RASĀYAN *J. Chem.*
Vol. 18 | No. 1 |141-150| January - March | 2025
ISSN: 0974-1496 | e-ISSN: 0976-0083 | CODEN: RJCABP
http://www.rasayanjournal.com
http://www.rasayanjournal.co.in

ELECTRONIC AND SENSOR PROPERTIES OF FURAN-PYRROLE COPOLYMER FOR DETECTING INH DRUG: A DFT STUDY

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ABSTRACT

A DFT-based computational approach was employed to investigate the sensing capabilities of furan-pyrrole copolymer for selective Isoniazid (INH) drug detection. The structural and electronic properties of the synthesized copolymer were optimized to evaluate its potential as a sensor material. Quantum chemical calculations revealed favorable electronic properties with a HOMO-LUMO gap of 1.58 eV, indicating high conductivity and chemical stability. The molecular energy spectrum analysis demonstrated strong binding interactions between the copolymer and INH molecules, with an adsorption energy of -0.65 eV, confirming efficient charge transfer mechanisms. Density of state (DOS) profiles exhibited significant electronic perturbations upon INH interaction, validating the sensing mechanism. The copolymer showed remarkable selectivity towards INH, with distinct changes in electronic characteristics and rapid recovery time, suggesting excellent reusability. These findings establish furan-pyrrole copolymer as a promising candidate for developing reliable INH detection systems, offering potential applications in pharmaceutical quality control and environmental monitoring.

Keywords: DFT Calculations, Furan-Pyrrole Copolymer, INH Detection, Electronic Properties, Molecular Energy Spectrum, Charge Transfer Analysis, Sensor Stability.

RASĀYAN *J. Chem.*, Vol. 18, No.1, 2025

INTRODUCTION

In recent times, the sensing capabilities of synthetic conducting polymers have received lots of attention due to their high electrical conductivity, profitability, and precise sensitivity. There have been significant efforts to improve the processability of these pristine polymers by integrating them with metals, as well as both organic and inorganic materials in the form of blends, composites, and interpenetrating polymer networks (IPNs). Owing to their low cost, facile synthesis, lightweight nature, good environmental stability, and high mechanical flexibility, conducting polymers have wide-ranging applications in batteries, supercapacitors, photovoltaic cells, and sensors.[1] Conducting polymers (CPs) offer several key advantages that make them economically valuable materials. These include their excellent stability, lightweight characteristics, ease of processing, corrosion resistance, and effective electrical conductivity. Several conducting polymers have been extensively studied, with the most prominent examples being polypyrrole (PPy), poly(3,4-ethylenedioxythiophene) (PEDOT), polyaniline (PANI), and polythiophene (PTH), along with their various derivatives.[2,3] Isoniazid (INH) serves as a primary antibiotic medication and is extensively used as a synthetic antimicrobial agent, particularly in treating tuberculosis. Looking at its molecular structure, INH consists of a hydrazine group connected to a pyridine ring, with the attachment occurring at the para position relative to the ring's nitrogen atom. It is also known as isonicotinic acid hydrazide. The drug's success stems from its high selectivity and potency against mycobacteria.[4,5] Isoniazid (INH) has been a mainstay of anti-tuberculosis treatment since 1952 because of its potency and good selectivity against Mycobacterium tuberculosis. For isoniazid (INH) to become active, it must undergo conversion through the enzyme KatG, a catalase-peroxidase, in the presence of molecular oxygen, making it a prodrug. While INH shows strong bactericidal effects against rapidly multiplying mycobacteria, it

