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Theoretical Insight of Excited States at Large Scale Organic/Organic Interface for Designing Novel Organic Electronic Devices

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Abstract

Revealing electronically excited states across organic/organic interfaces is important to speculate the charge photo-generation mechanisms in organic devices. As organic solar cells are large and unorganized systems so it is very tough to access it using conventional quantum chemical approaches. To unearth the charge separation mechanism a massive scale of excited states should be considered. For this purpose in this study, we have applied recently developed fragment molecular orbital (FMO) method that can effectively consider large-scale molecular aggregates. In our model, we have treated for different configurations of pentacene/C_{60} bilayer hetero-junction structures. Here, we have also discussed the charge delocalization effect, structural deformations. The measured energy dynamics low-lying interfacial CT states are in well match with experimental reports.

Keywords: Excited states, Charge transfer, Pentacene, C_{60} ,OSC.

Introduction

Recently, organic solar cells have shown extensive interest as they offer the potential for competitive renewable energy through direct photo-electron conversion of lavishly available sun light. In organic solar cells, charge transfer (CT) states at the donor-acceptor (D/A) interface have been focused because of its potentially enabling extensive area and flexible photovoltaic devices (Clarke and Durrant, 2010; Ostroverkhova, 2016). Figure 1 shows schematic diagram of charge transfer donor acceptor level. Electron–hole pair is created due to photon consumption of organic solar cells (OSC). In an organic/organic hetero-junction the exciton splits into free charge carriers after relocating donor, acceptor of electron. In the this the produce charge pairs can reunite to the initial state that reduce open-circuit voltage (Benduhn et al., 2017; Vandewal et al., 2010).

Charge carriers (electron-hole pair) generated across the donor/acceptor coupling plays a major role in charge photo-generation as it is an transition charge generation and reunited mechanism in a charge transfer state (CT) [Lin et al. 2018, Vandewal 2016]. Thus, investigation of dynamic and mood of the ICT states is important to reveal the charge photo-generation. In OSCs one of the major concern is the produce of free charge breeding (Gao and Inganäs, 2014; Yoshida et al., 2015). Some previous findings (Cornil et al., 2013; Reid et al., 2014; Vandewal et al., 2014) suggested that charge creation can occurs due to thermally relaxed ICT states.

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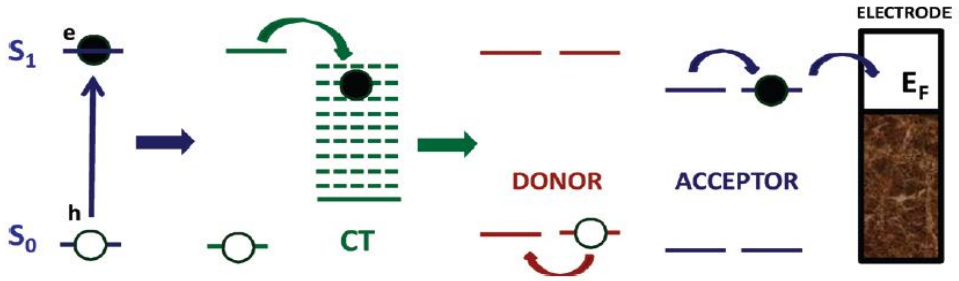

Figure 1. Schematic diagram of charge transfer.

Some scientific reports explain which the existence of massive concentrated C_{60} guide to fast charge generation (Gélinas et al., 2014; Jakowetz et al., 2016).

They attributed their reports to enhance relocation of the electron in the C_{60} clusters that boost dividation of charge pair (electron–hole pair) by diminishing the exciton bond energy. It measures directly the low-lying ICT states measurements and electro luminescence spectroscopy (Bernardo et al., 2014; Brigeman et al., 2016; Kitoh-Nishioka and Ando, 2016; Tvingstedt et al., 2009; Vandewal et al., 2010) in excessive CT states, that may play major role in charge dissociation process which is tough to portray experimentally.

