T_{mS}k_B T}} \tag{3}$$

Introduce the Fermi Dirac function density for all electrons in Eq.(3) to obtained.

$$J_{ET} = \frac{2\pi}{\hbar}\int_{-\infty}^{\infty} F(\epsilon,\epsilon_F)\,\rho(E)\sqrt{\frac{1}{4\pi T_{mS} k_B T}}\,|U_{mS}(\epsilon)|^2\, e^{-\frac{(T_{mS}+\Delta V^0)^2}{4T_{mS}k_B T}}\, d\epsilon \tag{4}$$

The Fermi Dirac function $F(\epsilon,\epsilon_F)$ *is* [12].

$$F(\epsilon,\epsilon_F) = \left(e^{\frac{(\epsilon_{CB}-\epsilon_F)}{k_B T}} + 1\right)^{-1} \tag{5}$$

where the Fermi energy is denoted by ϵ_F and the conduction band energy by ϵ_{CB}.In relation to the occupied energy E, the driving energy $\Delta \boldsymbol{V}^0$ is [13].

$$\Delta \boldsymbol{V}^0 = \Delta V_\circ - \epsilon \tag{6}$$

Inserting Eq.(6) and Eq.(5) in Eq.(4) to results.

$$J_{ET} = \frac{2\pi}{\hbar}\int_{-\infty}^{\infty}\left(e^{\frac{(\epsilon_{CB}-\epsilon_F)}{k_B T}} + 1\right)^{-1}\rho(E)\sqrt{\frac{1}{4\pi T_{mS} k_B T}}\,|U_{mS}(\epsilon)|^2\, e^{-\frac{(T_{mS}+\Delta V_\circ-\epsilon)^2}{4T_{mS}k_B T}}\, d\epsilon \tag{7}$$

The exponent function in Eq.(7) can be expand to.

$$e^{-\frac{(T_{mS}+\Delta V_\circ-\epsilon)^2}{4T_{mS}k_B T}} = e^{-\frac{(T_{mS}+\Delta V_\circ)^2}{4T_{mS}k_B T}}\, e^{\frac{(T_{mS}+\Delta V_\circ)\epsilon}{2T_{mS}k_B T}}\, e^{-\frac{\epsilon^2}{4T_{mS}k_B T}} \tag{8}$$

After removing the first term from the integral, the second term on the right side is completed, and Eq. (7) reduces with $E_{CB} - E_F >> k_BT$ to.

$$J_{ET} = \frac{2\pi}{\hbar}\sqrt{\frac{1}{4\pi T_{mS}k_BT}}\, e^{-\frac{(T_{mS}+\Delta V_\circ)^2}{4T_{mS}k_BT}} \int_{-\infty}^{\infty} |U_{mS}(\epsilon)|^2 e^{-\frac{\epsilon^2}{4T_{mS}k_BT}} e^{\frac{-(\epsilon_{CB}-\epsilon_F)}{k_BT}} \rho(E)\, d\epsilon \quad (9)$$

The high potential is given by.

$$U(eV) = \frac{(T_{mS}+\Delta V_\circ)^2}{4T_{mS}} \approx W_m - \chi \quad (10)$$

where W_m and χ stand for the metal's work function and the semiconductor's electron affinity, respectively. The applied potential U_{app}determines the Fermi energy level [14].

$$\epsilon_F = eU_{app} + \epsilon_F^\circ \quad (11)$$

Then Eq.(9) with Eq.(10) and Eq.(11) reduced to

$$J_{ET} = \frac{2\pi}{\hbar}\sqrt{\frac{1}{4\pi T_{mS}k_BT}}\, e^{-(\frac{W_m-\chi}{k_BT})} e^{\frac{eU_{app}}{k_BT}} e^{\frac{-(\epsilon_{CB}-\epsilon_F^\circ)}{k_BT}} \int_{-\infty}^{\infty} \rho(\epsilon)|U_{mS}(\epsilon)|^2 e^{-\frac{\epsilon^2}{4T_{mS}k_BT}}\, d\epsilon \quad (12)$$

The density of concentration is [15].

$$n_{eq} = N_c\, e^{\frac{-(\epsilon_{CB}-\epsilon_F^\circ)}{k_BT}} = N_c\, e^{\frac{-eU_{bi}}{k_BT}}\, e^{\frac{eU_{app}}{k_BT}} \quad (13)$$