http://doi.org/10.31788/RJC.2025.1819072

demonstrates limited efficacy against dormant or latent forms of these organisms. It was first produced in 1912, but researchers from Hoffmann-La Roche, E. R. Squibb & Sons in the United States, and Bayer in Germany independently discovered its antitubercular capabilities in the early 1950s.[6,7] Furan [C_4H_4O] and pyrrole [C_4H_5N] are aromatic organic heterocyclic compounds having ring structures with carbon and heteroatoms (nitrogen in pyrrole, and oxygen in furan) with conjugated systems. Delocalized π-electron systems result in increased stability and special electronic properties like conductivity and optical qualities. When furan and pyrrole are used as monomers in copolymerization, the resulting copolymer inherits both of their conjugated structures, providing far more useful electrical characteristics.[8] The detection of drugs has been significantly advanced through the use of copolymer matrices, which are created by combining multiple types of monomers. These materials stand out because their electrical properties can be precisely tuned during synthesis, leading to improved accuracy and sensitivity in drug-sensing applications. The electrical properties of copolymers, such as conductivity, dielectric constant, and charge mobility, can be precisely controlled by adjusting the ratio and type of monomers involved. This versatility allows for the design of copolymer-based sensors that can operate under various conditions and detect a wide range of drug molecules with high accuracy. Therefore, copolymerization of the conjugated monomers is a strategy to optimize their properties at the molecular level for targeted applications. The synthesis of furan-pyrrole copolymer enables the development of materials with customizable electronic and physical properties, suitable for applications in organic electronics, sensors, and energy storage devices.[9,10] Research has led to the development of a copolymer combining furan and pyrrole monomers with comparable oxidation potentials.[11] The structural, electronic, and photovoltaic characteristics of these materials were investigated using DFT calculations based on ab initio methods. Researchers evaluated the effects of both electron-donating and electron-withdrawing groups in head-to-head substituted arrangements. The polymer structure was characterized through analysis of intramolecular bond lengths, distances between rings, and dihedral angles. Additionally, electronic characteristics including HOMO, LUMO, their energy gap, and reorganization energy were examined. Using the DFT-based ab initio software package ATK-VNL, we investigated the structural and electrical characteristics of furan-pyrrole copolymer both with and without Isoniazid (INH). The study examined various properties including binding energy, adsorption energy, global molecular descriptors, electronic properties, detection range, and recovery time. These calculations help understand the system's stability, molecular interactions, and its potential applications as a sensor for INH.

EXPERIMENTAL

The study explored the potential of a furan-pyrrole copolymer for isoniazid (INH) detection through advanced computational methods based on density functional theory (DFT).[12] The molecular structure was optimized using the Perdew-Burke-Ernzerhof (PBE) exchange-correlation functional within the generalized gradient approximation (GGA). Electronic characteristics were analyzed using double zeta polarized (DZP) basis sets, combined with a 1x1x1 k-point grid for energy spectrum evaluation.[13,14] To achieve high-quality electron density maps, researchers implemented a 75-Hatree mesh cut-off. The optimization process involved periodic relaxation of cell constraints, maintaining force tolerances set at 0.05 eV/Å³.

RESULTS AND DISCUSSION

This research constructed a computational model using density functional theory in the Atomistix toolkit virtual nanolab platform to study a copolymer created from furan and pyrrole monomers. The material's sensing capabilities for INH were evaluated by examining different molecular configurations and their electronic characteristics. Their analysis focused on several key parameters: molecular energy spectrum (MES), density of states (DOS), electron density distribution, and Mulliken population data. These measurements revealed critical information about electron behavior within the molecular system, providing fundamental insights into the material's sensing mechanism.

Structure Stability Analysis

The optimized geometry of copolymer as conducting material, with or without the presence of Isoniazid (INH), is illustrated in Fig.-1. With the copolymer exhibiting a greater number of atoms compared to furan and pyrrole host polymers, there's a consequent increase in the surface-to-volume ratio. Prior to initiating

the adsorption process of Isoniazid (INH), it's imperative to establish furan-pyrrole copolymer-based sensing materials. The interaction mechanisms between furan-pyrrole copolymer and isoniazid were investigated by analyzing various structural properties. The study examined bond angles, bond lengths, and types of interactions to understand how the copolymer and isoniazid molecules orient and interact with each other. This structural analysis provided insights into the nature of their chemical interactions at multiple molecular orientations. When the isoniazid drug interacts with the furan-pyrrole copolymer, slight changes in the bond angles and lengths occur due to the introduction of new interactions. The specific adsorption sites on the copolymer where isoniazid has been adsorbed, potentially alter the bond angles and lengths near the interaction sites. Between pure copolymer and other orientations of copolymer with drug, minute changes have been observed in bond lengths and bond angles. In Table-1, the observations suggest that the structure is relatively stable, with slight flexibility in certain angles and dihedral configurations.

