Retraction

Retraction: Crossover from static to dynamic Non-Condon effect on charge Transport in Organic Semiconductors (J. Phys.: Conf. Ser. 1916 012230)

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This article (and all articles in the proceedings volume relating to the same conference) has been retracted by IOP Publishing following an extensive investigation in line with the COPE guidelines. This investigation has uncovered evidence of systematic manipulation of the publication process and considerable citation manipulation.

IOP Publishing respectfully requests that readers consider all work within this volume potentially unreliable, as the volume has not been through a credible peer review process.

IOP Publishing regrets that our usual quality checks did not identify these issues before publication, and have since put additional measures in place to try to prevent these issues from reoccurring. IOP Publishing wishes to credit anonymous whistleblowers and the Problematic Paper Screener [1] for bringing some of the above issues to our attention, prompting us to investigate further.

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Crossover from static to dynamic Non-Condon effect on charge Transport in Organic Semiconductors

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Abstract. The computed charge transport key parameters like, charge transfer integral, site energy and reorganization energy are used to study the hole and electron transport in dialkyl substituted thienothiophene caped benzobisthiazole (BDHTT-BBT) and methyl-substituted dicyanovinyl-capped quinquethiophene (DCV5T-Me) molecular crystals. The effect of structural fluctuation on charge transport in these molecules is analysed by Monte-Carlo simulations. To estimate the equilibrium speed during the charge transport process in these molecular solids, we have introduced the parameters such as, potential equilibrium rate and density flux rate. Here, the density flux rate is directly related with the drift force which facilitates the charge transfer along the consequential hopping sites. Our theoretical study reveals that the charge transfer up to the crossover point (or disorder drift time) is exponential, non-dispersive and it follows the static non-Condon effect. Beyond the disorder drift time, the charge transfer is partially exponential, dispersive and it follows the dynamic non-Condon principle. The expressions of density flux and diffusion shows their dependency on dynamic disorder and is in agreement with the Troisi’s model on diffusion limited by thermal disorder.

Keywords: Crossover, Transport, Organic, Semiconductors

1. Introduction
Over the last few decades the organic electronics is an emerging field in science and technology due to its application in organic semiconducting devices, such as field-effect transistors [1], light-emitting diodes [2], solar cells [3] and in nanoscale electronics [4]. The organic materials have soft condensed phase property and easily tunable electronic property through suitable functional group substitution [4]. In addition, they are environmentally friendly, mechanically flexible, having self-assembling character. The weak intermolecular interaction and structural disorder in the organic materials increases the electron-phonon coupling which is responsible for localized electronic states [5]. Therefore, the thermally activated polaron hopping mechanism is used to describe the charge transfer (CT) process in the organic molecules and the Marcus theory of charge transfer is used to study CT along the sequential localized sites [4]. Berlin et al. [6] studied the effect of static and dynamic fluctuations on charge transfer kinetics in the donor-bridge-acceptor systems and concluded that the dynamic fluctuation facilitates the non-dispersive band-like charge transport due to static non-Condon effect. Böhlin et al. [7] found that the localized charge carrier on the dynamically disordered system does not significantly influenced by electron-phonon coupling. Troisi’s charge transport models [5, 8] for disordered systems show that the dynamical disorder leads to the intermediate charge transfer
mechanism between localized hopping and delocalized band transport, and is termed as diffusion limited by dynamic disorder.

In our previous studies [9, 10], we found that the dynamic disorder facilitates the density flux along the sequential localized sites and is responsible for hopping conductivity. Kocherzhenko et al. [11, 12] concluded that the charge carrier dynamics in the short range molecular order follows the coherent band model and in the long range the charge carrier follows incoherent hopping mechanism. Many experimental studies also evidentially support that the charge transport in the dynamically disordered system does not fully hopping or band-like [11]. That is, the charge transport in organic molecules follows the partially coherent band-like due to static non-Condon (SNC) effect and partially incoherent hopping mechanism due to the effect of dynamic non-Condon (DNC) principle. The vibrational spectroscopic studies also shows that the band-like SNC transport is possible in highly ordered organic crystals, like pentacene [5]. Therefore, this intermediate CT mechanism and the effect of nuclear and electronic degrees of freedom on CT are to be studied further to understand the CT in organic molecules.