The aim of the current investigations is to reveal elaborate findings about the CT-state using ab initio method for excited-state computation. We have taken into account PEN/C_{60} where PEN for electron donor and C_{60} for electron donor interfaces have been widely considered both experimentally theoretically (Ahmed, 2015; Fu et al., 2014; Hasan et al., 2018; Minami et al., 2013; Minami and Nakano, 2011; Verlaak et al., 2009; Yang et al., 2014; Zheng et al., 2017, Fujita et al., 2018), (Brigeman et al., 2016; Congreve et al., 2013; Dimova et al., 2009; Howe et al., 2011; Nakayama et al., 2016; Yamamoto et al., 2015).

Although many previous reports about OSCs applied bulk hetero-junction devices, the usage of a hetero-junction bilayer is more pertinent for straightly corresponding the frontier models with electronic mechanisms. Previous published reports have directed to monitor the credence of the interfacial CT energies on different morphological status (Bernardo et al., 2014; Ndjawa et al., 2017), (Kästner et al., 2017; Lin et al., 2016) at the PEN/C_{60} interfaces.

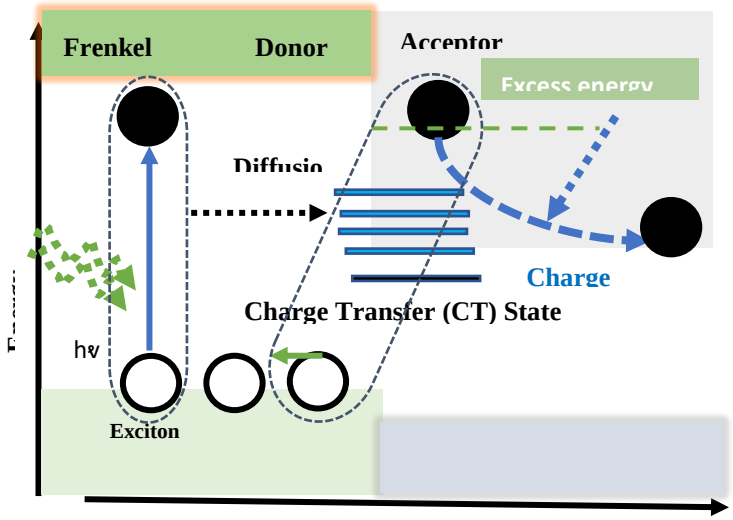

Figure 2. Schematic diagram of Electron-Hole separation

In this report, we have designed bilayer hetero-junction structures composed of large number of atoms to understand clearly the structural change, charge delocalization effects of excited state computations. Fig. 2 shows the schematic diagram of electron-hole separation.

Method and Modeling

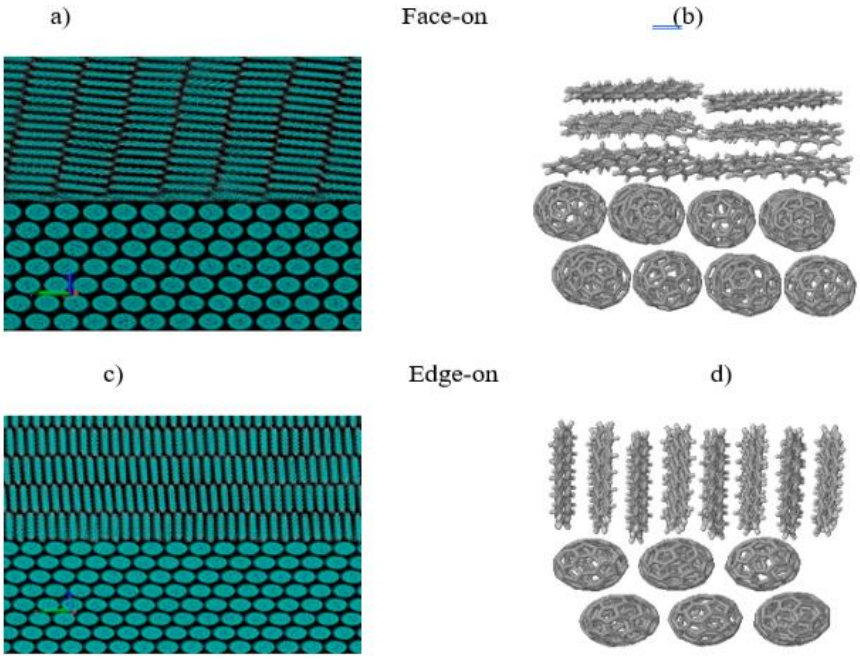

Figure 3. Atomistic structure of the (a) face on and (b) edge on interfaces included in the calculation (b and d) local interface structure.

