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Structural and electronic properties of FeO-decorated polythiophene-poly 3-methylpyrrole composite copolymer: DFT study

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The current study investigates the structure and electronic properties of the FeO-decorated polythiophene-poly 3-methylpyrrole composite copolymer using a density functional theory-based *ab initio* approach. The synthesized composite copolymer has a high stability with a binding energy of –5.2 eV compared to polythiophene-poly 3-methylpyrrole copolymer. The synthesized copolymer exhibits a 58.5% reduction in bandgap due to the formation of composite with FeO, and increased conductivity. The structural and electronic properties of FeO decorated polythiophene-poly 3-methylpyrrole composite copolymer are analysed *via* electron density, density of states, HOMO-LUMO gap, and Mulliken population. The enhanced conductivity and stability of the FeO-decorated composite copolymer make it a promising candidate for various applications, including polymeric sensors, energy storage, photovoltaic and electronics devices.

Keywords: Composites, Electronic properties, Sensor applications, Stability, Copolymerization

Conducting polymers (known as organic synthetic metals) have significant attention in polymer science over the past several decades due to their intrinsic conductivity, which arises from a conjugated π electron system in their structures[1]. This property, resulting from the availability of mobile electrons, has made CPs highly relevant in nanoscience, nanotechnology, and electrochemistry. Conducting polymers and their derivatives are prime candidates for thermoelectric materials owing to their non-toxicity, lightweight nature, low synthetic cost, environmental stability, and flexibility for integration into various forms. Additionally, they exhibit significantly lower thermal conductivity, making them highly attractive for various applications. Polyacetylene, ply vinyl carbazole, polyfuran, polythiophene, polypyrrole *etc.* conducting polymers are reported. Among these polymers, polyaniline, polypyrrole, and polythiophene are the most extensively studied because of its environmental stability, low monomer cost, ease of synthesis, and unique doping chemistry[3].

In addition, conjugated polymer nanoparticles (CPNs), a new class of fluorescence nanomaterials, have attracted significant interest due to their excellent brightness, photostability, low cytotoxicity, and good biocompatibility. These properties have enabled CPNs to be utilized in various applications, including sensing, bioimaging, and drug delivery. While traditional organic or polymeric fluorophores have been widely used for fluorescent bio- and chemosensors. The CP-based electrochemical biosensors can be modified to detect different environmental pollutants[4–7].

Furthermore, incorporating metal nanoparticles into polymer matrices create nanocomposites with enhanced physical properties. Various synthesis methods for metal or metal oxide nanoparticle-conducting polymer nanocomposites have been developed, each offering unique advantages in terms of material performance and potential applications.

Metal/Metal oxides gained much attention due to their magnificent properties and promising applications, as well as because of their different behavior from corresponding bulk materials. Metal oxides are pivotal in addressing environmental concerns through remediation and pollutant detection. Moreover, they hold strategic significance across various domains, such as energy production, conversion, and storage. Metal oxide nanoparticles, such as ZnO, CuO, TiO_2, MgO, NiO, FeO and

ZrO_2exhibit unique properties due to their small size and high surface area-to-volume ratio. As the size of these nanoparticles decreases, the increasing proportion of surface atoms compared to bulk atoms leads to altered electronic, optical, magnetic, and catalytic properties [8]. Metal oxides have different properties and are used in electronic structures, special dielectric properties, semiconductor properties, *etc.* It is important in many fields of science and engineering. In technical and practical applications, oxides are used in microelectronic circuits, in the production of sensors, in fuel cells, in anti-corrosion coatings, and as catalysts. In particular, the effectiveness of metal oxide nanoparticles in reducing environmental pollutants in air, water, and soil is increasingly known. Recent research has shown that they can enhance colors. Metal oxides, in particular, have become popular since the 1990s, with applications ranging from medicine and biotechnology to environmental remediation and photocatalysis. Over the past few decades, a variety of physical, chemical, and biological methods have been used to produce metal oxide nanoparticles, and their use in various ecological cleanup strategies has been investigated [9].

