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Electronic Structure–Conductivity Relationships in Schiff Base Compounds: A Computational Chemistry Study

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Abstract

Computational investigations carried out in this work provided valuable insights into the electronic behavior of the Schiff base compounds studied. The calculated HOMO, LUMO, energy gap, and related molecular descriptors varied considerably among the investigated structures, indicating the influence of substituent groups on electron distribution and molecular stability. Comparison of the computational data with the experimental conductivity values revealed strong associations between several electronic parameters and charge-transport behavior. Among the examined descriptors, HOMO energy and heat of formation exhibited the strongest contribution to conductivity prediction. These findings support the application of computational and statistical approaches as practical tools for estimating the electrical properties of Schiff base compounds and guiding the development of materials with desirable electronic characteristics.

Keywords: Schiff base, HOMO, LUMO, energy gap, conductivity.

Introduction

Interest in Schiff base derivatives has increased due to their versatile structural features and importance in various chemical applications [(1)]. Their behavior largely depends on the nature of the substituent groups and their influence on the distribution of electron density within the molecule [(2),] which, in turn, affects molecular stability (3). Computational chemistry has witnessed remarkable development in recent years[(4)] and has become an effective tool for studying molecular structures[(5)] and predicting electronic properties using various computational methods, including semi-empirical approaches such as AM1, PM3, and MM2, as well as the Hartree–Fock (HF) method[(7)], which provides a balance between computational accuracy and calculation speed[(8)].

This study focuses on analyzing the electronic properties of a series of Schiff base compounds using several computational approaches[9]. These properties are correlated with electrical conductivity through statistical analysis [10], thereby better understanding the behavior of these compounds and predicting their characteristics without the need for extensive experimental investigations [11].

Materials and Methods

Molecular Structure Construction

The molecular structures of the Schiff base compounds (S1–S16) were initially drawn in two-dimensional form using ChemOffice 2010 software. The structures were subsequently converted into three-dimensional models to obtain accurate spatial representations of the molecules.

Geometry Optimization

An initial geometry optimization of the molecular structures was performed using the Molecular Mechanics (MM2) method to obtain the lowest-energy configuration, corresponding to the most stable molecular structure.

Semi-Empirical Calculations

Theoretical calculations were carried out using the AM1 and PM3 semi-empirical methods. The energies of the Highest Occupied Molecular Orbital (HOMO) and the Lowest Unoccupied Molecular Orbital (LUMO) were determined, along with the energy gap (ΔE), the heat of formation, and the total energy.

Calculation of Chemical Descriptors

Based on the HOMO and LUMO energy values, several important chemical descriptors were calculated, including chemical hardness (η)[12], chemical potential (μ)[13], and the electrophilicity index (ω)[14]. These descriptors were used to evaluate molecular stability and reactivity according to the equations below

Where:

$\eta = ½ (I – A)$ --------- (1) I = Ionization Potential A = Electron Affinity.

$\mu = -1/2(I + A) = ½(E_{HOMO} + E_{LUMO})$--------(2)

$\omega = \frac{\mu^2}{2\eta}$ ---------- (3)

Calculations Hartree–Fock (HF)

The Hartree–Fock (HF) method was employed to improve the accuracy of the calculated results. This approach was used to investigate the electronic distribution and molecular properties in greater detail and to compare the obtained results with those derived from the semi-empirical methods.

Statistical Analysis

Statistical analysis was performed using SPSS software (Version 25) to investigate the relationship between the electronic properties and electrical conductivity. The analysis included calculating the correlation coefficient (R) and the coefficient of determination (R^2). In addition, both simple and multiple linear regression models were applied to identify the most suitable predictive model.

Results and Discussion

The two-dimensional structures of the synthesized compounds were drawn, as shown in Figure 1, to illustrate the structural differences among them. These differences arise from the nature and position of the substituent groups and play an important role in determining the electronic properties of the compounds. The electronic properties were investigated using the semi-empirical methods (AM1 and PM3) and the Hartree–Fock (HF) method, as presented in the following table.

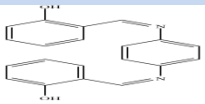
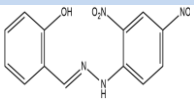
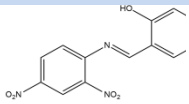
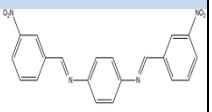
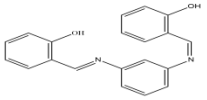
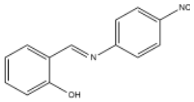
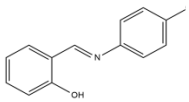
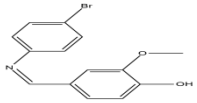
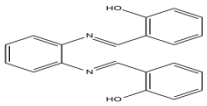
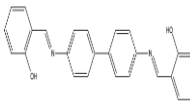
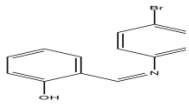
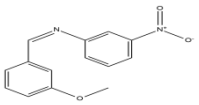
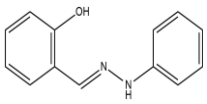
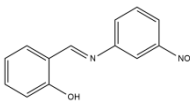
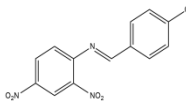
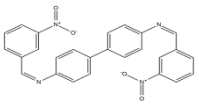
Comp	St. Comp	Comp	St. Comp	Comp	St. Comp	Comp	St. Comp
S1		S5		S9		S13	
S2		S6		S10		S14	
S3		S7		S11		S15	
S4		S8		S12		S16	

Figure 1. Two-dimensional (2D) structures of the sixteen Schiff base compounds (S1–S16).