In the present study, we have studied the dynamic disorder effect on charge transport properties of dialkyl substituted thienothiophene capped benzobisthiazole (BDHTT-BBT) and methyl-substituted dicyanovinyl-capped quinque thiophene (DCV5T-Me) molecules [13, 14]. The detailed energetic disordered charge transport and structure-property relationship were extensively studied for these molecules in our earlier paper [15]. To this extent, to calculate the equilibrium time during the charge transport along the π-stacked organic molecules, we have proposed the expression of rate of density flux and time-dependent potential energy. From time-dependent potential energy expression, we can find the equilibrium speed during the charge transport in the molecular systems. That is, from our method, one can elaborate that how much quickly the molecule reaches the equilibrium during the charge propagation. Also, the CT mechanism is studied on the basis of SNC and DNC-based rate coefficient, which can be analysed by the parameters, disorder drift time and dispersive parameter.

2. Method
The charge transfer rate \( k \) can be calculated through semi-classical Marcus theory, and is expressed as [4, 9],

\[
k = \frac{2\pi}{\hbar} |J_{eff}| \rho_{RCT}
\]

where, \( J_{eff} \), \( \hbar \) and \( \rho_{RCT} \) are the effective charge transfer integral, reduced Planck constant and Franck-Condon factor, respectively. The parameter \( \rho_{RCT} \) provides the information about the weightage of density of states and is given as [9],

\[
\rho_{RCT} = \frac{1}{\sqrt{4\pi kj_0 T}} \exp\left[\frac{-\left(\Delta \varepsilon_j + \lambda\right)^2}{4\lambda kj_0 T}\right]
\]

where, \( k_0 \), \( T \), \( \lambda \) and \( \Delta \varepsilon_j \) are the Boltzmann constant, temperature, reorganization energy, and the site energy difference between final and initial states, \( \Delta \varepsilon_j = \varepsilon_j - \varepsilon_i \). For our calculation, the charge transport parameters \( (J_{eff}, \lambda, \Delta \varepsilon_j) \) and the information of molecular conformational disorder are taken from our earlier study [15]. In this paper, we reproduce the numerical simulation using Monte-Carlo (MC) technique. In the present study, we have performed the MC simulation to study the charge carrier dynamics in studied molecules. During the simulation, the charge is propagated on the basis of rate of charge transfer calculated from Equations (1) and (2). Along with reorganization energy, the effective charge transfer integral and site energy difference calculated for 300 conformations and the stacking angle ranges from 0 to 180º are given as the input to the MC simulation to analyse the CT kinetics along the π-stacked molecules. In this simulation, the structural fluctuation time is fixed as 0.1 ps. In this model, we assume that the charge transport is along the sequence of π-stacked molecules and the charge carrier does not reach the end of molecular chain within the time scale of simulation. In
each step of MC simulation, the most probable hopping pathway is found out from the simulated trajectories based on the charge transfer rate at a particular conformation.