Among the various kinds of metal and metal oxide NPs, iron oxide NPs are one of the most prominent metal oxide NPs. Many biological applications have found IONPs to be suitable for use due to their unique characteristics, like a low environmental impact, catalytic behavior, biological compatibility, and multi-reaction method [10]. In recent decades, there has been increasing research attention directed towards iron oxide nanoparticles (IONPs). Iron's inherent reactivity and its ability to adopt various oxidation states make it conductive to form coordination bonds with other elements. The term IONP covers a range of chemical and structural forms ($FeO \leftrightarrow FeO \leftrightarrow Fe_3O_4 \leftrightarrow \alpha\text{-}Fe_2O_3) \leftrightarrow \gamma\text{-}Fe_2O_3 \leftrightarrow FeOOH$) [11]. Magnetite ($Fe_3O_4$), hematite ($\alpha$-$Fe_2O_3$), and maghemite ($\gamma$-Fe2O3) are probably the most common oxide forms in which IONPs exist in nature. It is a black solid and is often found in the form of a mineral called wüstite [12]. IONPs have been extensively studied for their diverse applications in various fields, such as biomedicine, information technology, and the environment. In the environment, IONPs are used for the removal or sensing of various air, water, and soil contaminants through adsorption, photo-degradation, and eco-friendly sensors. Iron oxide nanoparticles are versatile materials with promising applications in diverse fields, and ongoing research continues to explore their potential in emerging technologies. Iron oxides also find uses in catalysts, pigments (such as red and yellow iron oxides), and in various environmental applications, including wastewater treatment and remediation. They are essential compounds both industrially and in nature, playing crucial roles in geological processes and human activities [13,14].

Polythiophene (PTh) has been one of the most promising materials since 1980 due to its exceptional environmental stability, thermal stability, optical, and electrical properties that offer better conductivity, photoconductivity, electrochromism, low density, ease of synthesis, and processing in versatile forms. Polythiophene finds many applications in the fields of photovoltaic cells, electronics, corrosion protection, electrocatalysis, actuators, sensors, supercapacitors, light-emitting diodes, and DNA detection [15,16]. On the other hand, polypyrrole (PPy) and its derivatives are organic polymers that are highly explored with unique uses, including gas sensors, electronic tongues, and supercapacitor electrodes.Many PPy derivatives have been created and used in the marketplace as novel functional materials so far due to their combined high electrical conductivity with polymeric qualities including flexibility, low density, and strong compatibility with the environment [17].

Copolymerization can improve the thermal stability, influence the solubility and compatibility of polymers, and enhance the processability, electrical, and mechanical properties[18]. The copolymer has been synthesized by the polymerization of polythiophene and poly 3-methylpyrrole to fine-tune the individual properties of each polymer. To further enhance these properties, an FeO-decorated composite copolymer has been synthesized. So, the current research proposed the FeO-decorated polythiophene-poly3-methylpyrrole copolymer composite using density functional theory employing an ab initio approach. In this study, the binding energy is calculated for finding the stability of the copolymer composite in relative to neat copolymer. The electronic properties such as HOMO-LUMO gap, density of states (DOS), molecular energy spectrum (MES), Mulliken population, and electron density also have been calculated. This comprehensive analysis provides crucial insights into the structural and electronic characteristics of the composite, guiding its potential applications in the field of sensors and electronics.

Computational details

The Density function theory (DFT) has been utilized for the synthesis and characterization of the FeO-decorated polythiophene-poly 3-methylpyrrole copolymer composite. The Quantum Atomistix Toolkit (ATK) software served as the platform for these analyses. Generalized gradient approximation (GGA) with Perdew-Burke-Ernzerhof (PBE) geometry optimization has been employed for calculating electronic properties [19]. The electronic states are represented using double-zeta-polarized (DZP) basis sets, while 1×1×1 k-point sampling is utilized for energy spectrum calculation. A mesh cut-off of 75 Hartree has been used for the amplified electron density on a systematic grid. For optimization of the geometry, the maximum force tolerance has been set to 0.05eV/Å^3 with a maximum force of 0.05eV/Å^3, respectively[20,21].