The model of the C_{60}/PEN interface as shown in Fig. 3 were constructed of C_{60}, in which the [111], [211], and [011] directions were considered for different configurations in simulation model. (II) The PEN thin film (Schiefer et al., 2007) was connected with the C60[111] surface with two different orientations. In the intersection model for edge-on and face-on models incorporate about thousands of atoms as Fig. 3(a and c).

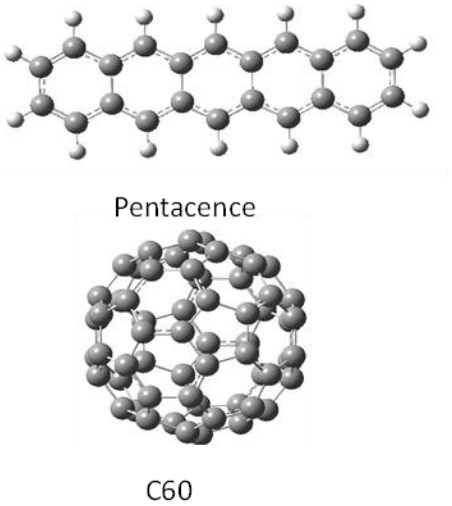

Figure 4. Single molecule of pentacene and C60

On the C_{60}/PEN interface structure molecular dynamics simulation was employed at 300 K temperature. In this simulation study considered time step of 10 ps. The molecular dynamics simulation package GROMACS (Berendsen et al., 1995) was considering AMBER force field (GAFF) model (Wang et al., 2004). The local frontier regions, as noticeable in Fig. 3(b and d), were considered by the excited state technique. The most bottom state is very important of CT state because of its energy obtained precisely from photoluminescence spectra. Total energy contributions were spilt into for the one-electron and two-electron, $E = E_{1e-}+E_{2e}$ in order to clear understanding the CT energy. For the different orientations measured energies are 1.383 eV and 1.142 eV, respectively of adiabatic states, indicates the extensive domination of interface arrangements. Fig. 4 shows single molecule of pentacene and fullerene.

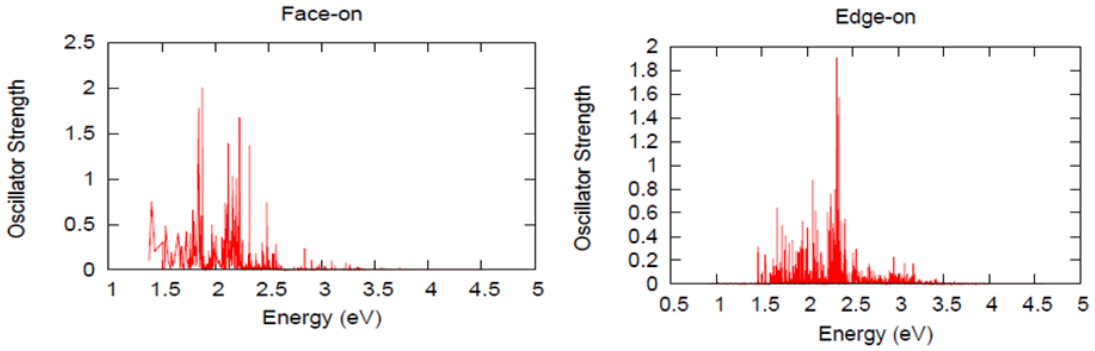

Figure 5. Absorption spectrum of face-on and edge-on

We have analyzed the absorption spectrum of pentacene/fullerene system for face-on and edge-on structures to know the stability and charge transfer states between the systems as shown in Fig. 5.

