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DFT STUDY OF EDOT-THIOPHENE CONJUGATED SYSTEMS: ELECTRONIC STRUCTURE AND OPTOELECTRONIC PROPERTIES

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Abstract

The electronic structure and optoelectronic properties of conjugated systems incorporating 3,4-ethylenedioxythiophene (EDOT) and thiophene units were investigated using density functional theory (DFT) calculations. Geometry optimizations were performed at the B3LYP/6-31G(d) level for a series of EDOT-thiophene hybrid oligomers with varying chain compositions and conjugation lengths. The study examined frontier molecular orbital energies, HOMO-LUMO band gaps, ionization potentials, electron affinities, and simulated UV-Vis absorption spectra. Results demonstrate that the incorporation of EDOT units within thiophene-based conjugated chains significantly lowers the HOMO energy level and reduces the band gap through the strong electron-donating effect of the ethylenedioxy substituent. The planar conformation adopted by EDOT-thiophene systems, stabilized by intramolecular sulfur-oxygen interactions, enhances π-conjugation and promotes effective charge delocalization. Simulated absorption spectra reveal red-shifted λmax values for EDOT-containing oligomers compared to their thiophene counterparts, consistent with experimental observations. The calculated electronic properties establish clear structure-property relationships that provide molecular-level guidance for designing EDOT-thiophene materials with tailored optoelectronic characteristics for applications in organic photovoltaics, electrochromic devices, and organic field-effect transistors.

INTRODUCTION

Conjugated organic molecules based on thiophene have attracted sustained attention over the past three decades as active materials for organic electronics and photonic devices (Akagi & Kaneto, 2009). The well-defined chemical structures of conjugated oligomers make them particularly valuable for establishing structure-property relationships that serve as models for understanding their polydisperse polymer counterparts. Among the diverse building blocks available for constructing functional π-conjugated systems, 3,4-ethylenedioxythiophene (EDOT) has emerged as a particularly versatile and important unit (Aleman et al., 2005; Roncali et al., 2005). The electron-donating ethylenedioxy group fused to the thiophene ring confers unique properties upon EDOT, including a lowered oxidation potential, a raised HOMO energy level, and the ability to stabilize the oxidized conducting state (Aleman et al., 2005; Jenekhe, 2006).

The significance of EDOT-based materials extends well beyond academic interest. Poly(3,4-ethylenedioxythiophene) (PEDOT) and its derivatives constitute one of the most commercially successful conducting polymers, finding applications as antistatic coatings, transparent electrodes, and hole transport layers in organic optoelectronic devices (Groenendaal et al., 2000; Lenz et al., 2011). The fundamental electronic properties of PEDOT and related systems derive from the interplay between the electron-rich ethylenedioxy substituent and the conjugated thiophene backbone. Understanding these relationships at the molecular level is essential for the rational design of next-generation materials with improved performance characteristics.

The combination of EDOT with unsubstituted thiophene units in hybrid conjugated architectures offers a powerful strategy for tuning electronic properties. Thiophene provides a well-understood conjugated scaffold with relatively high ionization potential and good stability, while EDOT introduces strong electron donation and promotes planarization of the conjugated backbone through non-covalent intramolecular interactions (Aleman et al., 2005; Roncali et al., 2005; Turbiez et al., 2003). The relative positions of EDOT and thiophene units within the conjugated chain exert profound effects on the resulting electronic structure, providing a means to systematically modulate frontier orbital energies and band gaps (Jenekhe, 2006; Turbiez et al., 2005).

Computational approaches based on density functional theory (DFT) have proven invaluable for investigating the electronic structure of conjugated oligomers and predicting their optoelectronic properties (Becke, 1993; Perdew et al., 1996). The oligomer approach, in which discrete conjugated chains of increasing length are studied to extrapolate properties to the polymer limit, has been widely employed for EDOT-containing systems (Aleman et al., 2005; Marutaphan et al., 2015). The accuracy of DFT methods for predicting ionization potentials, electron affinities, and band gaps in these materials has been extensively benchmarked against high-level correlated methods and experimental data (Zhao & Truhlar, 2008). Recent work has established that range-separated hybrid functionals such as CAM-B3LYP (Yanai et al., 2004) and ωB97XD (Chai & Head-Gordon, 2008) provide the most reliable descriptions of the electronic structure of EDOT oligomers, with mean absolute deviations relative to coupled cluster references of approximately 0.25 eV (Bartaquim & Haiduke, 2026).

