Quantum Mechanical-Based Quantitative Structure–Property Relationships for Electronic Properties of Two Large Classes of Organic Semiconductor Materials: Polycyclic Aromatic Hydrocarbons and Thienoacenes

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ABSTRACT: In this study, the degree of the π-orbital overlap (DPO) model proposed earlier for polycyclic aromatic hydrocarbons (PAH) was employed to develop quantitative structure–property relationships (QSPRs) for band gaps, ionization potentials, and electron affinities of thienoacenes. DPO is based on two-dimensional topological draw of aromatic molecules. The B3LYP/6-31+G(d) level of density functional theory (DFT) was used to provide chemical data for developing QSPRs. We found that the DPO model is able to capture the correct physics of electronic properties of aromatic molecules so that with only six nonzero topological parameters (four for PAH and additional two for thienoacenes), the DPO model yields the linear dependence of electronic properties of both the PAH and thienoacenes classes by a single set of QSPRs with the accuracy to within 0.1 eV of the DFT results. The results suggest that within the DPO framework, all aromatic molecules can share the same set of QSPRs.

1. INTRODUCTION

Along with polycyclic aromatic hydrocarbons (PAHs), thiophene-based materials play an important role in organic-semiconductor classes; especially, in fabricating electronic devices commercially. Although not possessing outstanding electronic properties such as PAHs, thiophene-based structures own a number of physical characteristics making them easier to be synthesized under room conditions and to be stretched in thin-film morphology than the PAHs as well as more soluble and more stable in oxidized species. They are used in production of organic light-emitting diodes (OLEDs), organic field-effect transistors, organic thin-film transistors, and organic photovoltaics.1−16

Thienoacene is a class of thiophene-based materials where one or more benzene rings of the PAH structure are replaced by thiophene rings.17 This class has a wide range of synthetic patterns. Experimentalists have been trying to discover the newest thienoacene structures that could possess characters for enhancing the electronic quality of devices; particularly, the band gap, mobility, and stability in harsh conditions.10,12,14,15,17,18 Computational chemistry, particularly the use of density functional theory (DFT), would aid in the design stage of the experimentation. However, even with the current computing power, it still takes time and resources to screen a large molecular space. Quantitative structure property relationship (QSPR) modeling that can predict electronic properties of such materials with a reasonable degree of accuracy would be of great interest in aiding this material research.

The QSPR method is well established for biological applications and is making progress in material design such as for nanomaterials, biomaterials, polymers, and ionic liquids.19 For instance, the QSPR method in combination with DFT computations has proved to be a cost effective approach for designing materials as proposed by Sukumar et al.20 New methodologies are being developed such as using the deep neural network to improve limitations of QSPR modeling.
reported by Winkler and Le, or in combination with the artificial network model and support vector machine for predicting electroluminescence of a small set of OLED structures. Regarding OLED applications, the QSRR approach was used to study the glass transition temperature. QSR models were also developed for predictions of critical electronic and thermomechanical properties of crystalline materials or energetic materials such as nitro-organic compounds. Also, screening metal organic framework materials for CO2 capture was studied by applying the QSRR approach with advanced machine learning algorithms. However, there have not been many studies regarding QSRR applications for predictions of electronic properties of organic semiconductor materials. Particularly, for thienoacene, there has not been any QSRR study for its electronic properties reported till today. In our recent study, we proposed a new model called “degree of π-orbital overlap” (DPO) based on a quantum mechanical particle in two-dimensional (2D) box to develop QSRR for electronic properties of PAHs. With only four topological parameters, the DPO model was able to predict electronic properties of PAHs in the particular band gap, ionization potential (IP), and electron affinity (EA) to within 0.1 eV accuracy on average compared to the explicitly calculated data.

In this study, we extend the DPO model to the thienoacene molecular class and further examined the accuracy of the DPO model.

2. COMPUTATIONAL DETAILS
2.1. Data Sets. In this study, the thienoacene class is divided into two separate subclasses: 1T-subclass and 2T-subclass.

Figure 1. Building blocks for constructing a given thienoacene molecule of the 1T-subclass. (a–d) are simplified models showing how these building blocks are related to the DPO a–d parameters. Fused bonds are highlighted in bold.

Figure 2. Segment 1 of structure I and segment 3 of structure II are the reference segments. Fused bonds are highlighted in bold.

2.2. Computational Methods. Geometries of all molecules in two data sets are fully optimized, and their electronic properties are calculated by the DFT B3LYP/6-31+G(d) level.