Results and Discussion

To reveal the exact feature at organic/organic interfaces junction for electronic structure is a difficult task, as charge relocations needs to consider. An electron or hole wave function is divided for a sizeable molecules to specify its using the inverse participation ratios (IPRs). CT energies remain same for the adiabatic and diabetic states of the face-on stuctures. One C_{60}-PEN pair is necessary for CT wave function because of their IPR for electron and hole. On the other hand, CT energy is reduced for the adiabatic than that of the diabatic for the edge-on system.

For both the adiabatic and diabatic CT states, it is visualized that comparing the E_{1e} and E_{2e} of the charge delocalization effect diminish for one-electron donation but does not change two-electron donation in edge-on model.

Table 1. Comparison of diabatic and adiabatic CT states (face-on vs edge-on)

Face on	*E* (eV)	*E*(2e) (eV)	*R*eh(A)	*Δ*eh(A^2)	*Δ*e(A^2)	*Δh*(A^2)
Diabetic CT	1.440	-1.803	7.4	0.0	0.0	0.0
Adiabatic CT	1.383	-1.830	7.5	4.2	3.4	2.0
	E (eV)	*E*(2e) (eV)	*R*eh(A)	*Δ*eh(A^2)	*Δ*e(A^2)	*Δh*(A^2)
Diabatic CT	1.452	-1.222	12.5	0.0	0.0	0.0
Adiabatic CT	1.142	-1.150	13.6	36.4	31.8	17.4

Here, we elucidate the outcome of the frontier morphologies hole delocalization. In previous studies, author et al. reported that the charge delocalization interactions increases with decreased electron-hole separation (D'Avino et al., 2016; Tamura and Burghardt, 2013).

We therefore, expect larger inverse participation ratios (IPRs) and standard abberation of electron-hole dissociation (σ_{eh}) to correlate with increased electron-hole separation (R_{eh}). However, irrespective of the larger IPR of wave functions for electron and hole (IPRe and IPRh), and σ_{eh} of the adiabatic state for the edge-on model, R_{eh} remain same in both wave functions (diabatic and adiabatic).

The bottom CT states are well balanced of short-range CT states whose R_{eh} are identical to one another, charge decentralization does not change distance of electron-hole wave functions. In previous theoretical reports, a tight-binding method (Ma and Troisi, 2014; Roth, 2015; Tamura and Burghardt, 2013) were applied for modeling the electronic states. Here, we have applied excited-state calculation for local conjoin configurations, with all external point charges. In this study, employed fragment based FMO (Nakano et al., 2002 Tanaka et al., 2014) method that is very effective for considering large systems.