Results and Discussion

The study examined the structural and electronic properties of synthesized FeO-decorated composite copolymer in comparison to neat copolymer. In this research, polythiophene, poly 3-methylpyrrole has been optimized to synthesize a copolymer (Fig. 1). After this, for further research FeO-decorated composites have been synthesized (Fig. 2). The structural and electronic properties have been computed in terms of their bond parameters, stability, conductivity, and electron charge distribution, respectively.

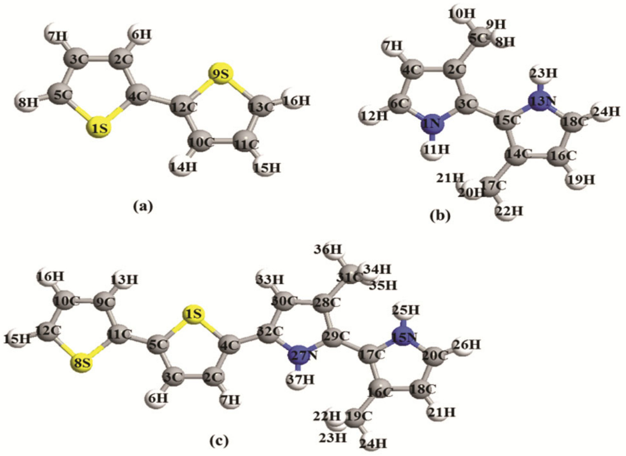
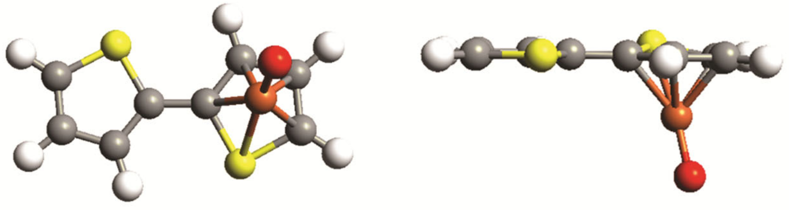
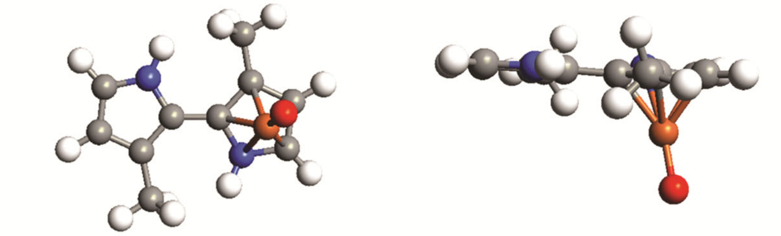


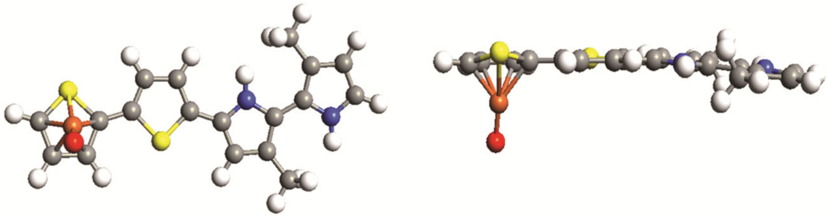
Fig. 1 — Optimized structures of neat (a) Polythiophene, (b) poly 3-methylpyrrole, and (c) copolymer.



(a) Front view of FeO-decorated PTh **(b) Side view of FeO-decorated PTh**



(c) Front view of FeO-decorated P3MPy **(d) Side view of FeO-decorated P3MPy**



(e) Front view of FeO-decorated composite copolymer **(f) side view of FeO-decorated composite copolymer**

Fig. 2 — Front and Side view of Optimized structures of FeO-decorated composite (a-b) Polythiophene, (c-d) poly 3-methylpyrrole, and (e-f) composite copolymer.

Structural analysis

The structural analysis of the polythiophene (PTh), poly3-methylpyrrole (P3MPy), and PTh-P3MPy copolymer and its FeO-decorated composites reveal significant changes in bond lengths, and bond angles shown in the Table 1. The copolymer's optimized structure showed specific bond lengths and angles that differ from those of the individual polymers, reflecting the new interactions within the copolymer structure. In the presence of FeO, the optimized structure of the FeO-decorated composite revealed specific changes that highlight the influence of FeO on the copolymer's structure. In the FeO-decorated composites, a noticeable elongation in bond length is observed. This can be attributed to the interaction between the electron-rich conjugated system of the copolymer and the FeO particles. The FeO nanoparticles act as electron acceptors, pulling the electron density away from the polymer backbone, causing an increase in bond lengths. The altered bond lengths and angles might influence the copolymer's conductivity and overall electronic behavior.