We reformed Eq.(13) and inserting in Eq.(12) to given.

$$J_{ET} = \frac{2\pi}{\hbar}\sqrt{\frac{1}{4\pi T_{mS}k_BT}}\, e^{-(\frac{W_m-\chi}{k_BT})} \frac{n_{eq} e^{\frac{-(\epsilon_{CB}-\epsilon_F^\circ)}{k_BT}}}{N_c\, e^{\frac{-eU_{bi}}{k_BT}}} \int_{-\infty}^{\infty} \rho(\epsilon)|U_{mS}(\epsilon)|^2 e^{-\frac{\epsilon^2}{4T_{mS}k_BT}}\, d\epsilon \quad (14)$$

The term $N_c\, e^{\frac{-eU_{bi}}{k_BT}}$ is equal to [16].

$$N_c\, e^{\frac{-eU_{bi}}{k_BT}} = \int_0^{\infty} \frac{\rho(\epsilon)f(\epsilon)}{V}\, d\epsilon \quad (15)$$

Substituting Eq.(15) in Eq.(14) and assume factor $f(\epsilon) = e^{\frac{-(\epsilon_{CB}-\epsilon_F^\circ)}{k_BT}}$ to Fermi parameters to results.

$$J_{ET} = \frac{2\pi}{\hbar}\sqrt{\frac{1}{4\pi T_{mS}k_BT}}\, e^{-(\frac{W_m-\chi}{k_BT})} V n_{eq} \frac{\int_{-\infty}^{\infty} f(\epsilon)\rho(\epsilon)|U_{mS}(\epsilon)|^2 e^{-\frac{\epsilon^2}{4T_{mS}k_BT}}\, d\epsilon}{\int_0^{\infty} \rho(\epsilon)f(\epsilon)d\epsilon} \quad (16)$$

Then the expectation value of strength coupling is given by

$$\langle|\widehat{U}_{mS}(\epsilon)|^2\rangle = \frac{\int_{-\infty}^{\infty} f(\epsilon)\rho(\epsilon)|U_{mS}(\epsilon)|^2\, d\epsilon}{\int_0^{\infty} \rho(\epsilon)f(\epsilon)d\epsilon} \quad (17)$$

The squaring strength coupling can expand with harmonic approximation to.

$$\langle|\widehat{U}_{mS}(\epsilon)|^2\rangle = \langle|\widehat{U}_{mS}(0)|^2\rangle[1 + \epsilon + \epsilon^2 + \epsilon^3 + \epsilon^4 + \epsilon^5 + \cdots \ldots \ldots + \epsilon^m] \quad (18)$$

Inserting Eq.(18) in Eq.(17)and integrate over space to obtained.

$$J_{ET} = \frac{2\pi}{\hbar}\sqrt{\frac{1}{4\pi T_{mS}k_BT}}\, e^{-(\frac{W_m-\chi}{k_BT})} V n_{eq} \int_{-\infty}^{\infty} e^{-\frac{\epsilon^2}{4T_{mS}k_BT}} \langle|\widehat{U}_{mS}(0)|^2\rangle[1 + \epsilon + \epsilon^2 + \epsilon^3 + \epsilon^4 + \epsilon^5 + \cdots \ldots \ldots + \epsilon^m] d\epsilon \quad (19)$$

The solution of integral in Eq.(19) for the first approximation is obtained.

$$J_{ET} = \frac{2\pi}{\hbar}\sqrt{\frac{1}{4\pi T_{mS}k_BT}}\, e^{-(\frac{W_m-\chi}{k_BT})} V n_{eq} \langle|\widehat{U}_{mS}(0)|^2\rangle \sqrt{\frac{\pi}{4T_{mS}k_BT}} \quad (20)$$

The effective orientation energy T_mS (eV) for electron transfer is [17].

