

Article

# Study and Calculation the Current Flow Rate of RUN3-ZnO Solar Cell Device

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**Abstract:** In this work, the current flow rate in a RUN3 solar cell was calculated using a [Ru(dcbpyH<sub>2</sub>)<sub>2</sub>(NCS)<sub>2</sub>] sensor where dcbpyH<sub>2</sub>-4,4'-dicarboxyl-2,2'-bipyridine when it came into contact with zinc oxide (ZnO) in a chloroform solution. A quantitative scenario was used to study the current flow rate in order to understand the efficiency of the RUN3-ZnO solar cell. The increasing demand for higher solar cell efficiency has led to the search for high current flow rate in solar cell systems. The electronic current flow rate played a significant role in characteristics of efficiency for RUN3-ZnO device. The current flow rate was evaluated using quantum processing with a connected model of the reorganization energy, and a quasi-quantum model of the electron drive energy, potential, and coupling interference. The current flow rate results showed a strong dependence on the reorganization energy, voltage, and coupling strength. These factors were calculated, and their effects on current density were discussed theoretically in this system using MATLAB software. The electrical current absorption spectra of the RUN3-ZnO compound, calculated at different values of reorganization energy and coupling strength, were analyzed to determine the appropriate solvent from among the seven solvents used, as well as the corresponding pKa values for its ground state. The current flow rate results show a strong dependence on the transfer energy and voltage. It increases as the transfer energy and voltage decrease, and vice versa. The data indicate that the electron current is high ( $\approx 10^7$  eV) for the N3/ZnO device when using chloroform solvent, compared to its lowest value ( $\approx 10^6$  eV) when using methanol solvent at an operating power  $\Delta FE^0 = 0.3$  eV.

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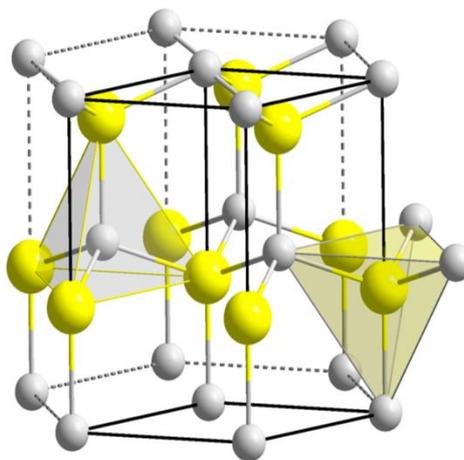
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**Keywords:** Current Flow Rate , RUN3 dye, ZnO Solar Cell

## 1. Introduction

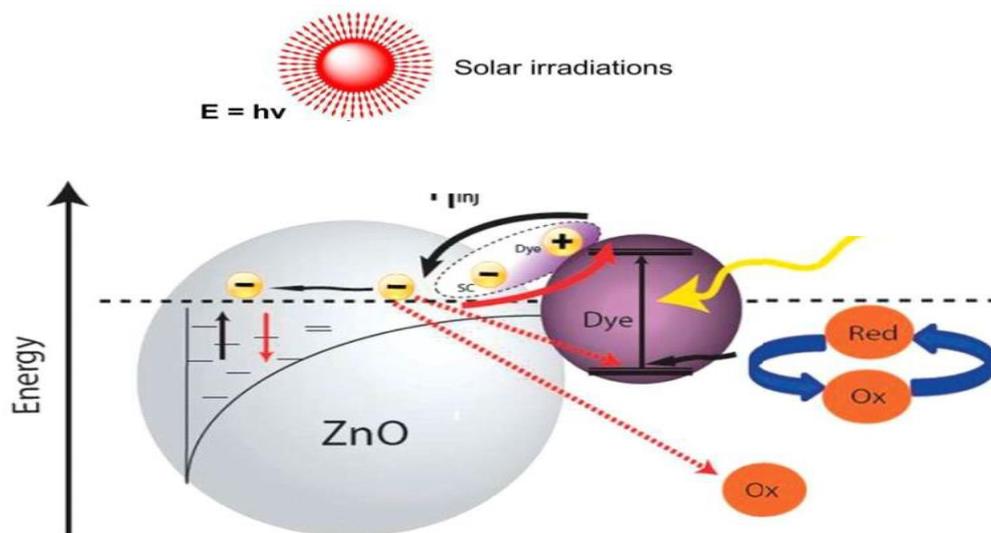
Global energy demand is increasing at an accelerating pace, making a clean and reliable energy source essential for the global economy. The environmental risks of fossil fuel use necessitates the search for alternative energy sources. Many variable renewable energy technologies have recently been developed with the aim of providing effective solutions for clean energy supplies[1]. Increasing the efficiency of equipment in energy conversion and developing efficient energy sources, solar energy is a clean energy source, an attractive tool, and receives great attention, and will not run out. [2]. Harnessing the solar spectrum is a formidable challenge to meet today's energy demands, and researchers together engineers continue to explore new materials and functional methods for photovoltaic cell applications. These efforts aim to improve overall energy conversion