Electronic properties analysis of copolymer with and without FeO

The electronic properties of copolymer and FeO-decorated composite copolymer are computed in terms of total energy, binding energy, HOMO-LUMO gap,

Table 1 — Optimized structural parameters, bond length (B.L), bond angle (B.A) and dihedral angle of neat and FeO-decorated composites of polythiophene (PTh), poly 3-methylpyrrole (P3MPy) and (PTh-P3MPy) copolymer.

Interacting atoms	PThB.L(Å)	FeO-PThB.L (Å)	Interacting atoms	PThB.A(°)	PTh-FeOB.A(°)
S1-C5	1.72	1.71	∠S1-C5-C3	111.6	111.7
C3-C5	1.38	1.38	∠C5-C3-C2	112.4	112.4
C2-C3	1.42	1.42	∠C3-C2-C4	113.01	112.7
C2-C4	1.39	1.39	∠C2-C4-S1	110.3	110.8
C4-S1	1.73	1.73	∠C4-S1-C5	92.4	92.2
C4-C12	1.45	1.45	∠C2-C4-C12	128.8	129.1
S9-C12	1.73	1.78	∠S1-C4-C12	120.7	120.1
S9-C13	1.72	1.77	∠C4-C12-S9	120.2	119.7
C11-C13	1.38	1.43	∠C4-C12-C10	129.2	128.1
C11-C10	1.42	1.43	∠C10-C12-S9	110.4	111.3
C10-C12	1.39	1.44	∠C12-C10-C11	112.9	112.5
			∠C10-C11-C13	112.4	111.3
			∠C11-C13-S9	111.6	112.4
			∠C12-S9-C13	92.4	89.8
			Dihedral angles		
			∠S1-C4-C12-S9	176.6	–170.7
			∠C2-C4-C12-C10	175.6	179.5
N1-C3	1.38	1.38	∠N1-C6-C4	107.4	107.5
C2-C3	1.41	1.41	∠C6-C4-C2	108	108
C2-C4	1.42	1.42	∠C4-C2-C3	106.9	106.8
C4-C6	1.38	1.39	∠C2-C3-N1	106.6	107.1
C2-C5	1.50	1.50	∠C3-N1-C6	110.8	110.5
C6-N1	1.37	1.37	∠C3-C2-C5	127.7	127.2
C3-C15	1.45	1.45	∠C4-C2-C5	125.9	125.9
C15-N13	1.38	1.49	∠C2-C3-C15	132.4	130.8
N13-C18	1.37	1.42	∠N1-C3-C15	120.9	121.9
C18-C16	1.38	1.43	∠C3-C15-N13	122.5	120.5
C16-C14	1.42	1.44	∠C3-C15-C14	130.74	132.1
C14-C15	1.41	1.45	∠C15-C13-C18	110.7	109.3
C14-C17	1.50	1.50	∠N13-C18-C16	107.5	106.2
			∠C18-C16-C14	107.9	108.2
			∠C15-C14-C16	107.1	107.4
			∠C14-C15-N13	106.7	106
			∠C16-C14-C17	125.8	125.3
			∠C15-C14-C17	127	127.2
			Dihedral angles		
			∠N1-C3-C15-N13	179.7	–168.4
			∠C2-C3-C15-C14	179.7	178.9

(*Contd.*)

Table 1 — Optimized structural parameters, bond length (B.L), bond angle (B.A) and dihedral angle of neat and FeO-decorated composites of polythiophene (PTh), poly 3-methylpyrrole (P3MPy) and (PTh-P3MPy) copolymer — (*Contd.*)