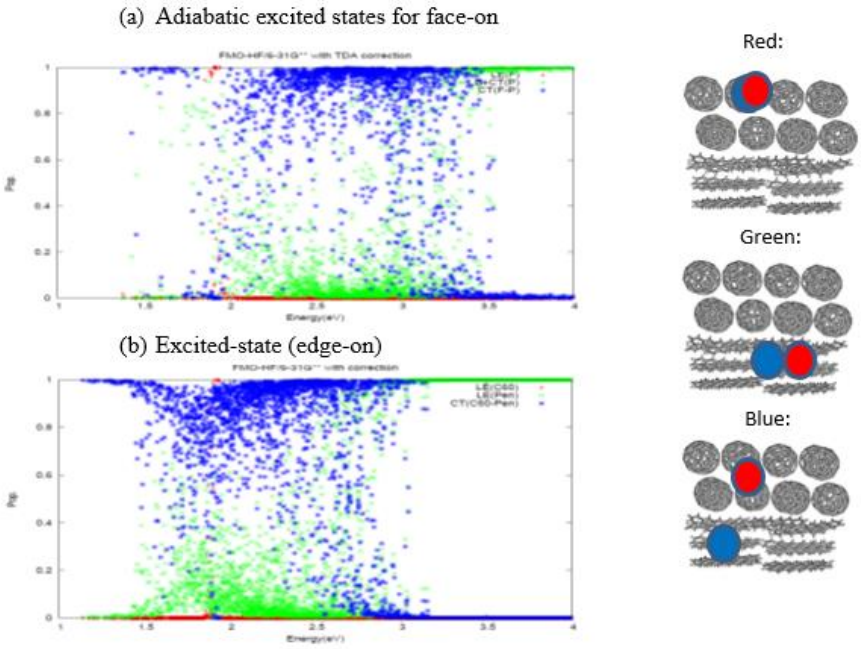

Figure 6. Character of excited states (a) face on and (b) edge on structure

FMO considered excited-state wave function for overlapping for both intramolecular and intermolecular (CT) excitations (Fujita et al., 2018) in diabatic states. The diabatic local excitations (LEs) state and the excited states for adiabatic of the system are accomplished by employing this equation $Hc = Ec$, [Here H is the Hamiltonian for excited-state and c indicates for coefficients for the diabatic states]. Computational particulars are shown in (Fujita et al., 2018). In the PEN/C_{60} interfaces excited-state wavefunctions are written as

$$|\psi\rangle = \sum c_k |\mathrm{LE}_k(C)\rangle + \sum c_k |\mathrm{CT}_k(C^-P^+)\rangle + \sum c_k |\mathrm{LE}_k(P)\rangle + \sum c_k |\mathrm{CT}_k(P^-P^+)\rangle \quad (1)$$

where |LEk(C) stands for first excited states of C_{60} and |LEk(P) denotes first excited states of PEN molecules, respectively.

This part in Fig. 6 indicates excitation energies and wave function of lowest CT states for different orientations (face-on and edge-on) of molecules (C60 and PEN). To get clear understanding into energy dynamics, CT states were divided into two parts where E_{1e} for one systems contributions and E_{2e} for two electron systems; total energy E= E_{1e}+E_{2e}. Here orbital energy difference (Band gap) for one electron contribution and the Coulomb attraction of electron and hole wave functions for two-electron contribution. The measured energies of ICT for the adiabatic are 1.383 eV and 1.142 eV for different orientations (face-on and edge-on) respectively, suggesting the considerable influence of interface models as shown in Table 1.