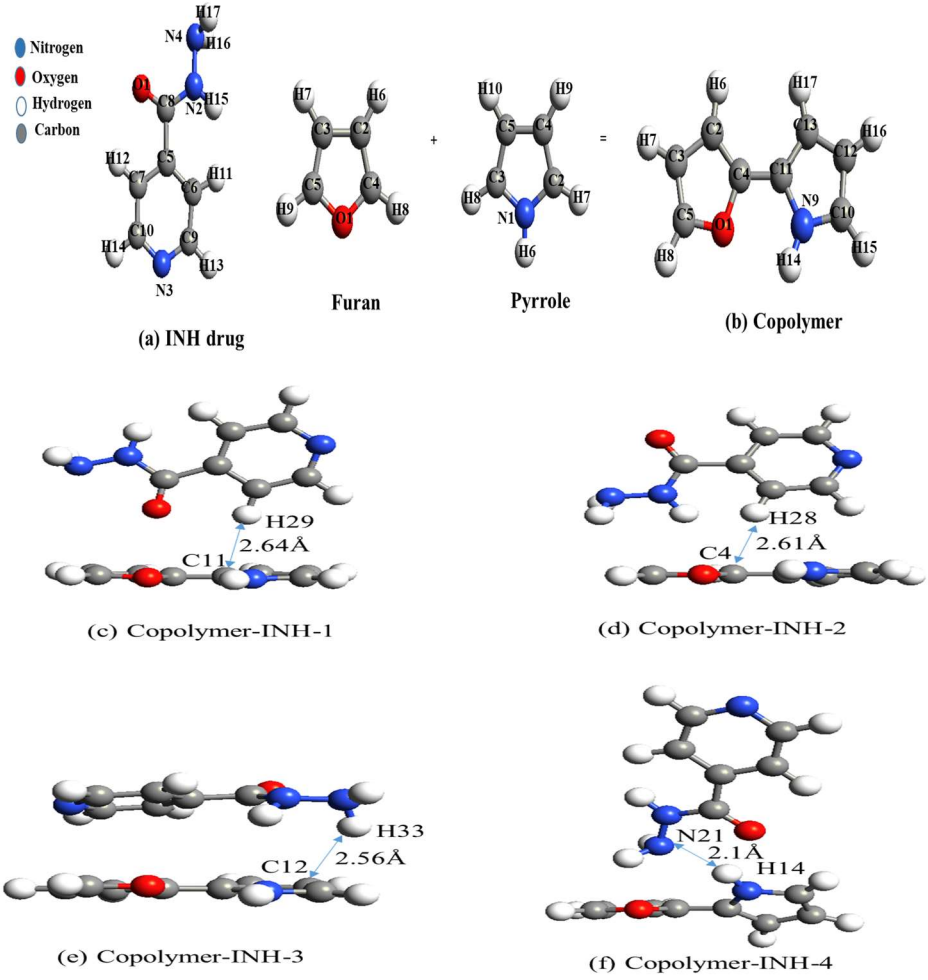

Fig.-1: Optimized Structures of (a) Isoniazid (INH) drug, (b) Fu-Py Copolymer, and (c-f) Copolymer -INH Drug

Table-1: Optimized Structural Parameters, Bond Length (B.L), Bond Angle (B.A) and Dihedral Angle of Fu-Py Copolymer, Copolymer - INH-1, Copolymer - INH-2, Copolymer - INH-3, And Copolymer - INH-4

Interacting atoms of copolymer	Fu-Py copolymer B.L.(Å)	Copolymer - INH-1 B.L.(Å)	Copolymer - INH-2 B.L.(Å)	Copolymer - INH-3 B.L.(Å)	Copolymer - INH-4 B.L.(Å)
O1-C5	1.36	1.36	1.36	1.37	1.37
C3-C5	1.37	1.37	1.37	1.37	1.37
C3-C2	1.43	1.42	1.43	1.43	1.43
C2-C4	1.38	1.38	1.38	1.38	1.38

C4-O1	1.37	1.37	1.37	1.38	1.38
C4-C11	1.44	1.44	1.44	1.45	1.45
C11-C13	1.40	1.40	1.40	1.40	1.40
C13-C12	1.42	1.42	1.42	1.42	1.41
C12-C10	1.39	1.39	1.39	1.39	1.39
C10-N9	1.37	1.37	1.37	1.38	1.36
N9-C11	1.38	1.38	1.38	1.38	1.38
	B.A.(º)	B.A.(º)	B.A.(º)	B.A.(º)	B.A.(º)
∠O1-C5-C3	110.4	110.5	110.4	110.6	110.6
∠C5-C3-C2	106.3	106.3	106.3	106.3	106.2
∠C3-C2-C4	106.3	106.2	106.2	106.2	106.8
∠C2-C4-O1	109.7	109.8	109.6	109.9	109.3
∠C4-O1-C5	107.1	107	107.3	106.8	106.9
∠O1-C4-C11	115.8	115.5	115.9	115.3	118.8
∠C2-C4-C11	134.4	134.5	134.4	134.7	131.8
∠C4-C11-C13	131.8	132.5	131.6	132.4	128.8
∠C4-C11-N9	120.9	120.4	121.1	120.3	123.7
∠C11-N9-C10	110.2	110.5	110.1	110.3	109.8
∠N9-C10-C12	107.6	107.4	107.8	107.4	108.4
∠C10-C12-C13	107.5	107.5	107.4	107.6	106.9
∠C12-C13-C11	107.3	107.4	107.3	107.4	107.3
∠C13-C11-N9	107.1	106.9	107.2	107.2	107.4
Dihedral angle					
∠O1-C4-C11-C13	174.9	-175.3	174.5	-170.7	142.1
∠C2-C4-C11-N9	174.3	178.5	174	-171.2	141.6