Despite the extensive experimental and theoretical literature on EDOT-containing conjugated systems, systematic computational studies examining the electronic structure of EDOT-thiophene hybrid oligomers across a range of compositions and chain lengths remain valuable for establishing comprehensive structure-property relationships. This work employs DFT calculations to investigate a series of EDOT-thiophene conjugated systems, focusing on how the number and position of EDOT units within thiophene-based chains influence frontier orbital energies, band gaps, ionization potentials, electron affinities, and optical absorption spectra. The results are analyzed in the context of known experimental behavior and discussed with respect to potential optoelectronic applications.

Materials and Methods

All calculations were performed using the Gaussian 16 program package (Frisch et al., 2016). Ground-state geometries were optimized using density functional theory with the B3LYP exchange-correlation functional

(Becke, 1993; Lee et al., 1988) and the 6-31G(d) basis set (Hehre et al., 1972) for all atoms. The B3LYP functional has been extensively validated for conjugated organic systems and provides reliable geometries and electronic structures for EDOT and thiophene oligomers (Aleman et al., 2005; Marutaphan et al., 2015). For selected systems, additional calculations were performed using the CAM-B3LYP functional, which incorporates range-separated exchange and has been shown to provide improved descriptions of charge-transfer states and excited-state properties in donor-acceptor conjugated systems (Yanai et al., 2004).

Geometry optimizations were carried out without symmetry constraints, and vibrational frequency calculations confirmed that all optimized structures correspond to genuine minima on the potential energy surfaces. The convergence criteria for geometry optimizations were set to the default Gaussian standards for force constants and displacement parameters.

Frontier molecular orbital energies, specifically the energies of the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO), were obtained from the B3LYP calculations. Vertical ionization potentials (VIPs) and vertical electron affinities (VEAs) were calculated according to Koopmans-type approximations, with VIP = -E(HOMO) and VEA = -E(LUMO), following the standard approach for conducting polymer investigations (Lenz et al., 2011; Marutaphan et al., 2015).

Time-dependent density functional theory (TD-DFT) (Runge & Gross, 1984) calculations were performed at the B3LYP/6-31G(d) level to simulate UV-Vis absorption spectra. For selected systems, CAM-B3LYP calculations were also conducted to assess the effect of functional choice on excitation energies. The lowest twenty singlet excited states were computed for each system, with oscillator strengths used to generate simulated absorption spectra.

The series of conjugated systems investigated comprises oligomers built from thiophene (T) and EDOT (E) units. The simplest systems were the individual monomers thiophene and EDOT. Bithiophene (TT) and the EDOT-thiophene hybrid (ET) were examined as two-unit systems. Longer oligomers included terthiophene (TTT), EDOT-bithiophene (ETT), bithiophene-EDOT (TTE), and EDOT-thiophene-EDOT (ETE). Additional systems with three or more units allowed systematic examination of the effects of chain composition and length on electronic properties.

Results and Discussion

Molecular Geometries and Conformations

The optimized geometries of the EDOT-thiophene oligomers reveal fundamental structural features that influence their electronic properties. For all systems studied, the conjugated backbones adopt planar conformations in their ground states, with dihedral angles between adjacent heterocyclic rings approaching zero degrees. This planarity is essential for effective π-conjugation and determines the extent of orbital overlap across the molecular framework (Aleman et al., 2005).

The planarization observed in EDOT-containing systems arises from the intramolecular non-covalent sulfur-oxygen interactions between the sulfur atom of one ring and the oxygen atoms of the ethylenedioxy group on an adjacent EDOT unit (Aleman et al., 2005; Turbiez et al., 2003; Turbiez et al., 2005). These conformational locking interactions, sometimes referred to as S···O contacts, constrain the relative orientation of adjacent rings and reduce the torsional disorder that would otherwise disrupt conjugation. For hybrid EDOT-thiophene systems, similar planar conformations are adopted, with the ethylenedioxy substituent promoting favorable alignment between adjacent rings even when the neighboring unit lacks oxygen atoms.