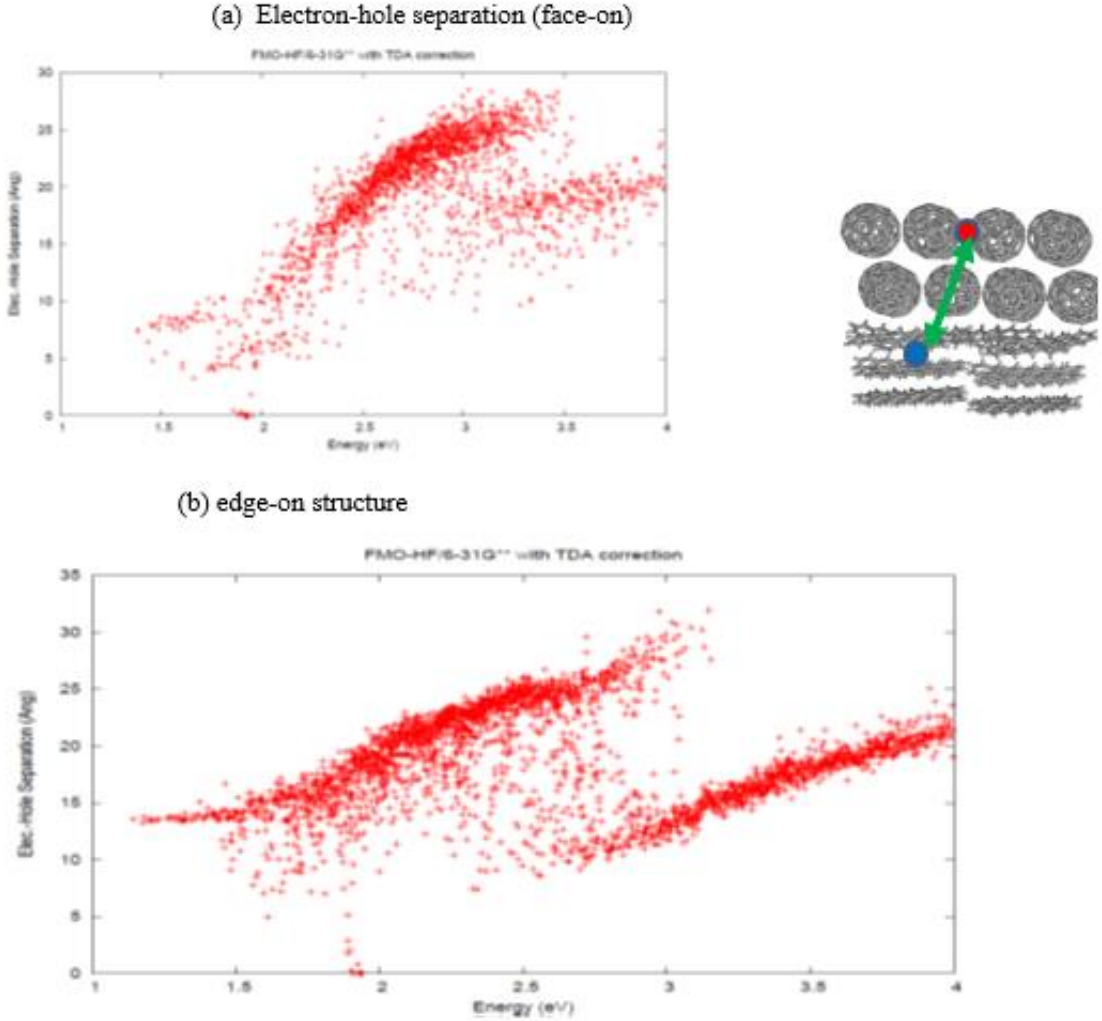

Figure 7. Electron-hole separation (a) (face-on) and (b) edge-on structure

To know the effects of morphology on the energy dynamics, here first focal point on the diabatic frontier CT energies. In case of one electron E_{1e}, the localized frontier CT states are 1.440 eV and 1.452 eV for both orientations (face on and edge on). On the contrary, of E_{2e} localized CT states are 1.830 eV, and 1.222 eV for both orientations. The difference in E_{1e} effectively develop from the pentacene quadrupole moments, which destabilize/stabilize the electron wave function on neighboring C_{60} molecules for different configurations (Verlaak et al., 2009). E_{2e}

corresponds to Coulomb attraction of the electron–hole and its value is measured based on intermolecular interspace of C_{60} and PEN. Results indicate the confined ICT energy is 1.1 eV for edge on that is lower that than of face-on structure (1.3 eV) as shown in Fig.6.

In this part we focus on the spatial extent of adiabatic ICT states. Here IPRs were proposed to consider large system and the charge carrier were divided. For the face-on structures the ICT energies remain unchanged for both adiabatic and diabatic states. Here, we analyze the effect of the interfacial morphologies for hole delocalization. Usually, the scope of relocations is more intensified by higher electronic pairings and smaller energy difference of complex systems. Here, the outcome of frontier dissection on the charge delocalization is ascribed essentially to the energy difference among heavily-collaborating charge transfer states.

The hole delocalization in the face-on orientation is repressed by the substabtial energy fluctuations in frontier CT states. On the other hand, the edge-on structure the PEN bundles run parallel to the interface where relocations over the heap does not increase distance between electron and hole as shown in Fig.7.