The stability of the systems has been computed based on binding and adsorption energy which is calculated by the system's total energy given in Table-2. The total energy of furan, pyrrole, and copolymer are -1127.14 eV, -980.42 eV, and -2075.95 eV, respectively. Subsequently, the total energy of the copolymer in the presence of INH drug at different orientations (Copolymer +INH-1, Copolymer+INH-2, Copolymer+INH-3, and Copolymer+INH-4) are -4380.02 eV, -4380.24 eV, -4380.20 eV, and -4380.42 eV, respectively. Consequently, there are reduction in the total energies in various orientations observed across various orientations from the copolymer at values 2304.07, 2304.29, 2304.31, and 2304.47 eV respectively. There is minute difference among the total energies of the given orientations. Based on total energies, the stability reveals the trend of Copolymer-INH-1< Copolymer-INH-2< Copolymer -INH-3< Copolymer -INH-4. Binding energy has been computed to study the interaction between monomers and copolymers. It helps to understand the stability of the copolymer. The binding energy is defined in equation-1.[15,16]

$$E_{BE} = E_{Furan} + E_{Pyrrole} - E_{copolymer} \qquad (1)$$

Where E_{Furan} , $E_{Pyrrole}$, and $E_{copolymer}$ are corresponding total energies of furan, pyrrole, and copolymer. The computed binding energy of the copolymer is 31.6, revealing a favorable interaction between them.

Table-2: Illustrate the Total Energy, Binding Energy Adsorption Energy, Interacting Atoms, Optimized Distance, and Type of Interaction of the Following

System	Total energy (eV)	Binding Energy (eV)	Adsorption energy (eV)	Interacting atoms between copolymer and drug	Optimized Distance (Å)	Type of Interaction
Isoniazid (INH)	-2303.82					
Furan (Fu)	-1127.14					
Pyrrole (Py)	-980.42					
Fu-Py copolymer	-2075.95	31.6				
Copolymer-INH-1	-4380.02		-0.25	C11-H29	2.64	Physisorption

Copolymer-INH-2	-4380.24		-0.47	C4-H28	2.61	Physisorption
Copolymer-INH-3	-4380.26		-0.49	C12-H33	2.56	Physisorption
Copolymer-INH-4	-4380.42		-0.65	H14-N21	2.1	Physisorption

To understand the type of interaction between the copolymer and INH drug, the adsorption energy (E_{ads}) of the interaction has been computed using equation 1.[14,17]

$$E_{ads} = E_{Y(X+I\quad)} - E_{Y(X)} - E_{Y(INH)} \qquad (2)$$

Where $E_{Y(X+INH)}$ is the total energy of the copolymer-INH system, where, $E_{Y(X)}$ is the total energy of furan-pyrrole copolymer and $E_{Y(INH)}$ is the total energy of the optimized Isoniazid (INH) drug. In equation 2, X is the corresponding copolymer. The adsorption energy of copolymer-INH-1, copolymer-INH-2, copolymer-INH-3, and copolymer-INH-4 are -0.25, -0.47, -0.49, and -0.65, respectively. The negative adsorption energies ($-E_{ads}$) indicating the release of energy during the process, confirm a physisorption interaction between the copolymer and INH drug. This type of interaction typically involves weak van der Waals forces, indicating that these forces contribute to the stability of the adsorption system. Moreover, the exothermic nature of the process further supports the presence of weak intermolecular forces, including van der Waals forces and π-π interaction between the copolymer and the drug. This approach suggests the interaction between the copolymer and the drug, providing valuable insights into their stability and behavior. The stability trend observed as-copolymer-INH-1< copolymer-INH-2< copolymer-INH-3< copolymer-INH-4. Recovery time (τ)[18] is the time required for an adsorbed molecule to desorb from a surface and for the surface to return to its original state. To evaluate the reusability of a sensor, it is a significant indicator associated with its physical adsorption energy (E_{ads}).

$$\tau = \vartheta^{-1} exp\left(\frac{E_{ads}}{K_b T}\right) \qquad (3)$$

Where K_b represents the Boltzmann constant and *v* symbolizes the attempt frequency of the sensor at the operational temperature T. The recovery time (τ) for a sensor is a crucial indicator of its reusability and is inversely related to the adsorption energy (E_{ads}). According to the calculated recovery times using equation 3, as the magnitude of the adsorption energy increases (i.e., becomes more negative), the recovery time significantly decreases. The observed trend in recovery times—copolymer-INH-1 > copolymer-INH-2 > copolymer-INH-3 > copolymer-INH-4 —demonstrates that recovery time is inversely proportional to adsorption energy. As the adsorption energy becomes more negative, the recovery time decreases exponentially. This suggests a rapid recovery time, thereby enhancing the sensor's reusability.

