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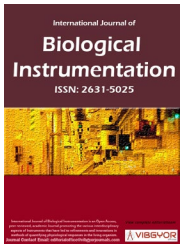
Study of Physical Properties of P3HT:DOCN-PPV Solar Cell by using Computer Simulation



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Abstract

In this paper, we try to study the physical properties and miscibility in P3HT/DOCN-PPV organic solar cell (OPV) by meaning of molecular dynamic (MD) simulation. The glass transition temperature (Tg) of P3HT, DOCN-PPV and P3HT/DOCN-PPV system were found by using the dilatometric procedure. In the general case, analyze of the thermal properties can be a good indicator to predict miscibility of a polymer bled. The solubility parameters δ of both P3HT and DOCN-PPV were calculated by using the modules Forcite and Van Kreleven of the semi empirical methods of Synthia. One single glass transition temperature (Tg) equal to 354 K is obtained for our blend system between the glass transition temperatures of P3HT/DOCN-PPV solar cel. The effect of some energies in the Tg process was studied. Other different physical properties for P3HT/CNPh-PPV system were simulated in order to improve our work.

Keywords

Miscibility, OPV, MD, Tg, Solubility Parameter, Blend

Introduction

Polymer blends are one of the best materials for using in economical electronics and organic photovoltaics (OPV) devices [1]. Mixing two polymers or more together to find a new blend system is an excellent technique to get desirable advantages which cannot be obtained by one single polymer of them [2]. In the last times, organic photovoltaic solar cell (OPV) were widely used in industry because of their different advantages, such as large-area devices, lightweight cells with flexibility, low cost and for their vast choice in the different domains [3,4]. In the general case, it is not possible to find the solubility parameter δ of a polymer from the experiment [5].

For a long time, molecular modeling (MM) has been used to study the physical properties of polymer blend [6,7]. All found methods have pursued with two different points: prediction of miscibility or miscible polymer blend properties.

The principal goal of our work is to study the physical properties of P3HT:DOCN-PPV solar cell. Whereas DOCN-PPV is a synthetic polymer obtained for the first time on 2006 and it was proposed to use as a good acceptor.

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The P3HT was used in the present work as an acceptor. P3HT presents different advantages such as: Low cost, better allocation of resources, with good yield, physical durability and also lightweight.

The P3HT:DOCN-PPV polymer system was studied for the first time on 2020 with other properties, and there are not other results in literature for the P3HT:DOCN-PPV blend in the best of our knowledge [6,7]. The cohesive energy density (CED) of both of P3HT and DOCN-PPV were employed to obtain the solubility parameters δ_{P3HT} and $\delta_{DOCN-PPV}$. Other different procedures were applied to determine the solubility parameter of both P3HT and DOCN-PPV $(\delta_{P3HT}$ and $\delta_{DOCN-PPV})$ in order to confirm our results.

Then, by using the united atom approximation, the molecular dynamic (MD) simulation of the P3HT/CNPh-PPV blend system (50%50) is performed to get the curve of the specific volume versus the temperature. The glass transition temperature (Tg) of the P3HT:DOCN-PPV blend was obtained. Furthermore, the theory of Fox was applied to calculate the glass transition temperature (Tg) of our system with another way.

In addition, the semi empirical method Synthia was also used in order to simulate the glass transition temperature (tg) of P3HT:DOCN-PPV system. The effect of total energy and potential energy in the Tg process were studied.

Other physical properties were calculated by using the semi empirical procedures (Synthia). In order to verify our results, the found values were compared with available results in other works.

Different previous publications were proved that the use of the computer simulation in the study of the properties of polymers gives good results [8-12].

Computational Details

Molecular dynamic (MD) Simulations were performed with the commercial software suite Materials studio (v 6.0) supplied by Accelrys. The Forcite (molecular mechanics and dynamics simulation), Synthia and Amorphous Cell program modules were used to perform the simulation in this paper.

Simulation of the solubility parameter δ

In the beginning, simple chains of P3HT and CNPh-PPV (DOCN-PPV) models are constructed. In each structure twenty monomers are involved. Then, ten amorphous polymer configurations are generated with periodic boundary conditions. From the ten configurations, we take the structure having the lowest potential energy given by molecular mechanic (MM) simulations as the initial configuration. To eliminate different undesirable interactions in our structure, 20,000 steps of energy minimization and Geometry optimization of Forcite calculation is employed. In this paper COMPASS was been chosen as a force field. The micro canonical ensembles NPT and NVT of 300 ps for each dynamic are applied to confirm the stability of our structure. The cohesive energy density (CED) is simulated by Appling Forcite.