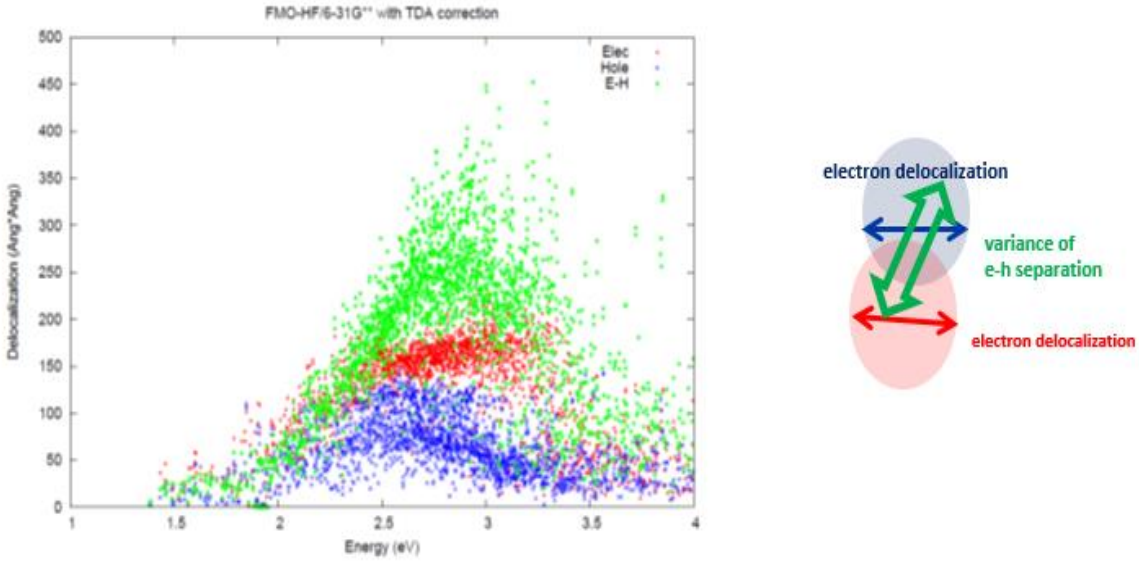

Figure 8. Variance of electron-hole separation, and delocalization of electron or hole wavefunctions

From the delocalization effects, now we target on the electron–hole partition. Decentralization was specified corresponding to the electron–hole separation. Previous report have recommended the charge decentralization reduces electron–hole electrostatic intercommunication and thus expands of its partition (D'Avino et al., 2016; Tamura and Burghardt, 2013). We, therefore, predicted spacious IPRs and deviation of electron hole partition S_{eh} to correlate with increased R_{eh}.

Fig. 8 shows clearly about the variance of electron-hole partition, and relocations of electron or hole wavefunctions. Experimental findings have indicated to outcome of the molecular coordination and bulk morphologies on energy dynamics of frontier CT states (Kästner et al., 2017; Lin et al., 2016, 2018). Main factors devoting to the ICT energies are columbic and cleavage outcomes on the orbital energy levels, that have been treated by the micro electrostatic model (Castet et al., 2014; Verlaak et al., 2009) and by photoelectron spectroscopy (Yoshida et al., 2015). Our first-principle study explains the elongated bilayer heterostructure, successfully narrating the conjoin reliant ICT energy shifts. Here, we have individually treated different structures (face-on and edge-on) orientations because target is to prepare bilayer heterojunction by connecting two crystal structures. Simulation study of charge partition

mechanism may be attained by merging a wide-ranging numerical method (Hoshi et al., 2013, 2017; Terao et al., 2013) with a quantum dynamics theory, (Fujita et al., 2016; Huh et al., 2014; Sawaya et al., 2015) that may provide clue for a future research.

Conclusions

In this study, we have examined the excited states of PEN/C_{60} interface junction structures, employing ab initio technique to atomistic models which was tailored by MD. We have partially recreated the energetics of experimental findings. Based on the wave function of electron–hole (partition, delocalization) and excited states of the PEN/C_{60} interfaces were analyzed. We have noticed that the PEN–ICT jointure findings of delocalized ICT states across the PEN/C_{60} frontier. From a computational point of view, we have exhibited the wide-ranging excited state measurements for the broaden bilayer hetero-junction model according to the newly introduced noble fragment-based method. We able to reveal a relation between frontier morphologies and optoelectronic development, which provides important clue for further research.

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Conflict of Interests

The authors have no conflict of interest declare.

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