Table-3: Calculated Recovery Time of Furan-Pyrrole Copolymer in the Presence of INH

Systems	Recovery time(μs)
Copolymer-INH-1	5.91×10^{-11}
Copolymer-INH-2	1.12×10^{-14}
Copolymer-INH-3	5.16×10^{-15}
Copolymer-INH-4	1.02×10^{-17}

The detection range of a copolymer in sensing a drug may be based on several significant factors including the specific copolymer composition, the nature of the drug being detected, and the sensing mechanism employed. The detection range has been calculated for all orientations, illustrated in Fig.-1(c-f). Results indicate that distance in the copolymer and INH system during interaction, the optimized distance copolymer-INH-1 is 2.64 Å, followed by copolymer-INH-2 at 2.61 Å, copolymer-INH-3 at 2.56 Å, copolymer-INH-4 at 2.1 Å. These distances represent the closest approach or strongest interaction between the copolymer and the drug. The shorter the distance, the stronger the interaction, potentially leading to more sensitive detection. Orientation 4, copolymer-INH-4 indicates strong interaction among all orientations.

Electronic Properties of Copolymer with/without Isoniazid (INH)

Upon adsorption of Isoniazid (INH), the changes in the electronic properties of the furan-pyrrole copolymer were examined using MES plots, HOMO-LUMO gaps, and DOS profiles. The band gap of the copolymer matrix in the presence/ absence of INH calculated as:

$$E_g = E_{LUMO} - E_{HOMO} \quad (4)$$

Where, E_{LUMO} and E_{HOMO} are the energies of LUMO and HOMO.

We also computed the percentage of relative energy gap changes (E_g%) of furan-pyrrole copolymer in the presence of INH.[19,20]

$$E_g\% = \frac{[E_X - E_{Y(X+INH)}]}{E_X} \times 100\% \quad (5)$$

The MES plot indicates that the computed HOMO-LUMO gap of the Fu-Py copolymer is 3.30 eV in the absence of INH. Upon interaction with INH, the HOMO-LUMO gaps copolymer-INH-1, copolymer-INH-2, copolymer-INH-3, and copolymer-INH-4 are found to be 2.04 eV, 3.08 eV, 2.70 eV, and 1.58 eV, respectively, as shown in Fig.-2. The percentage changes in the relative energy gaps for these orientations are 38%, 6.67%, 18.2%, and 52.1%, respectively. The MES plots demonstrate the enhanced conductivity of the Fu-Py copolymer upon the adsorption of INH, indicating that the copolymer exhibits better conductive properties in the 4th orientation compared to the pure Fu-Py copolymer. Furthermore, the Density of States (DOS) profiles were also computed to understand the impact of INH on the Fu-Py copolymer. The DOS profiles show that the maximum energy gap is reduced by 52.1% in the 4th orientation upon INH adsorption. This reduction is consistent with the changes observed in the MES profiles. Analysis of the density of states (DOS) shows that when adsorption occurs, the HOMO and LUMO energy levels shift closer to the Fermi level across all systems, leading to changes in the HOMO-LUMO gap (Fig.-2's right panel). In this analysis, the Fermi energy represents the kinetic energy separation between the highest and lowest occupied single-electron states at absolute zero temperature. To further confirm the HOMO-LUMO gap reduction, we calculated the ionization energy (IE) and electron affinity (EA) of the copolymer both with and without isoniazid (INH), with results presented in Table-4. IE measures the energy needed to remove an electron from a neutral molecule to form a positive ion, while EA represents the energy released when a neutral molecule accepts an electron to form a negative ion. The results demonstrate that adding INH reduces the copolymer's HOMO-LUMO gap. This corresponds to enhanced electron affinity, shown by an approximately 1 eV increase in the EA of the copolymer-INH complex. Meanwhile, the IE stays relatively stable compared to the original furan-pyrrole. IE and EA calculations used formulas (6) and (7), incorporating total energies for neutral, negative ion, and positive ion states respectively (represented as $E_{neutral}$, E_{anion}, and E_{cation}).[21,22]

$$IP = E_{cation} - E_{neutral} \quad (6)$$
$$EA = E_{neutral} - E_{anion} \quad (7)$$

Table-3: Illustrate the HOMO, LUMO, Energy Gap, Reduction Gap%, energies of Ionic States, Ionization Potential (IP), Electron Affinity (EA), and Addition Energy of Following Given in Below