Interacting atoms	PThB.L(Å)	FeO-PThB.L (Å)	Interacting atoms	PThB.A(°)	PTh-FeOB.A(°)
S8-C12	1.72	1.77	∠S8-C12-C10	111.4	112.1
C12-C10	1.38	1.43	∠C12-C10-C9	112.5	111.3
C10-C9	1.42	1.43	∠C10-C9-C11	113.2	112.6
C9-C11	1.39	1.44	∠C9-C11-S8	110.1	111.2
C11-C4	1.44	1.44	∠C11-S8-C12	92.5	89.8
C4-S1	1.73	1.73	∠C9-C11-C4	127.6	128
S1-C5	1.73	1.73	∠S8-C11-C4	122.1	120
C5-C3	1.39	1.39	∠C11-C4-C2	130.1	129.2
C3-C2	1.41	1.41	∠C11-C4-S1	119.6	120.1
C2-C4	1.39	1.39	∠C4-S1-C5	92.8	92.5
C5-C33	1.38	1.38	∠S1-C5-C3	110.4	110.6
C30-C29	1.41	1.41	∠C5-C3-C2	113	113
C31-C33	1.4	1.4	∠C3-C2-C4	113.4	113.1
C29-C32	1.5	1.5	∠C2-C4-S1	110.2	110.5
C33-N28	1.37	1.37	∠S1-C5-C33	118.9	119.1
C30-N28	1.38	1.38	∠C3-C5-C33	130.6	130.1
C30-C18	1.45	1.45	∠C5-C33-C31	129.8	130.1
C18-N16	1.38	1.38	∠C5-C33-N28	123.8	123.3
N16-C21	1.37	1.37	∠N28-C33-C31	106.3	106.5
C21-C19	1.39	1.39	∠C33-C31-C29	108.8	108.6
C19-C17	1.42	1.42	∠C31-C29-C30	106.9	106.9
C17-C18	1.41	1.41	∠C29-C30-N28	106.8	106.9
C20-C17	1.50	1.50	∠C30-N28-C33	111	110.9
			∠C31-C29-C32	125	125.1
			∠C30-C29-C32	127.9	127.9
			∠N28-C30-C18	122.5	121.7
			∠C29-C30-C18	130.5	131.3
			∠C30-C18-N16	120.9	131.5
			∠C30-C18-C17	132.3	131.5
			∠C30-C18-N16	120.9	121.6
			∠C18-N16-C21	110.8	110.6
			∠N16-C21-C19	107.3	107.5
			∠C21-C19-C17	108.1	108
			∠C19-C17-C18	106.9	106.9
			∠C17-C18-N16	106.6	106.7
			∠C19-C17-C20	125.1	125.5
			∠C18-C17-C20	127.9	127.5
			Dihedral angles		
			∠S8-C11-C4-S1	175.05	–167
			∠C9-C11-C4-C2	175.3	–176.2

Mulliken population analysis, and electron density analysis, respectively.

Stability analysis of polythiophene, poly 3-methylpyrrole copolymer with and without FeO

The stability analysis is based on the total energy and Binding energy of the optimized systems shown in Table 2. The total energies of the systems are decreased and the stability of the systems is increased. The composite polymer has the more negative total energy and higher binding energy which indicates a

Table 2 — Illustrated the total energy and binding energy of the optimized systems

Systems	Total energy(eV)	Binding energy(eV)
FeO	–1187.21	–
PTh	–2069.81	–
P3MPy	–2308.81	–
PTh-P3MPy	–4346.98	-
FeO-PTh	–3262.1	–5.08
FeO-P3MPy	–3500.69	–4.68
FeO- PTh-P3MPy	–5539.39	–5.2

stronger binding between the components of the composite copolymer. The total energies of the neat polythiophene, poly3-methylpyrrole, and copolymer are –2069.81 eV, –2308.81 eV, and –4346.98 eV, respectively. While they optimized in the form of composites, their total energies decreased by 1192.29 eV, 1191.88 eV, and 1192.41 eV for FeO-decorated composites of polythiophene, poly 3-methylpyrrole, and copolymer.