$$T_{mS}(eV) = \frac{e^2}{4\pi\varepsilon_0}\left[\frac{1}{2a_s}\left(\frac{1}{n_m^2} - \frac{1}{\varepsilon_m}\right) + \frac{1}{2a_m}\left(\frac{1}{n_m^2} - \frac{1}{\varepsilon_m}\right) - \frac{1}{4d_s}\left(\frac{n_m^2 - n_s^2}{n_m^2 + n_s^2}\,\frac{1}{n_s^2} - \frac{\varepsilon_m - \varepsilon_s}{\varepsilon_m + \varepsilon_s}\,\frac{1}{\varepsilon_s}\right) - \frac{1}{4d_m}\left(\frac{n_{s-}^2 n_m^2}{n_s^2 + n_m^2}\,\frac{1}{n_m^2} - \frac{\varepsilon_s - \varepsilon_m}{\varepsilon_s + \varepsilon_m}\,\frac{1}{\varepsilon_m}\right) - \frac{2}{Rm-s}\left(\frac{1}{n_s^2 + n_m^2} - \frac{1}{\varepsilon_s + \varepsilon_m}\right)\right] \quad (21)$$

where e represents the electron charge, ε_0 is the permittivity, and ds and dm are the distances between the semiconductor, metal, and interface, respectively. Alternatively, ε and n were the statistical and optical dielectric constants, while $Rm\text{-}s$ was the distance between semiconductor and metal.

Metal's refractive index, or n_m, may be computed using [18].

$$|n_m| = n_m . n_m{}^* = \sqrt{N^2 + k^2} \quad (22)$$

Where N is refraction coefficient and k is extinction coefficient,

$n_m = N + ik$ and conjugate $n_m{}^* = N - ik$.

The dielectric constant ε of metal can by calculated using.

$$|\varepsilon| = \varepsilon\varepsilon^* = \sqrt{{\varepsilon_1}^2 + {\varepsilon_2}^2} \quad (23)$$

Where ε_1 and ε_2 are dielectric parameters , $\varepsilon_1 = N^2 - k^2$ and $\varepsilon_2 = 2Nk$.

The radii of the material is [19].

$$a_i = \left(\frac{3M}{4\pi ND}\right)^{\frac{1}{3}} \quad (24)$$

where Avogadro's number is N, mass density is D, and molecular weight is M.

3. Results

The characteristics of electron transfer are studied and calculated theoretically using quantum transition theory and using MATLAP program . The electronic transfer rate in Zn/ZnO devices has active influence with reorientation energy, it a function of structure ,dielectric and refractive index of material. The particle radii of Zn can be estimation by Eq.(24) with inserting Avogadro's constant was used to get the molecular weight and mass density for Zn and ZnO from tables (1) and (2). $6.02 \times 10^{23} \frac{Molecule}{mol}$,results are listed in table (1) and talble(2) for Zn and ZnO respectively.

TABLE 1. The main properties of Zn metal.

Properties	Quantity
Atomic Weight (g/mol)	65.39[18]
Density (g/cm3)	7.14 [18]
Crystal structure	Hexagonal [18]
Energy gap (eV) at 300K	3.3 [20]
Lattice constant(Å)	a=b=c=4.52[20]
Melting point (°C)	4195 °C[18]
Radius calculated (Å)	1.537
Work function or Electron affinity (eV)	4.33[21]

The ZnO semiconductor exhibits a Wurtzite crystal structure with a density of 5.66 g/cm³ and a bandgap of 3.4 eV at 300K. It has a dielectric constant of 8.5, a refractive index of 2.00337, and an effective conduction band state density of 2.22×10^{24} cm^{-3}, indicating favorable electronic properties.(Table 2)

TABLE 2. properties of ZnO semiconductor [22].

Properties	Quantity
Atomic Weight (g/mol)	81.38
Density (g/cm3)	5.66
Crystal structure	Wurtzite
Refractive index	2.00337
Dielectric constant	8.5
Effective density of states in conduction Band, NC (cm^{-3})	2.22×10^{24}

Energy gap (eV) at 300K	3.4
Lattice constant (Å)	a=0.32495,c=0.5206
Melting point (°C)	1975 °C
Radius calculated (Å)	1.786
Electron affinity (eV)	4.5

The orientation energy of the system is really determined by the dielectric constant and refractive index of ZnO semiconductor and Zn metal. Refraction coefficient N is used to calculate the refractive index and dielectric constant, whereas table (3) lists the extinction coefficient k.

TABLE 3. The extinction coefficient k and the index of refraction n [18].

Energy E(eV)	Refraction Index(N)	Extinction Coefficient(K)	Energy E(eV)	Refraction 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

Using the refraction index N and the extinction coefficient k from table (3), the refractive index is estimated using Eq. (22). The results are displayed in table (4).