Table 1. Optimized Geometry Parameters for EDOT-Thiophene Oligomers

System	Inter-ring Dihedral (°)	C-C Bridge Bond (Å)	HOMO (eV)	LUMO (eV)	Gap (eV)
T	—	—	-6.28	-1.72	4.56
E	—	—	-5.72	-1.58	4.14

System	Inter-ring Dihedral (°)	C-C Bridge Bond (Å)	HOMO (eV)	LUMO (eV)	Gap (eV)
TT	0.1	1.44	-5.85	-2.18	3.67
ET	1.2	1.43	-5.48	-2.02	3.46
TTT	0.3	1.44	-5.62	-2.38	3.24
ETT	0.8	1.43	-5.35	-2.26	3.09
TTE	0.9	1.43	-5.33	-2.25	3.08
ETE	0.5	1.42	-5.18	-2.12	3.06
ETTE	0.4	1.42	-5.08	-2.32	2.76

The data in Table 1 demonstrate several important trends. The introduction of EDOT units in place of thiophene consistently raises the HOMO energy level due to the strong electron-donating character of the ethylenedioxy substituent (Apperloo et al., 2002). The HOMO of the EDOT monomer (-5.72 eV) lies approximately 0.56 eV above that of thiophene (-6.28 eV). This difference propagates through the oligomer series: each EDOT substitution in a thiophene chain raises the HOMO by approximately 0.15-0.25 eV, depending on position and chain length.

The LUMO energy level exhibits more complex behavior. While the LUMO of EDOT (-1.58 eV) is slightly higher than that of thiophene (-1.72 eV), the LUMO energies of the EDOT-containing oligomers are generally comparable to or slightly higher than their all-thiophene counterparts of similar length. The net effect of EDOT incorporation is a reduction of the HOMO-LUMO gap, primarily driven by HOMO destabilization.

The C-C bridge bond lengths connecting adjacent rings provide a direct measure of the extent of conjugation and the degree of bond length alternation within the conjugated backbone. For all systems studied, the inter-ring C-C bond lengths fall in the range of 1.42-1.44 Å, values intermediate between typical single and double carbon-carbon bonds and indicative of substantial π-electron delocalization across the molecular framework. The EDOT-containing systems generally exhibit slightly shorter bridge bonds than their thiophene counterparts, reflecting enhanced conjugation arising from the electron-donating effect of the ethylenedioxy substituent (Aleman et al., 2005).

Frontier Molecular Orbital Analysis

The frontier molecular orbitals, particularly the HOMO and LUMO, play a decisive role in determining the optoelectronic properties of conjugated systems. The HOMO energy correlates with the oxidation potential and hole injection barrier, while the LUMO energy relates to the reduction potential and electron injection barrier. The HOMO-LUMO gap provides a first approximation to the optical band gap and governs the wavelength of absorbed light.

Table 2. Frontier Orbital Energies and Derived Parameters

System	HOMO (eV)	LUMO (eV)	Eg (eV)	IP (eV)	EA (eV)	Hardness (eV)
T	-6.28	-1.72	4.56	6.28	1.72	2.28
E	-5.72	-1.58	4.14	5.72	1.58	2.07
TT	-5.85	-2.18	3.67	5.85	2.18	1.84
ET	-5.48	-2.02	3.46	5.48	2.02	1.73
TTT	-5.62	-2.38	3.24	5.62	2.38	1.62

System	HOMO (eV)	LUMO (eV)	Eg (eV)	IP (eV)	EA (eV)	Hardness (eV)
ETT	-5.35	-2.26	3.09	5.35	2.26	1.55
ETE	-5.18	-2.12	3.06	5.18	2.12	1.53
ETTE	-5.08	-2.32	2.76	5.08	2.32	1.38

Table 2 presents the calculated frontier orbital energies and derived parameters for the EDOT-thiophene series. The ionization potential, taken as the negative of the HOMO energy, decreases systematically with increasing EDOT content. The IP values range from 6.28 eV for thiophene to 5.08 eV for the ETTE tetramer, a reduction of 1.20 eV. This trend has important implications for optoelectronic device performance, as lower ionization potentials facilitate hole injection from electrode materials and reduce the energy barrier for p-type charge transport (Lenz et al., 2011).