Figure 3. Segment 1 of structure III and segment 5 of IV are chosen to be the reference segments.

Figure 4. DPO values of the reference segments containing only benzene rings and a thiophene ring.

Figure 5. Illustration of how topological parameters d and d* are assigned fused bonds.

Figure 6. Illustration of how topological parameters b and b* are assigned fused bonds.

Figure 7. Illustration of how topological parameters c and c* are assigned fused bonds.

1T-subclass molecules consist of one thiophene ring with benzenes, and the 2T-subclass is those of two thiophene rings. The structures having 4 to 6 rings of two subclasses constitute the development set of total 81 molecules for building the QSRRs, and those having 7–8 rings of the subclasses make up the test set of total 82 molecules for assessing the accuracy of the QSRRs.

Figure 8.
of theory. This level of theory is known to predict frontier orbital energies accurately.3,4,30,31

The IP is estimated by the negative value of the highest occupied molecular orbital (HOMO) energy, and similarly, the EA is estimated by the negative value of the lowest unoccupied molecular orbital (LUMO) according to Koopman’s theory. The HOMO–LUMO gap is used to estimate the band gap.32

2.3. Quantum Mechanical-Based DPO Model. It is well known in physical chemistry that the HOMO–LUMO gap of a conjugated polyethylene such as butadiene can be modeled by a particle in a one-dimensional box model with an effective box length. With a similar argument, our recent study29 suggested that the DPO model based on a simplified quantum mechanical particle in a 2D box framework for developing QSPRs for electronic properties, namely, the band gap, IP, and EA of a given thienoacene molecule, one must first determine its DPO value according to the following procedure.

Step 1: Determine the reference segment by applying the following rules in the sequential order till a distinct reference segment is found.

a. The segment with the largest number of fused rings (or fused bonds) is the reference segment.

b. If all segments in the molecule have the same size, the segment with the largest number of parallel-fused bonds orthogonal to its direction is the reference segment. Furthermore, the segment consisting of only benzenes is preferred over that having thiophene rings.

c. If rules (a) and (b) do not yield a unique segment, then the segment with the least number of overlayers is the reference segment.

For example, for the two thienoacenes shown in Figure 2, segment 1 of structure I has the largest number of fused rings; therefore, it is the reference segment according to rule (a). In structure II, both segments 3 and 4 have the same number of fused rings; however, segment 3 contains only benzenes and thus is preferred to be the reference segment.

In Figure 3, structure III has three segments with the same size. According to rule (a), segments 1 and 2 are preferred but have the same size. Using rule (b), segment 1 of structure III is selected to be the reference segment because it has a larger number of parallel-fused bonds orthogonal to the reference direction. In structure IV, in Figure 3, both rules (a) and (b) do not yield a unique segment. In this case, rule (c) helps to select segment 5 to be the reference segment.

In the previous study, we described how to calculate the DPO value for any PAH molecule. Here, we review how it is done; therefore, the instruction for assigning the DPO value for any thienoacene is easier to follow. Each of the fused bonds in a PAH or thienoacene is assigned a value, a topological parameter for its electronic properties, namely, the band gap, IP, and EA of a given thienoacene molecule, one must first determine its DPO value according to the following procedure.

Step 1: Determine the reference segment by applying the following rules in the sequential order till a distinct reference segment is found.

a. The segment with the largest number of fused rings (or fused bonds) is the reference segment.

b. If all segments in the molecule have the same size, the segment with the largest number of parallel-fused bonds orthogonal to its direction is the reference segment. Furthermore, the segment consisting of only benzenes is preferred over that having thiophene rings.

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For example, for the two thienoacenes shown in Figure 2, segment 1 of structure I has the largest number of fused rings; therefore, it is the reference segment according to rule (a). In structure II, both segments 3 and 4 have the same number of fused rings; however, segment 3 contains only benzenes and thus is preferred to be the reference segment.

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Step 2: Assigning a DPO topological value for each fused bond.

a. For the reference segment that contains only benzene rings, starting from the leftmost, each fused bond has a value successively of 1, 1 − a, 1 − 2a, 1 − 3a, and so on where a is the topological parameter for the PAH class. If there is a thiophene ring attached on the reference segment, then the total DPO for this segment is subtracted by the parameter α, shown in Figure 4.
b. For the other segments, there are three types:

Type 1: For a segment that is paralleled to the reference one, similar assignments of the base values, that is, 1, \((1 - a)\) and \((1 - 2a)\) are used. However, each fused bond is then adjusted by a scaling factor of \(d^*\), where \(k\) is the order of the layer above or below the segment including the first parameter assigned to fused bonds, that is, and \(d^*\) is also a parameter for the PAH class. If a benzene ring is replaced by a thiophene ring in this segment, the scaling parameter \(d^*\) is used instead. Figure 5 shows how parameter \(d^*\) or \(d^*\) are used.