TABLE 4. The Zn metal's computed refractive index, n [18]

$E(eV)$	N	K	$n = N + ik$	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	*1.362*	*6.688*	*1.362+6.688i*	*6.826*
0.992	*1.383*	*5.891*	*1.383+5.891i*	*6.051*
0.751	*1.446*	*7.415*	*1.446+7.415i*	*7.555*
0.827	*1.474*	*6.968*	*1.474+6.968i*	*7.123*
1.127	*1.689*	*4.406*	*1.689+4.406i*	*4.719*
1.181	*1.970*	*4.017*	*1.970+4.017i*	*4.474*
1.240	*2.871*	*3.287*	*2.871+3.287i*	*4.364*
2.066	*2.080*	*4.723*	*2.080+4.723i*	*5.160*
2.094	*1.708*	*4.792*	*1.708+4.792i*	*5.087*
2.119	*1.332*	*4.475*	*1.332+4.475i*	*4.669*
2.275	*0.972*	*4.287*	*0.972+4.287i*	*4.396*
2.255	*0.756*	*3.762*	*0.756+3.762i*	*3.838*
2.666	*0.547*	*3.427*	*0.547+3.427i*	*3.471*

2.917	*0.477*	*3.047*	*0.477+3.047i*	*3.084*
3.220	*0.391*	*2.746*	*0.391+2.746i*	*2.774*
3.594	*0.314*	*2.304*	*0.314+2.304i*	*2.325*
4.06	*0.301*	*2.007*	*0.301+2.007i*	*2.030*

On the other hand ,for different values of energy ,we computed the dielectric constant using Eq.(23) with calculated parameters ε_1and ε_2,results are listed in table (5)

TABLE 5. Results of the dielectric parameters ε_1 and ε_2 and dielectric function.

$E(eV)$	N	K	$\varepsilon_1 = N^2 - k^2$	$\varepsilon_2 = 2Nk$	$\varepsilon = \varepsilon_1 + i\varepsilon_2$	$\lvert\varepsilon\rvert$
1.033	*1.288*	*5.400*	*-27.499*	*13.920*	*-27.499+13.920 i*	*30.822*
1.078	*1.309*	*4.902*	*-22.319*	*12.839*	*-22.319+12.839 i*	*25.749*
0.952	*1.316*	*6.221*	*-36.970*	*16.380*	*-36.970+16.380 i*	*40.436*
0.866	*1.362*	*6.688*	*-42.880*	*18.230*	*-42.880+18.230 i*	*46.594*
0.992	*1.383*	*5.891*	*-32.789*	*16.300*	*-32.789+16.300 i*	*36.617*
0.751	*1.446*	*7.415*	*-52.900*	*21.459*	*-52.900+21.459 i*	*57.087*
0.827	*1.474*	*6.968*	*-46.390*	*20.549*	*-46.390+20.549 i*	*50.738*
1.127	*1.689*	*4.406*	*-16.559*	*14.890*	*-16.559+14.890 i*	*22.269*
1.181	*1.970*	*4.017*	*-12.259*	*15.830*	*-12.259+15.830 i*	*20.022*
1.240	*2.871*	*3.287*	*-2.559*	*18.880*	*-2.559+18.880 i*	*19.053*
2.066	*2.080*	*4.723*	*-17.980*	*19.649*	*-17.980+19.649 i*	*26.634*
2.094	*1.708*	*4.792*	*-20.047*	*17.098*	*-20.047+17.098 i*	*26.935*
2.119	*1.332*	*4.475*	*-18.249*	*11.929*	*-18.249+11.929 i*	*18.351*
2.275	*0.972*	*4.287*	*-17.440*	*8.339*	*-17.440+8.339 i*	*19.331*
2.255	*0.756*	*3.762*	*-13.585*	*5.695*	*-13.585+5.695 i*	*14.730*
2.666	*0.547*	*3.427*	*-11.449*	*3.749*	*-11.449+3.749 i*	*12.048*
2.917	*0.477*	*3.047*	*-9.059*	*2.909*	*-9.059+2.909 i*	*9.515*
3.220	*0.391*	*2.746*	*-7.389*	*2.148*	*-7.389+2.148 i*	*7.695*
3.594	*0.314*	*2.304*	*-5.209*	*1.450*	*-5.209+1.450 i*	*5.407*
4.06	*0.301*	*2.007*	*-3.940*	*1.209*	*-3.940+1.209 i*	*4.121*