System	HOMO (eV)	LUMO (eV)	Gap (eV)	Reduction gap% (eV)	Total Energy			IP	EA	E_{add}
					Neutral	cation	anion			
Fu-Py copolymer	-1.65	1.65	3.30	-	-2075.95	-2069.29	-2074.36	6.66	-1.59	8.25
Copolymer-INH-1	-1.02	1.02	2.04	38	-4380.02	-4373.87	-4380.43	6.15	0.41	5.74
Copolymer-INH-2	-1.54	1.54	3.08	6.67	-4380.24	-4374.09	-4380.33	6.15	0.09	6.06
Copolymer-INH-3	-1.35	1.35	2.70	18.2	-4380.26	-4373.12	-4380.37	7.14	0.11	7.03
Copolymer-INH-4	-0.79	0.79	1.58	52.1	-4380.42	-4374.51	-4380.67	5.91	0.25	5.66

Electron addition energy[23] (E_{add}) helps us to understand the molecule's reactivity and stability when an electron is added. It is represented as the difference between the ionization potential (IP) and the electron affinity (EA). Electron addition energy has been calculated by equation-8.

$$E_{add} = IP - EA \quad (8)$$

The electron addition energy of various configurations of copolymer-INH systems is reduced in comparison to the Fu-Py copolymer. The electron addition energy of copolymer-INH-1, copolymer-INH-2, copolymer-INH-3, and copolymer-INH-4 reduced by 2.51, 2.19, 1.22, and 2.59, respectively. These values indicate

how the presence of the INH drug influences the electronic characteristics of the copolymer. In orientation 4, lower electron addition energy suggests a higher reactivity and potential for enhanced sensor performance, making this parameter crucial in designing efficient sensing materials.

Global Descriptive Parameter of Fu-Py Copolymer in the Absence/Presence of the Isoniazid (INH)

Global descriptive parameters were calculated using ionization potential and electron affinity measurements (Table-4). These parameters include hardness (η), softness (S), Mulliken electronegativity (χ), chemical potential (π), and maximum charge transfer parameter (ΔNmax). The properties provide valuable theoretical insights into the system's chemical reactivity and selectivity characteristics.[24] Hardness represents a material's resistance to electron cloud deformation or polarization when exposed to mild chemical stimuli. The inverse property, softness, shows an increase with the addition of INH, indicating enhanced molecular reactivity.[25]