Simulation of the system's Tg

Each studied polymer chain in this work contains twenty repeat unites (Rus). The Amorphous_Cell© code [13] is used to generate our chains imbedded in a cell with periodic boundary conditions. The procedure is depends on the knowing of the conditional probability to increment repeat unites in the same time of structure generation.

Experimentally, the dilatometic techniques if used to found the Tg. By applying the module Forcite of Accelrys and the ensemble NPT by fixing the pressure and the temperature in al simulation time to get the density of equilibrium. This last will be used to calculate the specific volume (sv) that can be employed to find the glass transition temperature (Tg). We take precedent over the NPT ensemble with NVT ensemble with 300 K in the goal to relax our chains. In the NPT, the system is maintained in atmospheric pressure witch (0.0001 GPA). The structure will be heat up going from an initial temperature equal to 300 K coming to 800 K as a mas; in the come up and the system will be cool down going from 800 K and coming to 200 K with a step of 25 K for 300 ps for each degree of temperature with a simple step of 1 fs. Both of the temperature and the pressure are fixed by applying the Brendsen Thermostat. This procedure was employed with the COMPASS force field in order to find the glass transition temperature (tg) for our system.

Flory-Huggins theory approach

To see if the polymer system is miscible or no, other method could be used. According to Hildbrand, the Flory-Huggins parameter χFH can

Table 1: Solubility parameters for P3HT and CNPh-PPV.

	MD Simulation ($cal^{1/2}/cm^{3/2}$)	Synthia Calculation ($cal^{1/2}/cm^{3/2}$)	Experimental
P3HT	15.66	18.71[a]	13.4 ± 0.3[b]
CNPh-PPV	15.02	17.98[a]	-

[a]Values calculated by using the method Van Krevelen of Synthia; [b]Experimental value from [18]

be calculated from the solubility parameters of the constituents of a polymer system by sing the relationship [14].

$$\chi FH = V_{seg}\frac{(\delta_A - \delta_B)^2}{RT} \quad (1)$$

Where V_{seg} is the volume taken to be close to the molar volume of the smallest monomer and δ_A and δ_B are solubility parameters of the constituents A and B, respectively.

Theory of fax

To compute the glass transition temperature (Tg) of our blend, the Fox theory [15] is used as follows:

$$1/\mathrm{Tg} = \mathrm{X_A}/\mathrm{Tg_A} + \mathrm{X_B}/\mathrm{Tg_B} \quad (2)$$

Results and Discussion

The solubility parameter δ is an important element in the study of the miscibility for polymer system. In the first time it was applied just for polymer/solvent system in different domains. After, the approach polymer/polymer blend was generated by Bohn [16]. The solubility parameter δ [17] can be found by using the relations:

$$\delta = \sqrt{\frac{E_{coh}}{v}} = \sqrt{\frac{(E_s - E_b)*C}{V_c}} = \sqrt{CED} \quad (3)$$

Where $\frac{E_{coh}}{v}$ is the cohesive energy density; E_s the single chain energy; E_b the energy of the same chain in periodic system; V_c the volume of the cell in cubic angstrom, C the unit conversion factor.

The simulated values of the solubility parameters δ of P3HT and CNPh-PPV $\left(\delta_{P3HT}\ and\ \delta_{DOCN-PPV}\right)$ are [18] presented in the Table 1. Two several methods were used to calculate by simulation the value of the solubility parameters of P3HT and CNPh-PPV, the first one by meaning of the MC simulation and other by using Van Kreleven of the semi empirical procedure (Synthia).

We can remark that for P3HT, our simulated results are a little greater than the experimental value. In the best of our knowledge, there is not an experimental or simulated value in other works for CNPh-PPV. Mason [19] says that if two different polymers have similar value of the solubility parameter δ, the blend between them will be miscible. In this paper the difference between both of simulated solubility parameters of P3HT and CNPh-PPV $\left(\delta_{P3HT}\ and\ \delta_{DOCN-PPV}\right)$ is 0.64 $cal^{1/2}/cm^{3/2}$, so P3HT and CNPh-PPV tend to be miscible.