The dynamic fluctuation effect on CT kinetics is characterized by using the rate coefficient, \( k(t) \) which is defined as in equation (3)

\[
k(t) = -\frac{d \ln P(t)}{dt}
\]

where, \( P(t) \) is the survival probability of charge at a particular site. Based on this analysis, the type of fluctuation (slow or fast) and corresponding non-Condon (NC) effect (dynamic or static) on CT kinetics is studied. The time dependency character of rate coefficient is analysed by using the power law [6, 16]

\[
k(t) = k^a e^{-t}, \quad 0 < a \leq 1
\]

Generally, the rate coefficient, \( k \) is calculated from the survival probability curve. The dispersive parameter, \( a \) is calculated by fitting the plotted curve of rate coefficient versus time on the Equation (4). As described in our previous studies [10, 16], the dynamic disorder effect is studied by using survival probability through the entropy relation.

\[
\sum S(t) = -k_B \sum t P(t) \log P(t)
\]

The previous studies [6, 16] show that the dynamic disorder kinetically drifts the charge carrier along the charge transfer path. The variation of disorder drift \( S(t)/k_B \) during charge transfer is numerically calculated by using the Equation (5). The disorder drift time, \( S \) is the time at which the disorder drift is maximum (see ref. 16). The timely varying disorder drift curve will provide the information about charge diffusion process and its dependency on dynamic disorder. The dynamic disorder dependent density flux equation is written as [10]

\[
\rho_S = \rho_{S_0} \exp\left(\frac{3S(t)}{5k_B}\right)
\]

where, \( \rho_{S_0} \) is the density flux in the absence of dynamic disorder.

To get further insight on charge transport in the dynamical system, we have formulated the expressions for density flux rate, time-dependent momentum distribution factor as well as the potential difference and dynamic disorder dependent diffusion coefficient (see Equations 7-11). These parameters will provide the information about charge distribution speed along the hopping path in the π-stacked molecules.

The earlier studies[10, 11] show that the dynamic disorder perturbs the localized charge carrier at a particular electronic site, which is responsible for density flux from site to site. Here, the rate of change of density flux along the CT path is described on the basis of perturbed charge carrier density (\( \rho \)) and the drift force (\( F_D \)) as [17],

\[
\frac{\partial \rho}{\partial t} = \frac{3}{h(3\pi^2 e)^{1/3}} \rho^{2/3} F_D
\]

where, \( e, F_D \) are the electronic charge, the drift force acting on the charge carrier. The drift force can be quantified from the momentum redistribution analysis.

As described in previous studies [9, 16], the momentum redistribution of the charge carrier along the CT path with respect to time is calculated by using the following equation [15, 17],

\[
P(t)_{mom} = P_{mom,0}\left(\exp(1 - P(t))\right)^{8/15}
\]

where, \( P_{mom,0} \) is the momentum distribution in the absence of dynamic disorder, and \( P(t) \) is the survival probability of the charge carrier.

In the present study, charge transfer process is the thermal diffusion because no external electric field is applied for CT. The presence of excess charge at one end of π-stacked molecular chain introduces the potential difference, \( V_d \). During the CT, the non-steady charge diffusion will occur up to
the point where the potential equilibrium is reached, that is, $V_d = 0$. The change in potential with respect to time is defined in terms of survival probability, $P(t)$ as [15, 17],

$$V_d(t) = \frac{k_BT}{e}\left(1 - \left(\exp(1 - P(t))\right)^{16/15}\right)$$

(9)

where, $k_BT$ is the thermal energy which is responsible for thermal diffusion. The above Equation (9) gives the information about the potential equilibrium speed of the studied molecules, (see Figure 4).

The rate change of potential difference is calculated from the solution of Poisson equation and is expressed as [15, 17],

$$\frac{\partial V_d}{\partial t} = \frac{\rho}{e}D$$

(10)

where, $\rho$ is the contributed $\pi$-electron density for charge transport. From the mean squared displacement and time-dependent potential distribution curves (see Figures 1 and 4), the diffusion coefficient and the potential equilibrium rate are calculated, which are used in Equation (10) to find $\rho$. The calculated charge density is used to calculate the momentum of the charge carrier, for detailed see ref. 15 and 17. From this momentum redistribution curve, the drift force acting on a carrier is calculated. Here, the calculated drift force ($F_D$) and perturbed charge density ($\rho$) are used in Equation (7) to study the density flux rate for hole and electron transport in the studied molecules.