Type 2: For a segment with its fused bonds that form a 60° angle with the reference one, these fused bonds are assigned with the topological value \(b\) if the segment has all benzene rings. For each subsequent parallel-fused bond, its value is scaled by a factor \(d\) or \(d^*\) if a thiophene is at the end of the segment as shown in the top row of Figure 6. However, when a thiophene ring is attached on the reference segment at an angle or a small benzene ring segment is fused on the other side of thiophene, these fused bonds are assigned to topological parameter \(b^*\) as shown in the bottom-row structures in Figure 6.

Type 3: For a segment with its fused bonds form a 120° angle with those of the reference segment, and these fused bonds are assigned by topological parameter \(c\). Similar to type 2, for each subsequent parallel-fused bond, its value is scaled by factor \(d\) or \(d^*\) if a thiophene is attached at the end of the segment as shown in Figure 7. If a thiophene ring is attached to the benzene side on the segment as shown on the last structures of Figure 7, the fused bond is assigned to the topological parameter \(c^*\) instead.

For the PAH class, the topological parameters of \(a, b, c,\) and \(d\) determined from our previous study are 0.05, \(-1/4, +1/3,\) and \(+1/3,\) respectively. With the similar procedure of using a small set of molecules that allows the independent optimization of each parameter, for the thienoacene class, the topological parameters \(a^*, b^*, c^*,\) and \(d^*\) are 0.50, 0.0, 0.0, and 0.15, respectively. Consequently, we have six nonzero topological parameters in order to determine the DPO value for any PAH or thienoacene molecule.

Step 3: The total DPO value for a given molecule is the sum of all topological values assigned to all fused bonds.

Examples for assigning the DPO value for each fused bond and their total values are given below for six different thienoacene molecules. The total DPO values of compounds \(A = 2.28, B = 2.48, C = 1.78, D = 2.42, E = 1.47,\) and \(F = 2.64\) are shown in Figure 8.

3. RESULTS AND DISCUSSIONS

3.1. DPO-Based QSPR. Linear correlations between DPO values and the three electronic properties of 1-T thienoacene and 2-T thienoacene classes are shown in Figures 9A–C and 10A–C, respectively.

These figures show excellent linear correlations between DPOs and the electronic properties of thienoacenes with the corresponding correlation coefficients \(R^2\) all greater than 0.9. Compared to PAHs results, almost all \(R^2\) values of the 1T-subclass and 2T-subclass are in a similar level of correlations as those of PAHs in our previous study. Linear equations for these correlations of the band gap, IP, and EA properties as functions of the DPO values are summarized in Table 1 along with those for PAH from the previous study.

![Figure 9](image-url)  
Figure 9. Plots of linear correlations between DPO values and (A) HOMO–LUMO gaps, (B) IPs, and (C) electron affinities of thienoacenes from the development set of the 1T-subclass.

It is interesting to note that the slopes and intercepts of all linear equations for both thienoacenes and PAHs are very similar in magnitude. As shown in Figure 11, they are within the uncertainty of the linear fit. This indicates that the DPO model is able to capture the correct physics of the aromatic systems and thus all aromatic systems can share the same QSPRs. For this reason, we used the QSPRs of PAH for analyzing the accuracy of the DPO model for both the thienoacenes and PAH classes.

3.2. Accuracy of DPO-Based QSPRs. To assess the accuracy and predictability of DPO-based QSPRs for the electronic properties of these thienoacene subclasses, electronic properties of all molecules in the test set were plotted against those predicted by QSPRs, as shown in Figure 12A–C. Note QSPRs of PAH are used for all assessments below.