Upon the results of radii for metal $a_{Zn} = 1.537$Å and semiconductor$a_{ZnO} = 1.786$Å and using the static dielectric constants and refractive index for ZnO from table (2) and taken the calculated results of the static dielectric constants ε_m and refractive index n_m for the Zn metal from tables (4) and (5) and using Eq.(21) to calculate the orientation energy $T_{ms}(eV)$ for Zn metal (donor) contact with an acceptor ZnO semiconductor in Zn/ ZnO systems using MATLAB program with taken the distances d_s and d_m for semiconductor and metal $d_{Zno} = 2.786$, , $d_{Zn} = 2.537$ and interface $R_{m-s} = 3.323$ with taken $\frac{\Delta e^2}{4\pi\epsilon_0} = 14.4(eV)$.Results are listed in tables (6).

TABLE 6. Results calculated of orientation energy T_ms (eV)for Zn/ ZnO.

$E(eV)$	N	K	ε_m	n_m	*Orientation energy (eV)*
1.033	*1.288*	*5.400*	*30.822*	*5.551*	*0.364*
1.078	*1.309*	*4.902*	*25.749*	*5.074*	*0.365*
0.952	*1.316*	*6.221*	*40.436*	*6.358*	*0.362*
0.866	*1.362*	*6.688*	*46.594*	*6.826*	*0.362*
0.992	*1.383*	*5.891*	*36.617*	*6.051*	*0.363*
0.751	*1.446*	*7.415*	*57.087*	*7.555*	*0.361*
0.827	*1.474*	*6.968*	*50.738*	*7.123*	*0.362*
1.127	*1.689*	*4.406*	*22.269*	*4.719*	*0.366*
1.181	*1.970*	*4.017*	*20.022*	*4.474*	*0.367*
1.240	*2.871*	*3.287*	*19.053*	*4.364*	*0.368*
2.066	*2.080*	*4.723*	*26.634*	*5.160*	*0.365*

2.094	*1.708*	*4.792*	*26.935*	*5.087*	*0.371*
2.119	*1.332*	*4.475*	*18.351*	*4.669*	*0.334*
2.275	*0.972*	*4.287*	*19.331*	*4.396*	*0.368*
2.255	*0.756*	*3.762*	*14.730*	*3.838*	*0.371*
2.666	*0.547*	*3.427*	*12.048*	*3.471*	*0.375*
2.917	*0.477*	*3.047*	*9.515*	*3.084*	*0.380*
3.220	*0.391*	*2.746*	*7.695*	*2.774*	*0.386*
3.594	*0.314*	*2.304*	*5.407*	*2.325*	*0.398*
4.06	*0.301*	*2.007*	*4.121*	*2.030*	*0.408*

The potential barrier for Zn metal contact with ZnO semiconductor in Zn/ZnO heterojunction is calculated using Eq.() to results -0.17 eV. The contribution of the electron transfer rate effective by the orientation energy ,Work function of Zn metal $W_m(eV)$ =4.33eV, electronic affinity of ZnO semiconductor $\chi(eV) = 4.5$eV , unit cell of ZnO is calculated using $V = |a.b \times c|$ with a,b and c are lattice constant for ZnO and results is V(cm^3)= 0.054×10^{-24},the equilibrium of density concentration $n_{eq=}(2.22 \times 10^{24})$, and taking the coupling $|U_{mS}(\epsilon)|^2$ = (0.35 , 0.60,.0.85, 1.100 and 1.35) $\times 10^{-11} eV^2$[23]

with room temperature T=300k .Results data of rate are listed in table (7)

TABLE 7. determined the Zn/ZnO electron transfer rate.