In this paper, the dynamic disorder dependent diffusion coefficient, $D_s$ is expressed as [15, 17],

$$D_s = D_{s_0} \exp\left(-\frac{2S(t)}{3k_BT}\right)$$

(11)

where, $D_{s_0}$ is the diffusion coefficient in the absence of dynamic disorder. The Equation (11) is in agreement with the Troisi’s model on diffusion limited by dynamic disorder [5, 18].

3. Results and discussion

The calculated charge transport key parameters such as effective charge transfer integral, site energy difference, reorganization energy and structural fluctuation in the form of stacking angle distribution are given as the input of MC simulation to study the charge carrier dynamics in the sequential $\pi$-stacked molecules of BDHTT-BBT and DCV5T-Me. As shown in Figure 1, the mean squared displacement (MSD), $\langle x^2(t)\rangle$, of the electron in the $\pi$-stacked BDHTT-BBT molecule is calculated using MC simulation. As described in earlier studies [10, 16], the diffusion coefficient, $D$ is obtained as half of the slope of the line of MSD. The calculated survival probability and disorder drift are shown in Figure 2, (for detailed analysis see ref 9, 10 and 16). In our previous study [9, 10], we have concluded that the disorder drift time ($S_t$) is acting as the crossover point (COP) between adiabatic band and non-adiabatic hopping transport.

![Figure 1](image-url) **Figure 1.** Mean squared displacement of electron in BDHTT-BBT molecule with respect to time.
Figure 2. Survival probability and disorder drift of electron in BDHTT-BBT molecule with time.

Table 1. Coherent rate coefficient ($k_1$), incoherent rate coefficient ($k_2$), dispersive parameter before and after the crossover point ($a_1$ and $a_2$), disorder drift time ($S_t$), drift force ($F_D$), potential equilibrium rate ($\frac{\partial V}{\partial t}$) and density flux rate ($\frac{\partial \rho}{\partial t}$) for hole and transport in BDHTT-BTT and DCV5T-Me molecules.

| Molecules   | $k_1$ (x10^{12}/s) | $k_2$ (x10^{12}/s) | $a_1$ | $a_2$ | $S_t$ (fs) | $F_D$ (x10^{10} N) | $\frac{\partial V}{\partial t}$ (x10^{9} V/s) | $\frac{\partial \rho}{\partial t}$ (x10^{9} C/m^3 s) |
|------------|---------------------|---------------------|-------|-------|------------|-------------------|-----------------------------------------------|-----------------------------------------------|
| Hole       |                     |                     |       |       |            |                   |                                               |                                               |
| BDHTT-BBT  | 1.64                | 1.47                | 0.9   | 0.81  | 592        | 1.38              | 3.54                                          | 0.65                                          |
| DCV5T-Me   | 0.784               | 0.780               | 0.92  | 1.81  | 1860       | 0.61              | 1.49                                          |                                               |
| Electron   |                     |                     |       |       |            |                   |                                               |                                               |
| BDHTT-BBT  | 18.7                | 11.2                | 0.96  | 0.81  | 42         | 16.22             | 40.11                                         | 19.12                                         |
| DCV5T-Me   | 4.7                 | 2.2                 | 0.93  | 1.87  | 184        | 4.95              | 10.52                                         | 7.18                                          |