efficiency, cell lifespan, stability, and reduce production costs[3]. Dye-sensitized solar cells (DSSCs) are gaining increasing appeal due to their high photocurrent conversion efficiency, good optical properties, low cost, ease of manufacturing, light weight, flexibility, and rapid energy recovery. They have been used in many technological fields [4]. Electronic transport reaction is the basic reaction in various molecular-semiconductor heterojunction devices, where electrons move from a donor state to an acceptor state [5-6]. Electron transfer at the contact surface between heterogeneous devices is of great importance and plays a key role between the dye and the semiconductor [7]. Electron transfer from ruthenium-based sensitizing dye compounds RUN3 named as  $[\text{Ru}(\text{dcbpyH})_2(\text{NCS})_2(\text{N}_3)]$  to semiconductor materials has shown high efficiency for heterogeneous devices in the solar spectral range [8]. The contact of dyes with semiconductors is a highly effective technique in various technological applications, thanks to electronic transport reaction. The process of electron transfer and light absorption achieves separation between the dye molecule and the wide bandgap semiconductor, where the dye acts as a light-absorbing material [9]. The efficiency of solar cells improves as their performance increases, and this efficiency depends on the materials used in their manufacture [10]. DSSC cells have received increasing attention in recent years due to the remarkable improvement in energy conversion efficiency using less expensive cells [11]. In general, RUN3 is a common organic ruthenium molecule from the well-known  $\text{Ru}(\text{bpy})$  family, and is used in the manufacture of DSSC cells. It is one of the most efficient dyes as a charge-transfer layer [12]. The RUN3 dye is a commercially available ruthenium dye and sensitizer, *cis*-di(thiocyanato)-bis[2,2'-bipyridyl-4,4'-dicarboxylic acid]ruthenium(II) (N3). It exhibits promising efficiency (11%) and is widely used in DSSC systems. It is also characterized by its low cost, organic sensitivity, as well as stability[13]. However, the ZnO semiconductor has become of most important in technical applications. It features an energy gap of 3.37 electron volts, as well as superior thermal conductivity, mechanical stability, high electronic mobility, and excellent optical transmittance. It also has excellent optical and electrical properties, making it a suitable material for a variety of applications, the lattice structure is shown in figure 1[14].



**Figure 1.** ZnO wurtzite cell

In this work, the current flow rate of an RUN3-ZnO solar cell system was studied and calculated. The electron transfer from an excited RUN3 molecule to the conduction band of ZnO upon photon absorption by the dye was investigated, as shown in Figure 2. This included evaluating the reorganization energy factor resulting from the solvent polarity. For the RUN3-ZnO system, the reorganization energy, electron density, potential, coupling strength, and current flow rate ( $t$ ) are all important factors.



**Figure 2.** The schematic of the energy levels in the RUN3-ZnO devices

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## 2. Theory

The charge current rate at dye-sensitized heterojunction is given by [15].

$$K_J(E) = \frac{4\pi^2 q}{h} \int_0^\infty F(E) |\langle \hat{M}_{NZ}(E) \rangle|^2 D_{NZ}(E) \delta(E_{RUN3} - E_{ZnO}) dE \dots (1)$$

Where  $q$ ,  $h$  and  $F(E)$  are charge, Planck constant and Fermi-Dirac function,  $\langle \hat{M}_{NZ}(E) \rangle$  and  $D_{NZ}(E)$  are the strength couple and density of state, ( $E_{RUN3}$  and  $E_{ZnO}$  are energy of RUN# donor and ZnO acceptor. The density of state  $D_{NZ}(E)$  is [16].

$$D_{NZ}(E) = \frac{e^{-\frac{(T_{NZ} + \Delta E^0)^2}{4T_{NZ}k_B T}}}{\sqrt{4\pi T_{NZ}k_B T}} \dots \dots \dots (2)$$