The binding energy of the FeO-decorated polythiophene, poly-3-methylpyrrole and copolymer composites are calculated using the following equation (1)[22].

$$\Delta E_{BE} = E_{X+FeO} - (E_X + E_{FeO}) \quad \text{... (1)}$$

where E_{X+FeO} is the total energy of the FeO-decorated polythiophene, poly3-methylpyrrole, and copolymer composites; E_X is the total energy of the polythiophene, poly3-methylpyrrole, and copolymer; and E_{FeO} is the total energy of FeO metal oxide. Negative binding energies signify energy release upon composite formation, indicating their better stability. This higher (more negative) binding energy suggests strong interactions between the FeO and the copolymer components, ensuring the composite's structural integrity.

HOMO-LUMO Analysis

To explore the electronic properties of the neat and composites, the computed values of the HOMO (ƸH) and LUMO (ƸL) energies are presented in Table 3. The energy gap between the HOMO and LUMO is commonly referred to as the ƸH-ƸL gap or bandgap. A reduced ƸH-ƸL gap denotes enhanced electrical conductivity in materials. Consequently, the smaller energy gap observed in the composite copolymer suggests superior electrical conductivity compared to the neat copolymer. The HOMO (Highest Occupied Molecular Orbital) and LUMO (Lowest Unoccupied Molecular Orbital) represent energy levels that delineate electron distribution within a molecule, offering insights into its electronic characteristics. In Fig. 3, DOS (Density of States) illustrates the distribution of electron states at different energy levels within a material, thereby illuminating its electronic

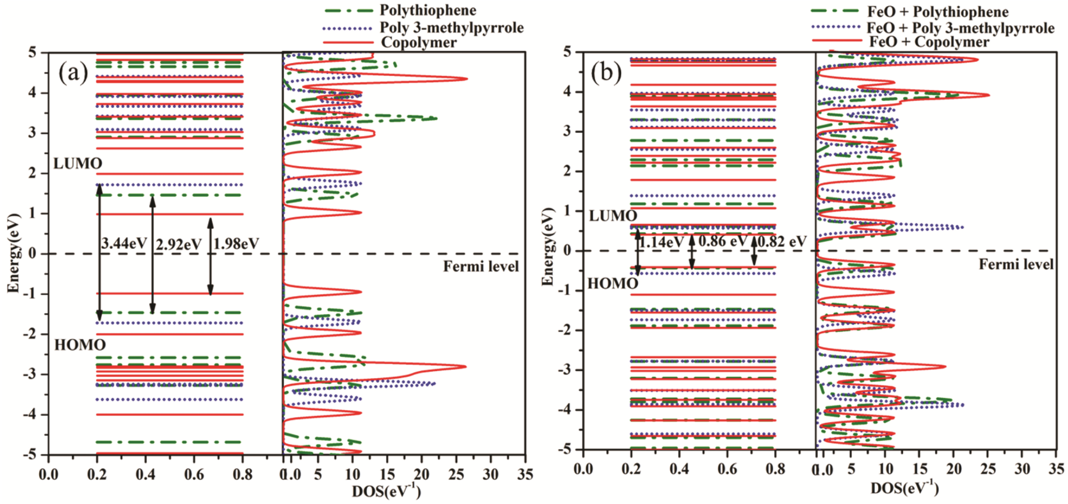


Fig. 3 — Schematic view of MES plot (Left panel) and DOS profile (right panel) of (a) neat and (b) FeO-decorated composite polythiophene, poly 3-methylpyrrole, and composite copolymer.

Table 3 — HOMO (ƸH), LUMO(ƸL), HOMO-LUMO gap (ƸH-ƸL), Energy (Neutral and Ionic states), Ionization potential (IP), Electron affinity (EA) of the optimized systems