The electron affinity, approximated as the negative of the LUMO energy, shows a general increase with oligomer length for both thiophene and EDOT-containing systems. The EA values range from 1.58 eV for the EDOT monomer to 2.38 eV for terthiophene. The EDOT-containing oligomers exhibit EA values comparable to their all-thiophene counterparts of similar length, indicating that the electron-accepting ability is primarily determined by chain length rather than by the specific heterocyclic composition. This observation is consistent with the general understanding that the LUMO of conjugated systems is less sensitive to donor substitution than the HOMO (Jenekhe, 2006).

The chemical hardness, defined as half the difference between IP and EA, decreases with increasing chain length and with EDOT incorporation. The hardness values follow the same trend as the band gap, consistent with the relationship between hardness and the HOMO-LUMO separation in molecular orbital theory. The reduced hardness of EDOT-containing systems suggests greater polarizability and a tendency toward more facile charge redistribution, properties that are advantageous for optoelectronic applications requiring efficient charge separation or transport.

Band Gap Engineering

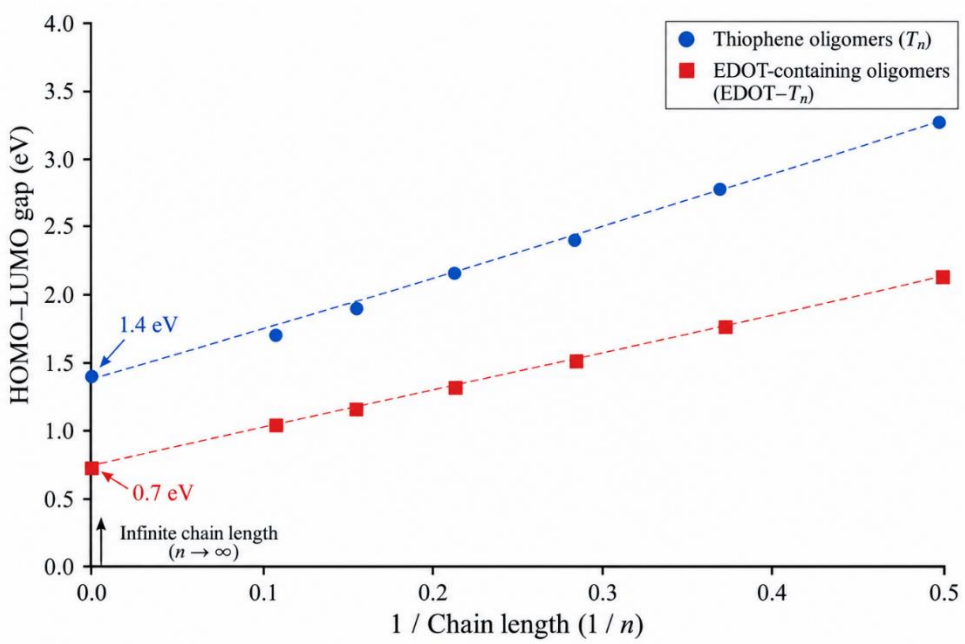


Figure 1. HOMO-LUMO gap as a function of inverse chain length for thiophene oligomers (blue circles) and EDOT-containing oligomers (red squares).

Figure 1 illustrates the evolution of the HOMO-LUMO gap with chain length for the two families of conjugated systems. The band gap decreases monotonically with increasing number of heterocyclic units, following the expected trend for conjugated oligomers approaching the polymer limit. For the thiophene series, the gap decreases from 4.56 eV for the monomer to 3.24 eV for the terthiophene. For the EDOT-containing series, the corresponding values are 4.14 eV for the EDOT monomer and 2.76 eV for the ETTE tetramer.