Where  $T_{NZ}$ ,  $k_B$  and  $\Delta E^0$  are reorganization energy, Boltzmann constant and driving energy and  $T$  is temperature. The activation electronic density of system is [17].

$$= \delta(E_{RUN3} - E_{ZnO}) \dots \dots \dots (3)$$

Inserting Eq.(2) and Eq.(3) in Eq.(1) assume constant  $\langle \hat{M}_{NZ}(E) \rangle \approx \langle \hat{M}_{NZ}(0) \rangle$  to give.

$$K_J(E) = \frac{4\pi^2 q}{h} \frac{|\langle \hat{M}_{NZ}(E) \rangle|^2}{\sqrt{4\pi T_{NZ}k_B T}} \int_0^\infty F(E) \rho_{ac}(E) e^{-\frac{(T_{NZ} + \Delta E^0)^2}{4T_{NZ}k_B T}} dE \dots (4)$$

Furthermore, the activation density of states is [18].

$$\rho_{ac}(E) = D_Z(E) d_Z^{-2/3} \frac{l_Z}{\delta_Z} \dots \dots \dots (5)$$

Where  $D_Z(E)$ ,  $d_Z$  and  $l_Z$  are the density of states, atomic density and effective length in ZnO semiconductor, and  $\delta_Z$  is the average diameter of atomic in lattice given by [18].

$$\delta_Z = \left(\frac{6}{\pi}\right)^{1/3} \dots \dots \dots (6)$$

Insert Eq.(6) together Eq.(5) into Eq.(4) with and reform to results.

$$K_J(E) = \frac{4\pi^2 q}{h} \frac{|\langle \hat{M}_{NZ}(E) \rangle|^2}{\sqrt{4\pi T_{NZ}k_B T}} e^{-\frac{(T_{NZ} + \Delta E^0)^2}{4T_{NZ}k_B T}} \int_0^\infty D_Z(E) d_Z^{-2/3} \frac{l_Z}{\delta_Z} F(E) dE \dots \dots (7)$$

The integral in Eq.(7) can be solved to given [19].

$$\int_0^{\infty} D_Z(E) d_Z^{-2/3} \frac{L_Z}{\delta_Z} F(E) dE = d_Z^{-2/3} \frac{L_Z}{\delta_Z} [n_Z] \dots \dots \dots (8)$$

Insert Eq.(8) in Eq.(7).

$$K_j(E) = \frac{4\pi^2 q}{h} \frac{|\langle \hat{M}_{NZ}(E) \rangle|^2}{\sqrt{4\pi T_{NZ} k_B T}} e^{-\frac{(T_{NZ} + \Delta E^0)^2}{4 T_{NZ} k_B T}} d_Z^{-2/3} \frac{L_Z}{\delta_Z} [n_Z] \dots \dots \dots (9)$$

The drive energy is function of conduction band energy  $E_{cb}$  and ionization energy  $qE_o$ , it is written by [20]

$$\Delta E^0 = (E_{cb} - qE_o) \dots \dots \dots (10)$$

Furthermore, the potential at the contact RUN3 dye and ZnO is given by an expression [21].

$$U(eV) = \frac{[T_{NZ} + (E_{cb} - qE_o)]^2}{4 T_{NZ}} \dots \dots \dots (11)$$

The reorganization energy  $T_{NZ}(eV)$  of the RUN3 dye contact with ZnO semiconductor is [22]

$$T_{NZ}(eV) = \frac{q^2}{4\pi\epsilon_0} \left[ \frac{1}{2r} \left[ \frac{1}{n^2} - \frac{1}{\epsilon} \right] - \frac{1}{4R} \left[ \left( \frac{n_Z^2 - n^2}{n_Z^2 + n^2} \right) \left( \frac{1}{n^2} \right) - \frac{\epsilon_Z^2 - \epsilon^2}{\epsilon_Z^2 + \epsilon^2} \frac{1}{\epsilon^2} \right] \right] \dots \dots \dots (12)$$

Where  $\epsilon_0$ ,  $n$  and  $\epsilon$  are free permittivity, refractive index and dielectric constant of solvent,  $r$  and  $R$  are radius of molecule and distance between dye and the semiconductor,  $n_{sem}$  is the refractive index of semiconductor and  $\epsilon_{sem}$  is dielectric constant of the semiconductor. The radius of the dye molecule can be evaluated from the apparent molar volumes using spherical approach [23].

$$r(nm) = \left( \frac{3}{4\pi} \frac{m}{N\rho} \right)^{\frac{1}{3}} \dots \dots \dots (13)$$

Where  $m$  is the molecular weight,  $N$  is Avogadro number, and  $\rho$  is the density of material.