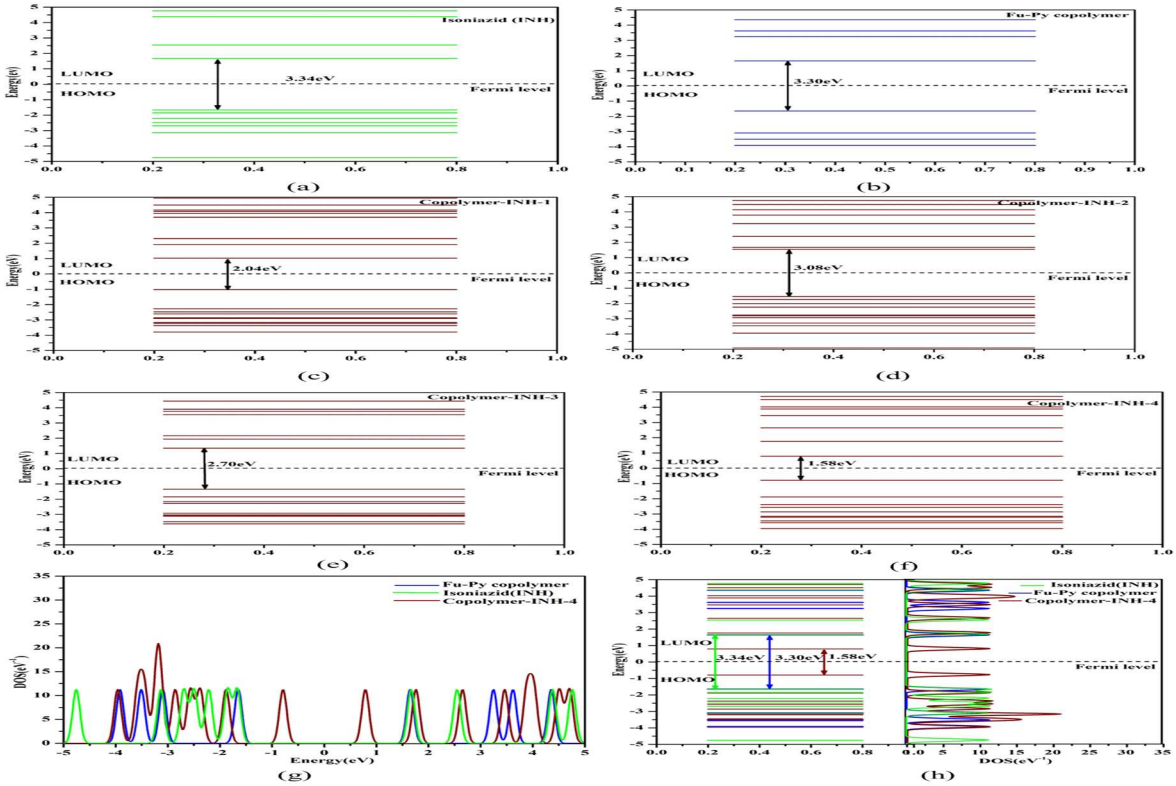

Fig.-2: MES Plot of Isoniazid (INH) (a), Fu-Py Copolymer (b), Copolymer-INH-1(c), Copolymer-INH-2(d), Copolymer-INH-3(e), Copolymer-INH-4(f), Dos Plot for Copolymer, INH, copolymer-INH-4(g), and MES and DOS Comparison of INH, Fu-Py Copolymer and Copolymer-INH-4

The electronegativity and chemical potential also change significantly, suggesting that the copolymer's ability to attract and interact with electrons is enhanced by the presence of INH. Maximum charge transfer increases for the copolymer-INH systems, indicating a higher capacity for charge transfer, which is beneficial for sensing applications.

$$\eta = \frac{I - A}{2} \ldots\ldots\ldots (9);\ s = \frac{1}{2\eta} \ldots\ldots\ldots (10);\ \chi = \frac{I + A}{2} \ldots\ldots\ldots (11);$$

$$\pi = -\frac{I + A}{2} \ldots\ldots\ldots (12);\ \Delta N_{Max} = (I + A)/2(I - A) \ldots\ldots\ldots (13)$$

Table-4: Calculated Chemical Activity Parameters of Furan-Pyrrole Copolymer in the Absence/Presence of INH

System	η (eV)	s (eV^{-1})	χ (eV)	π (eV)	ΔN_{Max}(eV)
Fu-Py copolymer	3.795	0.132	2.205	-2.205	0.581

Copolymer-INH-1	2.87	0.174	3.28	-3.28	1.143
Copolymer-INH-2	3.03	0.165	3.12	-3.12	1.03
Copolymer-INH-3	3.515	0.142	3.625	-3.625	1.031
Copolymer-INH-4	2.83	0.177	3.08	-3.08	1.089

Global chemical activity parameters including hardness, softness, electronegativity, chemical potential, and maximum charge transfer parameter were calculated using Equations 9-13. Comparing the copolymer-INH systems to the pure copolymer reveals decreases in hardness of 0.925 eV, 0.765 eV, 0.28 eV, and 0.965 eV for copolymer-INH-1 through copolymer-INH-4 respectively. Correspondingly, softness increased by 0.042 eV, 0.033 eV, 0.01 eV, and 0.045 eV. Since hardness reflects a system's resistance to electron distribution changes, these results suggest INH's presence makes the copolymer more reactive by reducing this resistance. Notably, copolymer+INH-4 shows a smaller reduction in hardness and a smaller increase in softness compared to other configurations, confirming its higher stability. Chemical potential decreased by 1.075 eV, 0.915 eV, 1.42 eV, and 0.875 eV for copolymer-INH-1 through copolymer-INH-4 respectively, with corresponding increases in electronegativity. Higher electronegativity values suggest INH's stronger electron-attracting tendency on the copolymer, favoring nucleophilic attack. The chemical potential values are negative, which indicates that the system is performing work, which suggests a higher likelihood of electrons moving away from their equilibrium state in the system. The presence of INH also enhances charge transfer phenomena in the copolymer, with the reactivity trend in the presence of INH on the copolymer as follows: copolymer-INH-4 > copolymer-INH-3 > copolymer-INH-2 > copolymer-INH-1. In contrast, the stability trend is copolymer-INH-1 > copolymer-INH-2 > copolymer-INH-3 > copolymer-INH-4.

Mulliken Population Analysis and Electron Density Analysis

The Mulliken population analysis calculates the distribution of electron density on individual atoms within a molecule. It is used to understand the charge distribution in furan, pyrrole, and its copolymer in the absence or presence of the drug. In the charge transfer analysis, the interaction intensity between the adsorbate (INH) and the adsorbent (copolymer) was assessed using Mulliken population analysis. Equation 13 has been employed for this analysis, and the results for further analysis were supported by the electron density plots:

$$\Delta\rho = \rho_{(X+INH)} - \rho_{(X)} - \rho_{(INH)} \qquad (14)$$

Where, $\Delta\rho$ indicates the charge transfer, $\rho_{(X+INH)}$ represents the charge on INH of the adsorbed system, and $\rho_{(INH)}$ represents the charge on INH in its original state and $\rho_{(X)}$ represents the host copolymer charge. The Mulliken charge population is analyzed to calculate the charge transfer before and after adsorption. The negative values of charge transfer indicate that INH drug transfers charge to the copolymer, as well as the positive value, shows that INH drug gain charge from the copolymer. Specifically, copolymer-INH-1, copolymer-INH-2, copolymer-INH-3, and copolymer-INH-4 exhibit a charge transfer of 0.002, 0.003, -2.998, and -2.996 respectively.