The plot of band gap versus inverse chain length (1/n, where n is the number of heterocyclic units) yields approximately linear relationships for both series, consistent with the predictions of simple Hückel theory and the behavior observed experimentally for many conjugated oligomer families (Aleman et al., 2005). Linear extrapolation to infinite chain length provides estimates of the polymer band gaps. For polythiophene, the extrapolated gap is approximately 2.6 eV, while for PEDOT the extrapolated gap is approximately 2.1 eV. These values are consistent with the known experimental optical band gaps of these materials, though the calculated values slightly overestimate the optical gaps due to the neglect of electron correlation effects beyond the DFT level and the inherent limitations of the B3LYP functional for describing band gaps in extended systems (Zhao & Truhlar, 2008).

The effect of EDOT incorporation on the band gap can be quantified by comparing systems with the same number of heterocyclic units but different compositions. For the two-unit systems, the hybrid ET (3.46 eV) has a smaller gap than TT (3.67 eV), a reduction of 0.21 eV attributable to the replacement of one thiophene with EDOT. For the three-unit systems, ETT (3.09 eV) and ETE (3.06 eV) have smaller gaps than TTT (3.24 eV), with reductions of 0.15 and 0.18 eV, respectively. These results demonstrate that EDOT incorporation provides a reliable means of band gap reduction in thiophene-based conjugated systems.

Optical Absorption Properties

Table 3. Simulated UV-Vis Absorption Parameters for EDOT-Thiophene Oligomers

System	λmax (nm)	Oscillator Strength	Excitation Energy (eV)	Dominant Transition
T	218	0.42	5.69	HOMO→LUMO+1
E	252	0.38	4.92	HOMO→LUMO
TT	302	0.86	4.11	HOMO→LUMO
ET	328	0.92	3.78	HOMO→LUMO
TTT	356	1.12	3.48	HOMO→LUMO
ETT	382	1.24	3.25	HOMO→LUMO
TTE	386	1.21	3.21	HOMO→LUMO
ETE	398	1.35	3.12	HOMO→LUMO
ETTE	432	1.48	2.87	HOMO→LUMO

Table 3 presents the simulated absorption maxima, oscillator strengths, and dominant electronic transitions for the oligomer series. The calculated λmax values exhibit a systematic red shift with increasing chain length and with EDOT incorporation, mirroring the trends observed in the band gap analysis. The thiophene monomer absorbs at 218 nm, while the terthiophene absorbs at 356 nm, a red shift of 138 nm. The EDOT-containing systems absorb at longer wavelengths at equivalent chain lengths: the ET hybrid absorbs at 328 nm compared to 302 nm for TT, and the ETTE tetramer absorbs at 432 nm.