### 3. Results

Due to quantum transition theory, the current flow rate of the RUN3-ZnO solar cell devices can calculate using electronic transport reaction. Firstly, the reorganization energy can be calculated depending on continuum model for energy levels with estimation the radii of sensitizer RUN3 molecule. The reorganization energy requires to start charge transport from RUN3 dye to conduction band in ZnO semiconductor. Seven solvents (Acetic acid, Methyl cellosolve, n-butanol, Methanol, Trichloromethane, Dimethylacetamide, and Ethanol) use a polar media with RUN3-ZnO device. The properties show in table (1).

**Table 1.** The physical properties of solvents [22].

| Solvents          | Chemical form                                | Density g/cm <sup>3</sup> | Boiling point(c <sup>0</sup> ) | Melting point(c <sup>0</sup> ) | Viscosity (cp) | Dielectric constant ( $\epsilon$ ) | Refractive index(n) |
|-------------------|--|---------------------------|--------------------------------|--------------------------------|----------------|------------------------------------|---------------------|
| Acetic acid       | C <sub>2</sub> H <sub>4</sub> O <sub>2</sub> | 1.049                     | 118                            | 17                             | 1.31           | 6.15                               | 1.37                |
| Methyl cellosolve | C <sub>3</sub> H <sub>8</sub> O <sub>2</sub> | 0.965                     | 124                            | 85                             | 1.70           | 16.90                              | 1.40                |
| n-butanol         | C <sub>4</sub> H <sub>10</sub> O             | 0.810                     | 117                            | -90                            | 2.95           | 17.80                              | 1.39                |
| Methanol          | CH <sub>4</sub> O                            | 0.792                     | 64.7                           | -98                            | 13.9           | 32.60                              | 1.32                |
| Trichloromethane  | CHCL <sub>3</sub>                            | 1.492                     | 61                             | -64                            | 0.58           | 4.81                               | 1.44                |
| Dimethylacetamide | C <sub>4</sub> H <sub>9</sub> N              | 0.937                     | 165                            | -20                            | 2.14           | 37.80                              | 1.43                |
| Ethanol           | C <sub>2</sub> H <sub>6</sub> O              | 0.816                     | 78                             | -114                           | 1.10           | 24.55                              | 1.36                |

The reorganization energy  $T_{NZ}(eV)$  is function of radii of RUN3 and ZnO, refractive index and dielectric constant of solvents as well as ZnO. Radii of RUN3 and ZnO estimate

using Eq.(13) by inserted molecule weight  $M(705.64)$  and density  $\rho(1.36g/cm^3)$  for RUN3 molecule dye and molecule weight  $M(81.38)$  and density  $\rho(5.66g/cm^3)$  for ZnO semiconductor from table (2). Results of radii are  $5.9A^0$  and  $3.8 A^0$  for RUN3 molecule and ZnO respectively.

**Table 2.** Properties of ZnO semiconductor [21].

| Properties                                  | ZnO[ 21]                              |
|---|---------------------------------------|
| Molecular weight g/mol                      | 81.38                                 |
| Dielectric Constant                         | 8.5                                   |
| Mass Density (g/cm <sup>3</sup> )           | 5.66                                  |
| Density of state $N_s/cm^3$ )               | $2.22 \times 10^{24}$                 |
| Crystal structure                           | Wurzite                               |
| Refractive index                            | 2.0033                                |
| Lattice constant( $\text{\AA}$ )            | $a=0.3.249, c=0.5206$                 |
| Radius( $\text{\AA}$ )                      | 3.8025                                |
| Conduction band energy(eV)                  | 4.5                                   |
| Energy gab eV                               | 3.37                                  |
| Refractive index                            | 2.0041                                |
| Electron concentration (1/cm <sup>3</sup> ) | n-type $10^{20}$ and p-type $10^{17}$ |
| Electron affinity (eV)                      | 4.3                                   |

However the reorganization energy  $T_{NZ}(eV)$  calculates using Eq.(12) by inserted the radii of RUN3 and ZnO, dielectric constant and refractive index of solvents from table(1) and dielectric constant and refractive index of ZnO semiconductor from table(2) with taken  $\frac{1}{2} \frac{e^2}{4\pi\epsilon_0} \approx 7.2eV$  and distance with each other materials is  $9.705 \text{ \AA}$  to result show in table(3).