The glass transition temperature (Tg) of a polymer system is an important value to enhance the miscibility of the constituents. Miscible polymer blend exposes one single glass transition temperature (Tg) between the glass transition temperatures of the compounds, where immiscible polymer blend may give two several glass transition temperature (Tgs) between those of the components. Then, we calculate the specific volumes (sv) of P3HT/CNPv-PPV blend system as a function of the temperature by using the molecular dynamic (MD) simulation. Figure 1 shows the curves of the specific volume versus the temperature for P3HT, CNPh-PPVand P3HT/CNPh-PPV blend system.

One glass transition temperature (Tg) of P3HT:CNPh-PPV polymer blend about 354 K takes place in the curve of the specific volume versus the temperature; it is between the simulated glass transition temperature (tg) of P3HT (about 360 K) and the simulated Tg of CNPh-PPV (about 344 K).

In the case of a miscible polymer blend just one glass transition temperature (Tg) can be found. The obtained Tg for our polymer blend lies between the two Tgs of compounds, whereas for no miscible polymer system, two different glass transition temperatures (tgs) can be shown in the curve of the specific bolume versus the temperature [17], in the present study, the molecular dynamic (MD) simulation shows that P3HT/DOCN-PPV (1:1 blends in terms of repeated units) blend has one single glass transition temperature (Tg) (Figure 2).

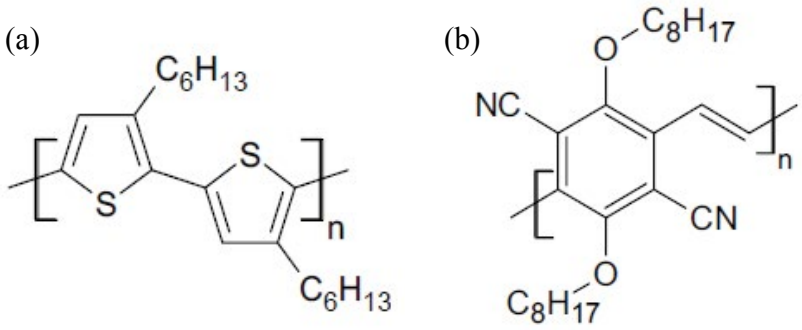

Figure 1: Chemical structures of (P3HT (a)) and (DOCN-PPV (b)) polymers used in our polymer blends for solar photovoltaic solar cells.