Electron density is a fundamental concept in the study of atoms and molecules, providing insights into their structure, behavior, and chemical properties. Electron density describes how electrons are arranged in the space around the nucleus of an atom, furnishing valuable information about the chemical behavior and interactions of atoms. Figure-3 shows the electron charge density plots for furan, pyrrole, and copolymer in the presence/absence of the INH drug, where the iso-surface plots at an iso-value of 1.9 are presented. The color scale from blue to red typically indicates regions with lower to higher electron density.

Electronegativity being the ability of an atom to attract the shared bonding electron pair in a chemical bond varies as per the specific chemical structures of the copolymer, pyrrole monomer, and furan monomer. The copolymer's electronegativity can be estimated based on the electronegativities of the constituent monomers and their respective contributions to the overall structure. As the heteroatoms oxygen and nitrogen are electronegative *p*-block elements, oxygen has a valence shell ($1s^2$,$2s^2$, $2p^4$) with two lone pairs and nitrogen has a valence shell ($1s^2$,$2s^2$, $2p^3$) with one lone pair. Oxygen has a strong electronegative nature in the optimized system and the trend for electronegativity over the Pauling scale is 2.20(H) < 2.55(C) < 3.04 (N) < 3.44(O), responsible for variation in the structural characteristics.

Table-5: Calculated Charge Transfer Values on INH after Adsorption on Fu-Py Copolymer

System	Q(e)[1]
Copolymer-INH-1	0.002
Copolymer-INH-2	0.003
Copolymer-INH-3	-2.998
Copolymer-INH-4	-2.996

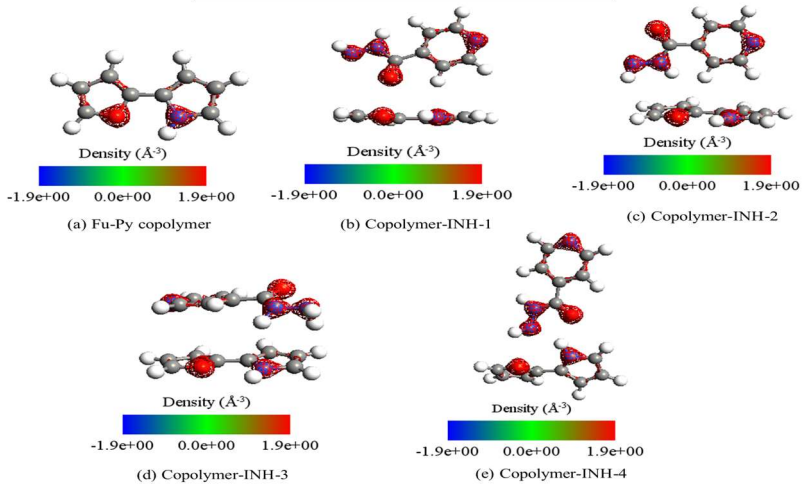

Fig.-3: (a -4) Electron Density Plots at Isovalue-1.9 of Fu-Py Copolymer, (b) Copolymer-INH-1, (c) Copolymer-INH-2, (d) Copolymer-INH-3, and (c) Copolymer-INH

CONCLUSION

The computational study indicates that the interaction between the furan-pyrrole copolymer and the isoniazid drug leads to significant changes in structural and electronic properties. The copolymer-INH-4 system is the most stable configuration, with the lowest total energy (-4380.42 eV) and adsorption energy (-0.65 eV), and a substantial charge transfer (2.996 eV). The electron affinity increased by 1.84 eV, and the energy gap decreased by 1.58 eV (a reduction of 52.1% compared to the unperturbed copolymer), indicating improved conductivity. It shows strong interaction among all orientations. These results suggest that the furan-pyrrole copolymer, especially in the copolymer-INH-4 configuration, is a promising candidate for INH detection, combining enhanced reactivity and stability for effective sensor applications.

ACKNOWLEDGEMENTS

The author expresses deep appreciation to the Materials Synthesis and Sensor Design (MSSD) Laboratory at ABV-IIITM Gwalior, for providing the computing facilities for this research.

CONFLICT OF INTEREST

The author states that there are no conflicts of interest with publishing this work.

AUTHOR CONTRIBUTIONS

All the authors contributed significantly to this manuscript, participated in reviewing/editing, and approved the final draft for publication. The research profile of the authors can be verified from their ORCID ids, given below:

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[RJC-9072/2025]