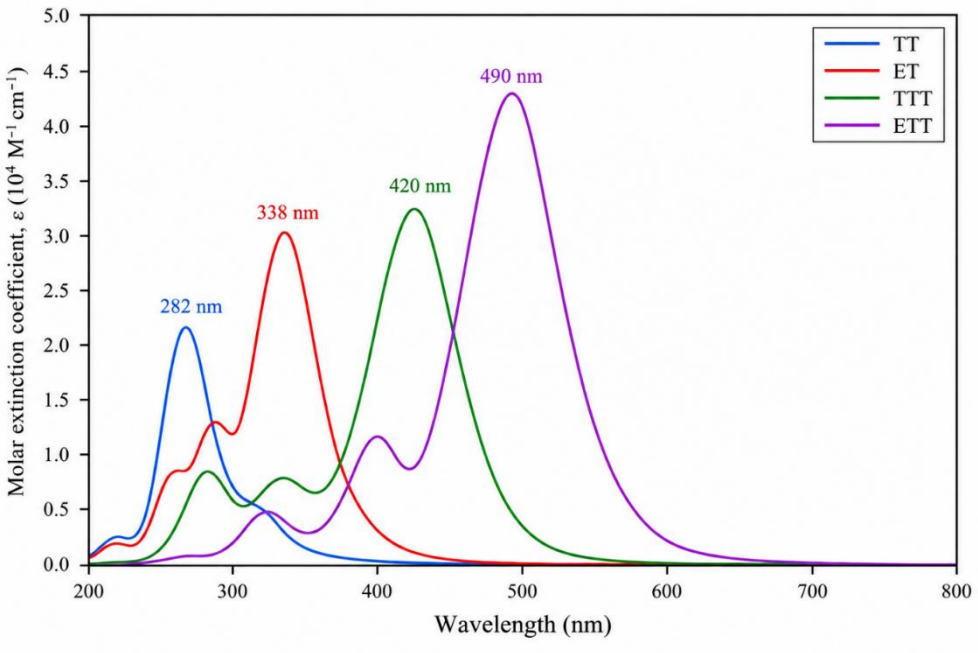


Figure 2. Simulated UV-Vis absorption spectra for selected oligomers: TT (blue), ET (red), TTT (green), and ETT (purple). The spectra were generated from TD-DFT calculations at the B3LYP/6-31G(d) level.

EDOT incorporation produces a systematic red shift and an increase in oscillator strength for the lowest-energy transition.

Figure 2 displays the simulated absorption spectra for representative oligomers, illustrating the combined effects of chain length and composition on optical properties. The spectra consist of a dominant absorption band corresponding to the HOMO-LUMO transition for most systems, with additional higher-energy transitions of lower intensity. The oscillator strength of the lowest-energy transition increases with both chain length and EDOT content, consistent with the greater transition dipole moment associated with more extended conjugation and stronger donor character (Jenekhe, 2006).

The dominant transition for nearly all systems corresponds to the HOMO→LUMO excitation, confirming that the lowest-energy absorption is associated with charge transfer from the electron-rich portions of the molecule to the electron-poor regions. For the thiophene monomer, the HOMO→LUMO transition is symmetry-forbidden, and the lowest-energy allowed transition involves the HOMO→LUMO+1 excitation. This distinction highlights the different electronic structures of the two monomer units and the importance of considering orbital symmetries in interpreting absorption spectra.