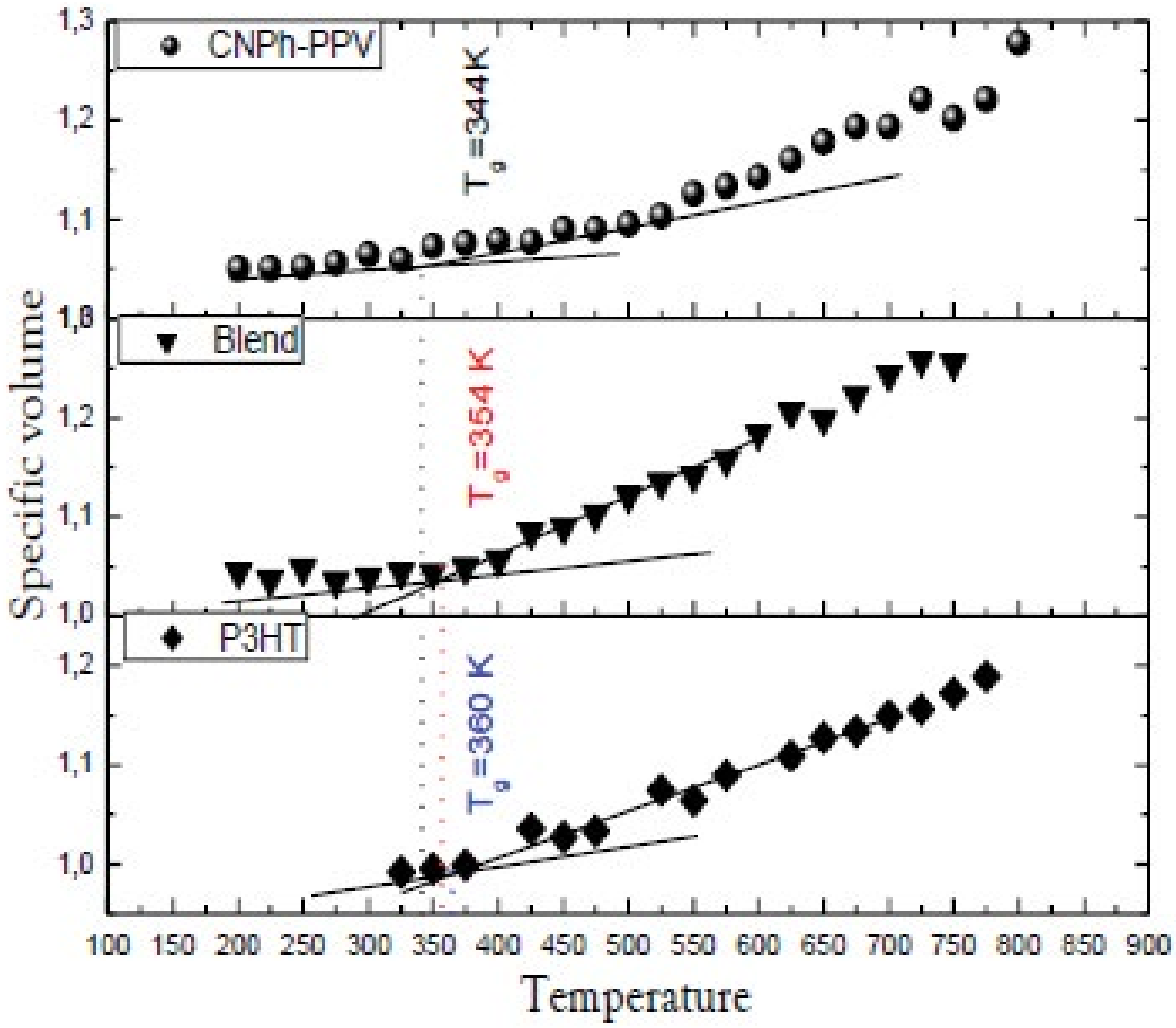

Figure 2: Specific volume versus temperature using atomistic simulation for blend system P3HT/CNPh-PPV (1:1 blends in terms of repeated units).

Considering the similar solubility parameters of tow polymers (P3HT and DOCN-PPV) and the single glass transition temperature (Tg) for our blend system, it can be concluded that the P3HT/DOCN-PPV blend system in miscible.

Table 2 shows glass transition temperature (Tg) of P3HT, CNPh-PPV and P3HT/CNPh-PPV blend by meaning of molecular dynamic (MD) simulation and by the semi empirical method Synthis [20,21]. The glass transition temperature (Tg) of P3HT/

Table 2: Glass transition temperatures (TGS) of P3HT, CNP_H-PPV and P3HT/CNP_H-PPV system.

	Our simulated Tg (K)	Tg by theory of Fox (K)	Synthia (K)	Other simulated Tg (K)	Experimental (K)
P3HT	360	/	347	-	340[a]
CNPh-PPV	344	/	335	344[b]	-
P3HT/CNPh-PPV	354	352	-	339[b]	-

[a]from [20]; [b]from [21]

Table 3: Some properties of P3HT/CNPh-PPV polymer blend by using synthia.

	Connectivity Index 0X($s.m^{-1}$)	Molar Volume ($m^3.mol^{-1}$)	Density (gm/cm^3)	Thermal Conductivity ($W.m^{-1}K^{-1}$)	Young's Modulus (Pa)	Crictical Molecular Weight (uma)
P3HT:DOCN-PPV	18.16	349.07	1.04	0.14	2.87e+003	1.32e+004