In this work, both the SNC and DNC based hopping charge transport mechanisms are studied through survival probability and disorder drift curve. Numerically computed charge transfer rate ($k(t)$) values by MC simulation are used to analyse the time dependency character of rate coefficient by using equation (3) and (4). From the survival probability curve, the calculated rate coefficient up to the disorder drift time ($S_t$) is $k_1$ and beyond that point is $k_2$. These rate coefficients ($k_1$ and $k_2$) are used in Equation (4) to calculate the dispersive parameters ($a_1$ and $a_2$). The calculated rate coefficients ($k_1$ and $k_2$) and corresponding dispersive parameters ($a_1$ and $a_2$) are summarized in Table 1. Based on dispersive parameters ($a_1$ and $a_2$), the rate coefficients $k_1$ and $k_2$ are referred as the coherent and incoherent rate coefficients, respectively, which is conceptually supported by the previous studies [6, 9, 10, 16]. The first one is associated with the SNC principle and the later one is related to the DNC principle. Calculated SNC and DNC based rate coefficients ($k_1$ and $k_2$), and the corresponding dispersive parameters ($a_1$ and $a_2$), and disorder drift time ($S_t$) are summarized in Table 1, for hole and electron transport in the BDHTT-BBT and DCV5T-Me molecular crystals.
Figure 3. Electron transfer rate in BDHTT-BBT molecule in (a) coherent (b) non-coherent regime.

It has been observed that the charge transfer up to the COP (or disorder drift time) is exponential, non-dispersive and hence charge transport follows the SNC transport mechanism, which leads to band-like transport. Beyond COP, the charge transfer is not exact exponential, partially dispersive and the charge transport now turns from band to incoherent hopping transport due to the crossover from SNC to DNC principle [11, 18]. It has been found that the charge transfer rate coefficient up to the COP \( k_1 \) is time-independent, beyond the COP the rate coefficient \( k_2 \) is time-dependent which is analyzed through dispersive parameter calculated by using Equations (3) and (4). For instance, the calculated rate coefficients \( k_1 \) and \( k_2 \) for electron transport in molecule BDHTT-BBT are \( 1.87 \times 10^{13} \) and \( 1.12 \times 10^{13} \) /s and their dispersive parameters \( a_1 \) and \( a_2 \) are 0.96 and 0.64 (see Figure 3 and Table 1), respectively. In principle, SNC-based transport is expected when the parameter \( a \) value is closer to unity. The DNC transport is anticipated in the molecular solids while the parameter \( a \) takes towards zero. That is, the dispersive parameter \( a_1 \) is nearly 1 which indicates that the rate coefficient \( k_1 \) is non-dispersive, time-independent, but, in the latter case the rate coefficient \( k_2 \) is dispersive and time-dependent. The molecule DCV5T-Me has lesser hole and electron transporting ability due to the higher reorganization energy of 0.33 and 0.29 eV. In this case, the calculated disorder drift time is 1860 and 184 fs. That is, the positive charge carrier spend longer time on a localized HOMO of DCV5T-Me which is responsible for lesser hole transport property.
To study the equilibrium speed during the charge transport in the BDHTT-BBT and DCVST-Me molecules, charge carrier momentum redistribution \( (P_m) \) and potential \( (V_i) \) variation are analysed with the aid of Equations (8) and (9). The momentum redistribution and rate of change of potential are plotted, which are shown in Figure 4. Here, the momentum distribution provides the information about the speed of charge distribution along the \( \pi \)-stacked units. The drift force \( (F_D) \) and potential equilibrium rate \( \left( \frac{\partial V}{\partial t} \right) \) are calculated from the charge carrier momentum distribution and potential rate curves (Figure 4), and are summarized in Table (1). The drift force \( (F_D) \) is the driving force for charge diffusion, and is inversely proportional to the disorder drift time, \( S \). The potential equilibrium rate \( \left( \frac{\partial V}{\partial t} \right) \) provides the information about the time required for reaching the potential equilibrium during the charge transfer process. That is, the charge diffusion will occur until the potential equilibrium is reached. After this equilibrium point, the potential energy difference between the adjacent molecular units is zero, at which the CT will not take place. The calculated potential equilibrium rate \( \left( \frac{\partial V}{\partial t} \right) \) is used in Equation (10) to calculate the \( \pi \)-electron density. As given in Equation (7), the density flux rate is calculated by using drift force \( (F_D) \) and density \( (\rho) \). The density flux rate expression gives the knowledge about the contributed charge density, due to perturbed effect of dynamic disorder, for CT mechanism within hopping time which is related to current density gradient.