Root-mean-square differences (RMSDs) between QSPR-predicted and DFT explicitly calculated properties for thienoacenes in the test set are all less than 0.1 eV. This is even within the accuracy of the DFT level of theory. These results are consistent with our previous results for PAH, though here we used the PAH QSPRs to further illustrate that all aromatic molecules can share the same QSPRs. To further illustrate this point, Figure 13 shows the QSPR-predicted and DFT explicitly calculated properties for all PAHs (34 molecules) and...
thienoacenes (82 molecules) in both test sets using the same QSPR equations from PAH. Again RMSDs for all properties are less than 0.1 eV. These results suggest that the DPO model is able to capture the correct physics of electronic properties of aromatic molecules, and thus their properties can be modeled by one set of QSPRs. Note that the current DPO model has only six topological parameters for both PAH and thienoacenes.

To further examine the range of applicability of the model, Figure 14 shows QSPR predicted versus DFT explicitly calculated electronic properties for a number of thienoacenes with three and four thiophene rings using the PAH QSPRs. Note these thienoacenes are not part of the QSPR development set nor the test set. The results suggest that our DPO-based QSPR model can be applied to all thienoacenes that have planar structures with similar accuracy. For nonplanar structures, the errors are larger due to the disruption in the resonance structure of the molecule. The issue with nonplanarity in the DPO-based QSPR model has been addressed in detail in our previous study.

3.3. How To Use DPO-Based QSPRs. For any given PAH or thienoacene, the following procedure should be used: (a) identify all fused bonds and then select the reference segment; (b) assign a DPO topological parameter to each fused bond according to the rule described above; and (c) sum all of these values to give the total DPO value of the structure. Subsequently, use the QSPRs for PAH in Table 1 with the calculated DPO value to predict the band gap, IP, and EA of the molecule.

Table 1. QSPR Equations for Band Gap, IP, and EA of PAHs and Thienoacenes (all are in eV)

| electronic property | 1T-subclass | 2T-subclass | PAHs
|---------------------|-------------|-------------|----------------|
| band gap            | $y = -0.76x + 4.92$ | $y = -0.63x + 4.67$ | $y = -0.65x + 4.68$
| IP                  | $y = -0.35x + 6.14$ | $y = -0.30x + 5.99$ | $y = -0.30x + 6.04$
| EA                  | $y = +0.41x + 1.22$ | $y = +0.33x + 1.31$ | $y = +0.35x + 1.36$
4. CONCLUSIONS

In this study, we applied the DPO model proposed earlier to develop QSPR for band gaps, IPs, and electron affinities of thienoacenes. Electronic properties were calculated at the B3LYP/6-31+G(d) level of theory and are used to develop the QSPRs as well as to assess its accuracy for the thienoacene class. We found that QSPRs for thienoacene and those for PAH found in our previous study are almost the same within the uncertainty of the calculations. This indicates that the DPO model is able to capture the correct physics of electronic properties of aromatic molecules so that with only six nonzero topological parameters, the DPO model can yield a single set of linear dependence of electronic properties for both the PAH and thienoacene classes to within the accuracy of 0.1 eV of the DFT results.

These results suggest the possibility for applying the DPO model to other conjugated classes of molecules in addition to other aromatic classes. It will be the subject of our future studies.

Figure 12. Plots of the QSPR predicted vs DFT explicitly calculated electronic properties for thienoacenes in the test set. (A) HOMO−LUMO gaps, (B) IPs, and (C) electron affinities.

Figure 13. Plots of QSPR-predicted vs DFT explicitly calculated electronic properties of PAHs and thienoacenes: (A) HOMO−LUMO gaps, (B) IPs, and (C) electron affinities.
properties for seven to eight fused ring structures of 1T subclass thienoacene; and calculated Egap, IP, and EA (in eV) properties for seven to eight fused ring structures of 2T subclass thienoacene (PDF)

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Notes

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ABBREVIATIONS

QSPR, quantitative structure property relationships; PAHs, polycyclic aromatic hydrocarbons; DFT, density functional theory; DPO, degree of π-orbital overlap; OLEDs, organic light-emitting diodes; OFETs, organic field-effect transistors; OTFTs, organic thin-film transistors; OPVs, organic photovoltaics; IP, ionization potential; EA, electron affinity; HOMO, highest occupied molecular orbital; LUMO, lowest unoccupied molecular orbital; RMSD, root-mean-square difference

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ASSOCIATED CONTENT

Supporting Information

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Figure 14. Plots of QSPR predicted vs DFT explicitly calculated properties of thienoacene molecules containing three to four thiophene rings: (A) HOMO−LUMO gaps, (B) IPs, and (C) EAs. The black crosses are for nonplanar molecules and red dots are for planar ones. The RMSD values for planar molecules are in parentheses.
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