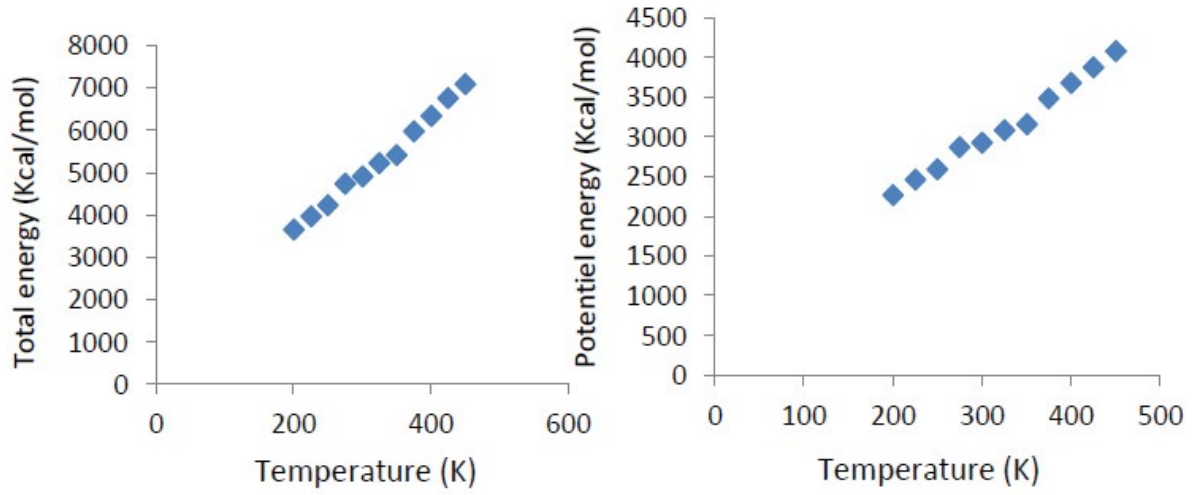

Figure 3: Plots of some energy compnents versus temperature for the P3HT/CNPh-PPV polymer blend (1:1 blends in terms of repeated units).

CNPh-PPV blend was calculated by using the Theory of Fox. The results found are compared between them and with the available experimental value.

The total and the potential energies versus the temperature of the P3HT/CNPh-PPV polymer blend are shown in Figure 3 In the goal to enhance the effect of the different interacting elements in a glass transition process. Hua, et al. [22] have studies different energies for some structures. They found little breaks in the curves of dihedral torsion energy and non-bond energy versus the temperature. Other studies also have detected a point break in the curve of the energy versus the temperature [23,24].

In other work no break point is detected in the curve of the energy versus the temperature [25].

In this paper, small breaks take place in the curves of total energy and potential energy versus the temperature. Above of the glass transition temperature of our blend system (Tg ≥ 350 °K), the energies mechanism decrease linearly with temperature decreasing. However under the glass transition temperature, the energies too decrease linearly with temperature decreasing. From the above analysis, the total energy and the potential energy have necessary effect in the glass transition process.

Optical properties

Some optical properties of P3HT/CNPh-PPV polymer system were studied by using MD simulation methods.

In order to improve our work, some physical properties of P3HT/DOCN-PPV were calculated and

listed in Table 3.

In the best of our knowledge, the physical properties for P3HT/CNPh-PPV polymer system were not studied and for this propose we could not compare our results with other values.

Conclusion

In this paper, different physical properties of P3HT/CNPh-PPV polymer system was studies by meaning of the computer simulation. The glass transition temperature (Tg) of P3HT, CNPh-PPV and P3HT/CNPh-PPV polymer system were calculated from the curves of the specific volume (vs) temperature. The study of the thermal properties can help to predict the miscibility of a polymer blend. The solubility parameters of both P3HT and CNPh-PPV $\left(\delta_{P3HT}\ and\ \delta_{DOCN-PPV}\right)$ were calculated by using Forcite and Van Kreleven of the semi empirical method Synthia. The difference between the solubility parameters $\left(\delta_{P3HT}\ and\ \delta_{DOCN-PPV}\right)$ equal to 0.64 $cal^{1/2}/cm^{3/2}$; that can be a good indicator of miscibility for P3HT:DOCN-PPV blend. The solubility parameters of P3HT and CNPh-PPV were compared with available experimental values in literature. One single glass transition temperature (Tg) equal to 354 K is obtained for our polymer blend. The effect of some energies in the Tg process was studied and analyzed. In the best of our knowledge, no experimental value for P3HT:DOCN-PPV is available in literature. From all above results we can confirm the miscibility of P3HT:CNPh-PPV polymer blend.

In order to improve our study, other different physical properties were simulated.

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