**Table 3.** The calculation of reorganization energy  $T_{NZ}(eV)$  for RUN3-ZnO solar cell.

| Solvents          | Chemical form | Dielectric constant ( $\epsilon$ )[21] | Refractive index( $n$ )[21] | $T_{NZ}(eV)$ |
|-------------------|---------------|--|-----------------------------|--------------|
| Acetic acid       | $C_2H_4O_2$   | 6.15                                   | 1.37                        | 0.364        |
| Methyl cellosolve | $C_3H_8O_2$   | 16.90                                  | 1.40                        | 0.467        |
| n-butanol         | $C_4H_{10}O$  | 17.80                                  | 1.39                        | 0.472        |
| Methanol          | $CH_4O$       | 32.60                                  | 1.32                        | 0.550        |
| Trichloromethane  | $CHCL_3$      | 4.81                                   | 1.44                        | 0.270        |
| Dimethylacetamide | $C_4H_9N$     | 37.80                                  | 1.43                        | 0.485        |
| Ethanol           | $C_2H_6O$     | 24.55                                  | 1.363                       | 0.514        |

The current flow rate  $K_j(E)$  is the main important parameters for the known the electronic properties devices that gives more knowledge about efficiency for the RUN3-ZnO device solar cell. It can be evaluated to understand of the electric properties of RUN3-ZnO device. The expression in Eq.(9) can be taken to evaluate the current flow rate  $K_j(E)$  for RUN3-ZnO device with the seven solvents by insert the reorganization energy  $T_{NZ}(eV)$  from tables (3), strength coupling strength  $\langle \hat{M}_{NZ}(E) \rangle = 0.212, 0.255, 0.291, 0.324, 0.353$  and  $0.380$  eV with taken energy  $\Delta E^0 =$

0.3,0.4 and 0.5eV, atomic density of ZnO  $d_z = 5.7 \frac{1}{\text{cm}^3}$ , effective length  $l_z = 3 \times 10^{-10}\text{m}$ [23] and taken carrier concentration  $[n_z] = 2.22 \times 10^{24}$ .Results as is shown in the Tables (4),(5) and (6) for RUN3-ZnO devices system.

**Table 4.** Calculated of the current flow rate  $K_J(E)$ for RUN3-ZnO with  $\Delta E^0 = 0.3\text{eV}$ .

| solvent           | Chemical form                    | $T_{NZ}(eV)$ | $K_J(E) \times 10^{+7}$                     |        |        |        |        |       |
|-------------------|----------------------------------|--------------|---|--------|--------|--------|--------|-------|
|                   |                                  |              | Strength coupling( $\hat{M}_{NZ}(E)$ ) (eV) |        |        |        |        |       |
|                   |                                  |              | 0.212                                       | 0.255  | 0.291  | 0.324  | 0.353  | 0.380 |
| Acetic acid       | $\text{C}_2\text{H}_4\text{O}_2$ | 0.364        | 8.520                                       | 1.230  | 1.609  | 1.988  | 2.366  | 2.745 |
| Methyl cellosolve | $\text{C}_3\text{H}_8\text{O}_2$ | 0.467        | 4.662                                       | 6.735  | 8.807  | 1.088  | 1.295  | 1.502 |
| n-butanol         | $\text{C}_4\text{H}_0\text{O}$   | 0.472        | 4.485                                       | 6.479  | 8.473  | 1.046  | 1.246  | 1.445 |
| Methanol          | $\text{CH}_4\text{O}$            | 0.550        | 2.483                                       | 3.587  | 4.691  | 5.795  | 6.899  | 8.003 |
| Trichloromethane  | $\text{CHCL}_3$                  | 0.270        | 1.068                                       | 1.543  | 2.018  | 2.493  | 2.968  | 3.443 |
| Dimethylacetamide | $\text{C}_4\text{H}_9\text{N}$   | 0.485        | 0.407                                       | 0.5886 | 0.7698 | 0.9509 | 1.132  | 1.313 |
| Ethanol           | $\text{C}_2\text{H}_6\text{O}$   | 0.514        | 0.3292                                      | 0.4755 | 0.6219 | 0.7682 | 0.9145 | 1.060 |