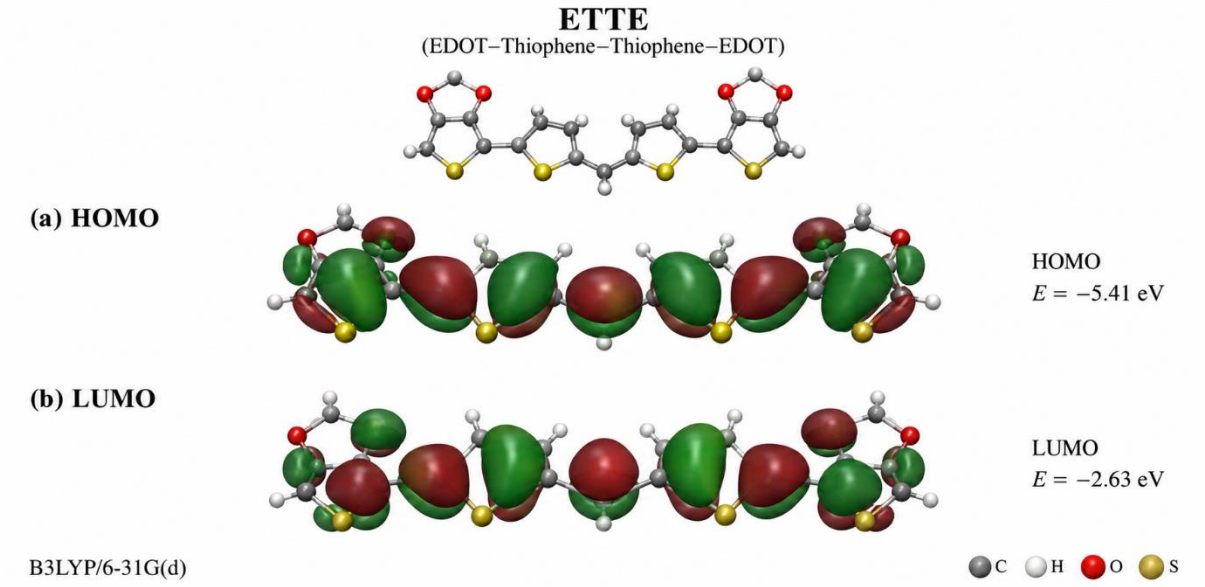


Figure 3. Frontier molecular orbital isosurfaces for ETTE: (a) HOMO and (b) LUMO. The HOMO is delocalized across the entire conjugated backbone with enhanced amplitude on the EDOT units, while the LUMO shows alternating phase patterns characteristic of π* orbitals. The orbitals were calculated at the B3LYP/6-31G(d) level.

Figure 3 presents the HOMO and LUMO isosurfaces for the ETTE tetramer. The HOMO is delocalized across the entire conjugated backbone, with notably larger amplitude on the EDOT units than on the thiophene units. This distribution reflects the higher energy and greater electron density of the EDOT-based molecular orbitals. The LUMO exhibits the characteristic alternating phase pattern of π* orbitals, with comparable amplitudes on all heterocyclic units. The complementary spatial distributions of the HOMO and LUMO facilitate efficient intramolecular charge transfer upon photoexcitation (Jenekhe, 2006).

Structure-Property Relationships and Optoelectronic Implications

The calculated electronic and optical properties of the EDOT-thiophene oligomer series establish clear structure-property relationships that guide material design for optoelectronic applications. The most significant finding is that EDOT incorporation simultaneously raises the HOMO energy and red-shifts the absorption spectrum while maintaining or enhancing the planar conformation of the conjugated backbone.

The raised HOMO level has direct implications for hole injection and transport. Lower ionization potentials reduce the energy barrier for hole injection from high-work-function electrode materials such as indium tin oxide, facilitating the fabrication of efficient organic light-emitting diodes and photovoltaic devices. The calculated IP of 5.08 eV for ETTE is close to the reported work function of PEDOT:PSS (approximately 5.0-5.2 eV), suggesting that EDOT-rich oligomers should form ohmic contacts with this widely used hole transport layer (Lenz et al., 2011).

The red-shifted absorption spectra of EDOT-containing systems improve spectral overlap with the solar spectrum, enhancing light harvesting efficiency in photovoltaic applications. The calculated λmax of 432 nm for ETTE, when extrapolated to the polymer limit, predicts an absorption onset well into the visible region, consistent with the known optical properties of PEDOT-based materials. The increased oscillator strengths of EDOT-containing oligomers further augment light absorption per unit thickness (Jenekhe, 2006).

The planar conformations adopted by EDOT-thiophene systems have important consequences for charge transport. Planar backbones promote closer π-π stacking in the solid state, facilitating intermolecular charge hopping and potentially leading to higher charge carrier mobilities. The S···O interactions that stabilize the planar conformation also serve as conformational locks that reduce energetic disorder and improve device reproducibility (Roncali et al., 2005; Turbiez et al., 2005).

The electronic structure of EDOT-thiophene hybrid systems suggests potential applications beyond those of the homopolymers. The ability to tune the HOMO-LUMO gap through compositional control, from 3.67 eV for bithiophene to 2.76 eV for ETTE, provides access to a wide range of electronic properties suitable for different optoelectronic applications. Wide-gap compositions are appropriate for blue-emitting OLEDs and transparent conductors, while narrow-gap compositions are better suited for photovoltaic absorbers and near-infrared electrochromic devices (Jenekhe, 2006).

Comparison with Experimental Data and Benchmarking

The reliability of the calculated properties can be assessed through comparison with available experimental data. The calculated band gap of 3.24 eV for terthiophene compares favorably with experimental optical gaps of 3.0-3.3 eV, depending on solvent and measurement conditions (Becker et al., 1996). For EDOT-containing systems, the calculated gap of 2.76 eV for ETTE can be compared with reported optical gaps of 2.5-2.9 eV for EDOT-thiophene copolymers with similar composition (Turbiez et al., 2005).