Systems	ƸH(eV)	ƸL(eV)	ƸH-ƸL(eV)	ƸH-ƸL%	Energy(eV)			IP	EA
					Neutral	Cation	Anion		
PTh	–1.46	1.46	2.92	–	–2069.81	–2068.98	–2062.83	0.83	–6.98
P3MPy	–1.72	1.72	3.44	–	–2308.81	–2306.85	–2302.71	1.96	–6.1
PTh-P3MPy	–0.99	0.99	1.98	–	–4346.98	–4346.78	–4341.71	0.20	–5.27
FeO-PTh	–0.43	0.43	0.86	70.5	–3262.1	–3262.27	–3256.11	–0.17	–5.99
FeO-P3MPy	–0.57	0.57	1.14	66.8	–3500.69	–3500.45	–3495.21	0.24	–5.48
FeO-(PTh-P3MPy)	–0.41	0.41	0.82	58.5	–5539.39	–5539.79	–5534.18	–0.40	–5.21

structure. The Molecular Energy Spectrum term encompasses the energy levels and electronic states within a molecule, often elucidated through quantum chemical computations, aiding in the comprehension of its electronic structure[21,23]. The changes in the Density of States (DOS) profiles of the adsorbed system correspond to their calculated Molecular Energy Spectrum (MES) profiles.

The ƸH-ƸL gaps of neat polythiophene, poly 3-methylpyrrole, and copolymer are 2.92 eV, 3.44 eV, and 1.98 eV, respectively. Similarly, in the presence of FeO, the ƸH-ƸL gaps of polythiophene, poly 3-methylpyrrole, and copolymer are 0.86 eV, 1.14 eV, and 0.82 eV, respectively.

We have also computed the percentage of relative energy gap changes (Eg%) of FeO-decorated polythiophene, poly 3- methylpyrrole, and copolymer composites [24,25].

$$E_g\% = \frac{[E_X - E_{Y(X+FeO)}]}{E_X} \times 100\% \qquad \text{... (2)}$$

where E_X denotes the energy gap of neat polythiophene, poly 3- methylpyrrole, and copolymer; and $E_{Y(X+FeO)}$ denotes the energy gap of FeO-decorated polythiophene, poly 3-methylpyrrole, and copolymer composites. The percentage of relative energy gap changes (Eg%) in FeO-decorated polythiophene, poly 3- methylpyrrole, and copolymer composites by 70.5%, 66.8%, and 58.5% from the neat polythiophene, poly 3-methylpyrrole, and copolymer, respectively. As a result, this decrease in bandgap is crucial because it implies that the FeO-decorated composite copolymer has enhanced electronic conductivity. The reduction in bandgap can be attributed to the introduction of FeO, which modifies the electronic structure and facilitates easier electron flow, making the material more conductive.

Further, the charging energies of the materials have been calculated by analyzing electron affinity (EA) and ionization potential (IP) of materials in Table 3. Here, the IP represents the energy required to remove an electron from a neutral atom or molecule to form a positively charged ion, while the EA represents the energy released when an electron is added to a neutral atom or molecule to form a negatively charged ion [26].

$$IP = E_{cation} - E_{neutral} \qquad \text{... (3)}$$

$$EA = E_{neutral} - E_{anion} \qquad \text{... (4)}$$

In the Table 3, the decrement of IE and EA values as the HOMO-LUMO gap reduces confirms the direct relationship between the electronic structure and these properties. Positive values of IP for neutral atoms indicate an endothermic ionization process, while negative values of EA indicate an exothermic electron attachment process. This trend demonstrates that modifications, such as FeO decoration, significantly influence the electronic properties of these materials, lowering the energy gaps and altering ionization and electron affinity behaviors.

Mulliken population analysis

The Mulliken population analysis provides insights into the charge distribution within the materials. The analysis reveals that the presence of FeO affects the charge distribution in the composite copolymer, indicating significant electron transfer between the copolymer and the FeO. This electron transfer is crucial for understanding the enhanced electronic properties of the composite. Equation (5) has been utilized to calculate the total charge difference between the systems *via* Mulliken population analysis[27].

$$\Delta\rho = \rho_{(X+FeO)} - \rho_{(X)} - \rho_{(FeO)} \qquad \text{... (5)}$$

where, Δρ indicates the charge transfer, $\rho_{(X+FeO)}$ represents the charge on metal oxide (FeO) of adsorbed system, and $\rho_{(FeO)}$ represents the charge on metal oxide (FeO) in its pure form and *X*represents corresponding to the host system (polythiophene, poly 3-methylpyrrole, and copolymer), respectively. Specifically, polythiophene exhibits a charge transfer of (–1.104e), poly 3-methylpyrrole shows a charge transfer of (–0.718e), and the copolymer displays a charge transfer of (–0.001e), respectively. Negative charge transfer values signify the transfer of charge from the copolymer to FeO, confirming the copolymer's donation of charge to FeO.