**Table 5.** Calculated of the current flow rate  $K_J(E)$  for RUN3-ZnO at  $\Delta E^0 = 0.4\text{eV}$ .

| solvent               | Chemical form                    | $T_{NZ}(eV)$ | $K_J(E) \times 10^{+5}$                     |       |       |       |       |       |
|-----------------------|----------------------------------|--------------|---|-------|-------|-------|-------|-------|
|                       |                                  |              | Strength coupling( $\hat{M}_{NZ}(E)$ ) (eV) |       |       |       |       |       |
|                       |                                  |              | 0.212                                       | 0.255 | 0.291 | 0.324 | 0.353 | 0.380 |
| Acetic acid           | $\text{C}_2\text{H}_4\text{O}_2$ | 0.363        | 1.681                                       | 2.429 | 3.176 | 3.924 | 4.672 | 5.419 |
| 2-Methoxyethanol      | $\text{C}_3\text{H}_8\text{O}_2$ | 0.465        | 1.404                                       | 2.028 | 2.652 | 3.276 | 3.900 | 4.524 |
| 1-Butanol             | $\text{C}_4\text{H}_0\text{O}$   | 0.471        | 1.375                                       | 1.986 | 2.597 | 3.208 | 3.819 | 4.430 |
| Methyl alcohol        | $\text{CH}_4\text{O}$            | 0.550        | 9.416                                       | 1.360 | 1.778 | 2.197 | 2.615 | 3.034 |
| chloroform            | $\text{CHCL}_3$                  | 0.269        | 1.078                                       | 1.558 | 2.037 | 2.517 | 2.996 | 3.476 |
| N,N-Dimethylacetamide | $\text{C}_4\text{H}_9\text{N}$   | 0.484        | 1.302                                       | 1.880 | 2.459 | 3.038 | 3.616 | 4.195 |
| Ethyl alcohol         | $\text{C}_2\text{H}_6\text{O}$   | 0.513        | 1.140                                       | 1.647 | 2.154 | 2.661 | 3.168 | 3.675 |

**Table 6.** Calculated of the current flow rate  $K_J(E)$ for RUN3-ZnO at  $\Delta E^0 = 0.5\text{eV}$ .

| solvent          | Chemical form                    | $T_{NZ}(eV)$ | $K_J(E) \times 10^{+3}$                     |       |       |       |       |       |
|------------------|----------------------------------|--------------|---|-------|-------|-------|-------|-------|
|                  |                                  |              | Strength coupling( $\hat{M}_{NZ}(E)$ ) (eV) |       |       |       |       |       |
|                  |                                  |              | 0.212                                       | 0.255 | 0.291 | 0.324 | 0.353 | 0.380 |
| Acetic acid      | $\text{C}_2\text{H}_4\text{O}_2$ | 0.363        | 1.915                                       | 2.766 | 3.618 | 4.469 | 5.321 | 6.172 |
| 2-Methoxyethanol | $\text{C}_3\text{H}_8\text{O}_2$ | 0.465        | 2.752                                       | 3.976 | 5.199 | 6.422 | 7.646 | 8.869 |

|                       |                                  |       |       |       |       |       |       |       |
|-----------------------|----------------------------------|-------|-------|-------|-------|-------|-------|-------|
| 1-Butanol             | C <sub>4</sub> H <sub>10</sub> O | 0.471 | 2.757 | 3.983 | 5.208 | 6.434 | 7.659 | 8.885 |
| Methyl alcohol        | CH <sub>4</sub> O                | 0.550 | 2.481 | 3.584 | 4.687 | 5.790 | 6.893 | 7.996 |
| chloroform            | CHCL <sub>3</sub>                | 0.269 | 5.187 | 7.493 | 9.799 | 1.210 | 1.441 | 1.671 |
| N,N-Dimethylacetamide | C <sub>4</sub> H <sub>9</sub> N  | 0.484 | 2.753 | 3.977 | 5.201 | 6.424 | 7.648 | 8.872 |
| Ethyl alcohol         | C <sub>2</sub> H <sub>6</sub> O  | 0.513 | 2.677 | 3.868 | 5.058 | 6.248 | 7.438 | 8.628 |