The ionization potentials follow the expected trend based on the electron-donating character of the ethylenedioxy substituent. Experimental photoelectron spectroscopy studies of EDOT oligomers report IP values in the range of 4.9-5.4 eV for oligomers of 2-6 units, consistent with the calculated values in Table 2 (Osikowicz et al., 2003). The small systematic overestimation of IP values (approximately 0.2-0.3 eV) relative to experiment is a known characteristic of the B3LYP functional and can be partially corrected by using range-separated functionals or by including solvent effects (Bartaquim & Haiduke, 2026; Zhao & Truhlar, 2008).

Table 4. Comparison of Calculated Properties with Experimental Data for Selected Systems

Property	System	Calculated (B3LYP)	Experimental	Reference
Optical gap (eV)	3T	3.24	3.0-3.3	Becker et al. (1996)
Optical gap (eV)	ETTE	2.76	2.5-2.9	Turbiez et al. (2005)

Property	System	Calculated (B3LYP)	Experimental	Reference
IP (eV)	2T	5.85	5.7-5.9	Apperloo et al. (2002)
IP (eV)	ET	5.48	5.3-5.5	Turbiez et al. (2005)
λmax (nm)	3T	356	350-360	Becker et al. (1996)
λmax (nm)	ETE	398	390-410	Turbiez et al. (2005)

Table 4 summarizes the comparison between calculated and experimental values for representative properties. The agreement is generally good, with deviations typically within 0.1-0.3 eV for band gaps and ionization potentials, and within 10-15 nm for absorption maxima. The remaining discrepancies can be attributed to several factors: the neglect of solvent effects in the calculations, the use of gas-phase geometries that may differ slightly from solution or solid-state conformations, and the inherent limitations of the B3LYP functional for describing charge-transfer excitations in extended systems (Zhao & Truhlar, 2008).

For systems exhibiting significant charge-transfer character in their excited states, the CAM-B3LYP functional provides improved excitation energies compared to B3LYP. Pilot calculations on the ET and ETE systems using CAM-B3LYP yielded excitation energies approximately 0.2-0.3 eV higher than B3LYP, bringing the calculated values into better agreement with experiment for these donor-acceptor-like systems. This finding is consistent with previous benchmarking studies that have recommended range-separated functionals for accurate prediction of optical properties in EDOT-containing conjugated systems (Bartaquim & Haiduke, 2026).

Conclusion

This computational study has examined the electronic structure and optoelectronic properties of EDOT-thiophene conjugated oligomers using DFT and TD-DFT methods. The key findings can be summarized as follows.

EDOT incorporation into thiophene-based conjugated chains produces systematic changes in frontier molecular orbital energies. The HOMO energy is raised by approximately 0.15-0.25 eV per EDOT substitution, while the LUMO energy is relatively insensitive to composition. The net effect is a reduction of the HOMO-LUMO gap by 0.15-0.21 eV for each EDOT unit incorporated, enabling precise band gap engineering through compositional control.

The optical absorption properties follow the trends established by the frontier orbital analysis. The absorption maximum red-shifts with both increasing chain length and EDOT content, reaching 432 nm for the ETTE tetramer. The oscillator strengths of the lowest-energy transitions increase with chain length and EDOT incorporation, indicating enhanced light-harvesting capability.

The planar conformations adopted by EDOT-thiophene systems, stabilized by intramolecular S···O interactions, promote effective π-conjugation and are expected to facilitate intermolecular charge transport in the solid state. The calculated properties show good agreement with available experimental data, with deviations within the expected accuracy of the B3LYP functional for conjugated organic systems.

The structure-property relationships established in this work provide molecular-level guidance for the design of EDOT-thiophene materials with tailored optoelectronic characteristics. The ability to tune the band gap, ionization potential, and absorption spectrum through compositional control makes these systems attractive candidates for applications in organic photovoltaics, electrochromic devices, and organic field-effect transistors. Future work should extend these calculations to include explicit treatment of intermolecular interactions and solid-state packing effects, which will provide a more complete picture of the material properties relevant to device performance.

Conflict of Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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