**Figure 4.** Momentum and potential redistributions for electron transport in BDHTT-BBT molecule.

**Figure 5.** Electron density variation with respect to time in BDHTT-BBT molecule.
Figure 6. Variation in diffusion coefficient for electron transport in BDHTT-BBT molecule

The potential equilibrium rate gives the information about how the ‘ion injected molecules’ quickly reaches the potential equilibrium within hopping time, which is associated with the ionic diffusion property of the molecules. The potential equilibrium rate is calculated from the time evolutions of potential distribution curve (see Figure 4) and is used in Equation (10) to study the perturbed localized charge density. As observed from Table (1), the molecule BDHTT-BBT has the larger value of potential equilibrium rate (4x10^{11} V/s), drift force (~1.62x10^{-12} N) and density flux rate (1.91x10^{20} C/m^3 s) for electron transport. Hence, the expected electron mobility in this molecule is high (see ref. 15). Note that in this case the disorder drift time (S_t) is lower (42 fs). That is, due to the larger drift force the charge carrier does not spend longer time on the particular localized site. The potential equilibrium rate and drift force for hole transport in the studied DCV5T-Me molecule is comparatively minimum, the values are 1.49x10^{10} V/s and 6.1x10^{-14} N, and hence the hole transporting ability of this molecule is poor (see Table 1). The above results clearly show that the dynamic disorder mediated SNC is mainly responsible for density flux along the charge transfer path which turns from hopping to band-like charge transport mechanism and is in agreement with the previous studies [5, 6, 9, 18].

Using the density flux and diffusion coefficient expressions 6 and 11, we have analysed the dynamic disorder-coupled charge localization property as well as diffusion mechanism. The main observation is that the localized charge density and diffusion coefficient are decreasing up to the disorder drift time, S_t (COP), beyond that the charge density and diffusion coefficient is increasing. This diffusion limitation indirectly suggests the SNC based coherent transport. It is noted that the dynamic disorder increases up to the disorder drift time, and then the dynamic disorder is decreased (see Figure 2). That is, the localized charge density and diffusion coefficient are decreasing when the dynamic disorder is increasing; and vice versa (see Figures 2, 5 and 6). That is, the values of localized charge density and hopping transport-based diffusion are decreased by dynamic disorder. Therefore, the dynamic disorder controls the localized hopping mechanism and turns the band-like CT mechanism due to SNC effect, which is in agreement with the earlier studies of Troisi’s model on diffusion limited by the dynamic disorder [5, 8, 18].

4. Conclusion
The charge transport properties of BDHTT-BBT and DCV5T-Me molecules are studied computationally. The charge transport integral, site energy and the stacking angle fluctuation are used to calculate the charge transfer kinetic parameters, such as SNC-based coherent and DNC-based incoherent rate coefficients, disorder drift time, drift force, potential equilibrium rate and density flux rate and are used to study the hole and electron transport in the BDHTT-BBT and DCV5T-Me molecules. The disorder drift time is acting as the crossover point between hopping and band transport mechanisms, due to the transformation from static to dynamic non-Condon effect. It has been found that the charge transport up to the crossover point (disorder drift time) is exponential, non-dispersive and it follows the static non-Condon principle (band-like transport). Beyond the disorder drift time the charge transport is partially exponential and it follows incoherent hopping transport due to the
dominancy nature of dynamic non-Condon effect. The proposed density flux and diffusion expressions show that the localized charge transport in these molecules is limited by dynamic disorder and is in agreement with the Troisi’s model on diffusion limited by thermal disorder. The BDHTT-BBT system has larger electron density flux rate and drift force of $1.9 \times 10^{20} \text{C/m}^3\text{s}$ and $1.62 \times 10^{-12} \text{N}$, respectively.

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