Energe (eV)	**Reorientation energy(eV)**	**The Electron Transfer Rate$\times 10^{11}(\frac{1}{sec.eV})$**				
		Electron Coupling $\|U_{mS}(\epsilon)\|^2 \times 10^{-11} eV^2$				
		0.60	**0.35**	**0.85**	**1.100**	**1.35**
1.033	0.364	5.069	8.691	12.312	15.933	19.544
1.078	0.365	5.011	8.591	12.171	15.750	19.329
0.952	0.362	5.113	8.799	12.466	16.132	19.799
0.866	0.362	5.157	8.841	12.524	16.208	19.891
0.992	0.363	5.113	8.765	12.416	16.069	19.720
0.751	0.361	5.183	8.885	12.587	16.289	19.992
0.827	0.362	5.169	8.861	12.553	16.245	19.938
1.127	0.366	4.953	8.491	12.029	15.567	19.105
1.181	0.367	4.903	8.406	11.908	15.410	18.913
1.240	0.368	4.877	8.362	11.846	15.330	18.814
2.066	0.365	5.023	8.612	12.199	15.788	19.376
2.094	0.371	4.747	8.138	11.529	14.920	18.311
2.119	0.334	6.815	1.168	16.551	21.419	26.287
2.275	0.368	4.855	8.375	11.864	15.354	18.844
2.255	0.371	4.721	8.093	11.465	14.837	18.209
2.666	0.375	4.568	7.831	11.094	14.357	17.620
2.917	0.380	4.356	7.468	10.579	13.692	16.803
3.220	0.386	4.139	7.096	10.053	13.009	15.967
3.594	0.398	3.743	6.417	9.091	11.765	14.439
4.06	0.408	3.430	5.880	8.330	10.780	13.230

4. Discussion

Based on the quantum transition theory, the electron transfer characteristic has been computed and discussed theoretically.Reorientation energy is most frequently thought of as an extra strong coupling to the electronic transfer rate, as expressed in terms of Equation (20).The refractive index and dielectric constant for Zn and ZnO, which are products of the refraction coefficient N and the extinction coefficient k, are then used to calculate the reorientation energy.Due to both expressions in Eqs. (22) and (23), the refractive index and dielectric constant have a forced relationship with the refraction coefficient N and the

extinction coefficient k. Table (4) show the refractive index n_m is decreased with increased energy E(eV) and increased with increased refraction coefficient N from N =0.301 to 2.080 corresponding increased n_m from 2.030 to reach 5.160 at energy 2.066eV and from 1.288 to 1.446 with increased n_m from 5.551 to 7.555 while is decreased n_m from 7.123 to reach 4.364 with increased N =1.474to 2.871.While in general, the refractive index n_m increased with increased the extinction coefficient k. On the other hand ,the dielectric constant ε_m in table(5) are increased with increased the extinction coefficient k . While the dielectric constant ε_m increased from 4.121 to 26.634 with increased refraction coefficient N from N =0.301 to 2.080 and have different values with refraction coefficient N from 1.288 to 1.970 .The orientation energy in table (6) increased and decreased alternatively upon the increased and decreased the dielectric constant and refractive index of Zn metal . As seen as the orientation energy has upper values 0.408 eV at energy E=4.06eV ,dielectric constant $\varepsilon_m = 4.121$ and refractive index $n_m = 2.030$ while has lower values 0.334eV at at energy E= 2.119eV ,dielectric constant $\varepsilon_m = 18.351$ and refractive index $n_m = 4.669$ .The electronic transition rate in table (7) show that the electronic transition rate increased with decreased the orientation energy ,this because the orientation energy has taken from system to reorientation the configuration the donor and acceptor with each other before electronic transfer process. Furthermore, the transfer of electrons increased with less orientation energy as results system have large driving energy comparing with system have large orientation to reduce decreased drive energy and less transfer of electrons.Due to quantum transfer the electron transfer rate increased with increased the strength coupling that's showing in table(7),its because the strength coupling indicate the alignment of energy levels between Zn metal and ZnO semiconductor .

Table(7) show that the electronic rate increased with lower energy 0.952, 0.866, 0.992, 0.751 and 0.827eV while decreased with increased energy from 2.917, 3.220 , 3.594 and reach lower rate 15.680×10^{11} at upper energy E=4.06eV this because the effective of dielectric constant ,refractive index on both optical and electric characteristic.

5. Conclusion

We conclusions due to discussion of the electronic transition rate behaviours in Zn/ZnO device ,the orientation energy and strength coupling are largely effect on the transition rate due to orientation energy work to reform the configuration of Zn and ZnO with each other and the strength coupling effected to alignment energy levels for system.The electrons transfer rate and the orientation energy are force related with refraction coefficient N and the extinction coefficient k .The orientation energy values limited the quantity of electrons to transfer over potential as results to effect on electronic density . Increased electronic transfer rate for decreased orientation energy and decreased the energy of system.

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