Electron density analysis

Fig. 4 displays electron density plots for polythiophene, poly 3-methylpyrrole, and copolymer in the absence/presence of FeO. Positive electron densities are depicted in green, while negative densities appear in red, with shades ranging from green to blue indicating regions of moderate electron density. Electron density plots reveal notable differences between the neat copolymer and the FeO-decorated composite copolymer. In these plots, dark green represents the electron density of the copolymer, while pale blue indicates the electron

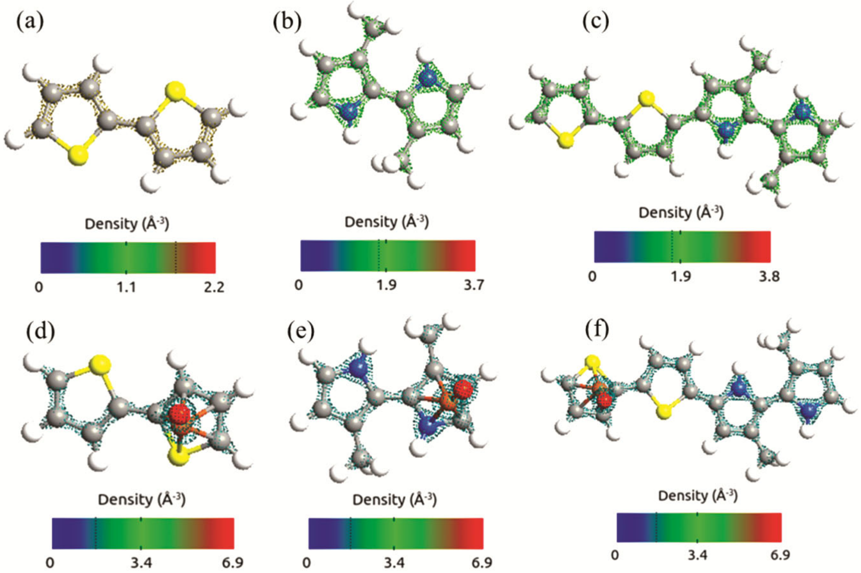


Fig. 4 — Electron density of neat and FeO-decorated (a, d) Polythiophene, (b, e) poly 3-methylpyrrole, and (c, f) copolymer.

density of the FeO-decorated composite. The transition from dark green to pale blue signifies a shift in electron charge due to the interaction with FeO. This charge transfer is likely due to the higher charge density of Fe characteristic of d-block elements. In terms of electron densities, neat polythiophene, poly 3-methylpyrrole, and copolymer have values of 1.1, 1.9, and 1.89, respectively. With FeO, these values become 3.4 for all components. Electronegativity in electron density plots measures an atom's ability to attract electrons in a chemical bond. Comparatively, oxygen, sulfur, and nitrogen are electronegative p-block elements. Sulfur has two lone pairs, nitrogen has one, and oxygen has two, akin to sulfur. In the optimized system, oxygen exhibits high electronegativity, following the trend Fe < H < C < S < N < Cl < O on the Pauling scale of 1.83 < 2.20 < 2.55 < 2.58 < 3.04 < 3.16 < 3.44. These variations influence structural parameters.

Conclusion

This study investigates the structural and electronic enhancements in FeO-decorated polythiophene-poly 3-methylpyrrole composite copolymer using density functional theory. The incorporation of FeO into the copolymer matrix significantly improves its stability and electronic properties. Key findings include a binding energy of –5.2 eV, indicating strong interactions within the composite, and a 58.5% reduction in the bandgap, which enhances conductivity. Detailed analyses, including electron density, Density of States (DOS), Molecular Energy Spectrum (MES), and Mulliken population, confirm the substantial impact of FeO on the composite's electronic structure. Specifically, charge transfer from the copolymer to FeO is observed, further improving the composite's electronic properties. The substantial improvements in stability and conductivity make the FeO-decorated composite a promising material for a range of advanced applications, including polymeric sensors, energy storage systems, photovoltaic devices, and electronic applications.

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