#### 4. Discussion

The current flow rate  $K_j(E)$  and reorganization energy  $T_{NZ}(eV)$  for RUN3-ZnO are calculated depending on quantum consideration due to electronic transport theory. Electronic current flow rate calculation can provide a good tool to enhance the efficiency of RUN3-ZnO device solar cell. Table(3) shows the reorganization energy  $T_{NZ}(eV)$  increases with decreases the refractive index and increases dielectric constant for RUN3-ZnO with all solvents. Furthermore, it was observed that the relationship between the reorganization energy and the dielectric constant is inverse. The reorganization energy of the data in Table (3) shows that contact of RUN3 with zinc oxide using chloroform solvent leads to the lowest value (0.269 eV), indicating that the dielectric constant of chloroform solvent is low (4.81). In contrast, the RUN3-ZnO device using Methyl alcohol solvent gives the highest value (0.550 electron volts) due to the high dielectric constant 32.6 of Methyl alcohol solvent.

For the data in Tables (4), (5) and (6), the current flow rate  $K_j(E)$  increases with increasing coupling strength from 0.212eV to 0.380eV electron volts. In addition, the current flow rate  $K_j(E)$  increased as the reorganization energy decreased for all solvents in the RUN3-ZnO device system. The RUN3-ZnO device features a high electronic current when using chloroform solvent, compared to a low current flow rate  $K_j(E)$  when using the low-power operating methanol solvent. Lower reorganization energy means that RUN3-ZnO device with the solvent need less energy to reorient energy levels to initiate electron transfer, thus increasing the electron current. The current flow rate  $K_j(E)$  reaches a maximum of  $\approx 10^{+7}$  at the effective driving energy  $\Delta E^0 = 0.3$  eV and reaches a minimum with chloroform ( $\approx 10^{+3}$ ) at the maximum driving energy  $\Delta E^0 = 0.5$  eV. In general, the current flow rate decreases as the stimulation energy increases, and the flow of electrons decreases, resulting in a lower current. As is evident, the electron current changes according to the stimulation energy. However, the current in Tables (4), (5) and (6) for the RUN3-ZnO devices decreased with increasing electromotive force (EMF) energy, reaching its lowest value at an EMF of  $\Delta E^0 = 0.5$  eV. The current flow rate  $K_j(E)$  increases when the coupling force approaches 0.380 eV. The  $K_j(E)$  reaches its maximum value with all solvents at an electromotive force energy  $\Delta E^0 = 0.3$  eV, compared to lower values at  $\Delta E^0 = 0.5$  eV. This indicates that the driving force energy is proportional to the relative electrochemical potential of the RUN3 dye, where the current increases as the driving force energy decreases and the electrochemical potential of the RUN3 dye increases. In addition, we can also show the current for RUN3-ZnO devices in Tables 4, 5, and 6, as well as its increase with increasing coupling energy levels. This indicates when increasing the coupling strength of the donor and acceptor energy levels leads to the transfer of more electrons across the potential at the interface.

$$K_j(E) = \frac{4\pi^2 q}{h} \frac{|\langle \hat{M}_{NZ}(E) \rangle|^2}{\sqrt{4\pi T_{NZ} k_B T}} e^{-\frac{(T_{NZ} + \Delta E^0)^2}{4 T_{NZ} k_B T}} d_z^{-2/3} \frac{l_z}{\delta_z} [n_z] \dots \dots (9)$$

## 5. Conclusion

In this study, we study and calculate the current flow rate  $K_f(E)$  for the sensitizer molecule RUN3 dye contact to ZnO semiconductor using quantum electronic transport theory. We have provided a method for calculating the rate of flux of the resulting current based on the reorganization energy, coupling strength, conduction band, ionization energy, excitation energy, and energy level overlap, using the theory of electronic transport. The results indicate that the current flow rate is dependent on the calculated reorganization energy, assuming that energy level interference leads to energy alignment. The reorganization energy plays a crucial role in influencing the current due to its effect on the limited electron transport through the system. Analysis of the data results shows that the current flow rate is highest in the RUN3-ZnO device with low reorganization power and low operating power. The current flow and transfer energy results indicate that the chloroform solvent exhibits its highest value at a low transfer energy ( $\Delta E^0 = 0.3$  eV) and reaches its lowest value at a high transfer energy ( $\Delta E^0 = 0.5$  eV).

The electron current flow increased with the increasing overlap of energy levels in the RUN3-ZnO devices, indicating good compatibility of the energy levels of both materials with more polar media.

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