Electrical Conductivity of Pure Organic Compounds

This study relied on the electrical conductivity values of the investigated compounds reported in our previous work, without reproducing the complete dataset to avoid redundancy. The results revealed significant variations in conductivity, with values ranging from 0.67×10^{-9} to 3.57×10^{-9} $S \cdot cm^{-1}$. Among the investigated compounds, S16 and S13 exhibited higher conductivity than the remaining members of the series, which may be attributed to more favorable electronic conditions for charge migration. Conversely, S3 and S15 exhibited comparatively weak conductivity, indicating limited charge mobility within their molecular structures. Examination of the

computational results suggests that conductivity is influenced by the molecules' electronic configuration. In particular, compounds characterized by relatively higher HOMO energies tended to exhibit improved conductive performance, whereas wider HOMO–LUMO separations were associated with less efficient charge transport.

Results Obtained Using the AM1 Method

The application of the AM1 semi-empirical approach yielded a set of electronic descriptors for the studied compounds. The calculated values are summarized in Table 1.

Table 1. Calculated electronic descriptors of the investigated compounds using the AM1 approach.

Comp	Heat Formation	Total Energy	ΔE	HOMO	LUMO	η	μ	W
S1	39.685	116.397	0.101	-0.201	-0.100	0.506	-0.151	0.022
S2	37.233	107.966	0.082	-0.165	-0.083	0.408	-0.124	0.019
S3	13.468	39.925	0.032	-0.063	-0.031	0.015	-0.047	0.007
S4	31.657	94.006	0.079	-0.157	-0.078	0.395	-0.197	0.017
S5	33.003	94.530	0.082	-0.163	-0.081	0.410	-0.122	0.018
S6	33.811	99.410	0.077	-0.154	-0.077	0.388	-0.116	0.017
S7	43.835	124.971	0.112	-0.214	-0.102	0.559	-0.158	0.022
S8	27.007	76.472	0.076	-0.152	-0.076	0.376	-0.114	0.017
S9	32.604	95.737	0.083	-0.166	-0.083	0.414	-0.124	0.018
S10	34.678	102.209	0.063	-0.127	-0.064	0.316	-0.096	0.014
S11	23.077	67.664	0.056	-0.114	-0.058	0.281	-0.086	0.013
S12	33.262	100.515	0.077	-0.154	-0.077	0.385	-0.116	0.017
S13	62.691	183.82	0.131	-0.318	-0.187	0.658	-0.252	0.048
S14	28.892	85.155	0.073	-0.146	-0.073	0.366	-0.110	0.016
S15	17.203	49.686	0.039	-0.075	-0.036	0.019	-0.056	0.019
S16	71.445	217.290	0.175	-0.352	-0.177	0.875	-0.264	0.039

Noticeable differences were observed in the calculated HOMO and LUMO energies for the studied compounds. The variation in the calculated values is mainly due to differences in the substituents attached to the molecular structure. These variations in electron distribution affected the calculated stability and reactivity parameters. Compounds characterized by lower HOMO energies tended to exhibit greater stability, whereas relatively higher HOMO values were associated with increased electronic activity. Variations in the energy gap were also evident among the investigated structures. In general, wider energy gaps corresponded to more stable and less reactive systems, while narrower gaps indicated a greater tendency toward electronic interaction. The observed trend is likely associated with the type and location of the substituent groups in the studied compounds.

Results Obtained Using the PM3 Method

The PM3 semi-empirical method was applied to further examine the electronic characteristics of the synthesized Schiff base compounds. The parameters calculated using this approach are summarized in Table 2.

Table 2. Electronic descriptors obtained from PM3 calculations for the synthesized Schiff base compounds.

Comp	Heat Formation	Total Energy	HOMO	LUMO	ΔE	η	μ	W
S1	41.830	116.397	-0.418	-0.053	0.365	0.182	-0.235	0.152
S2	35.758	107.966	-0.360	-0.030	0.330	0.165	-0.195	0.116
S3	13.149	39.925	-0.109	-0.042	0.067	0.033	-0.075	0.085
S4	20.936	94.006	-0.210	-0.029	0.181	0.090	-0.120	0.080
S5	30.722	94.530	-0.377	-0.029	0.348	0.174	-0.203	0.118
S6	30.869	99.410	-0.331	-0.039	0.292	0.145	-0.185	0.118
S7	42.849	124.971	-0.301	-0.044	0.257	0.128	-0.172	0.116
S8	28.509	76.472	-0.254	-0.024	0.230	0.115	-0.139	0.084
S9	29.605	95.737	-0.247	-0.022	0.225	0.112	-0.134	0.080
S10	24.516	102.209	-0.289	-0.023	0.266	0.132	-0.156	0.092
S11	22.507	67.664	-0.295	-0.024	0.271	0.136	-0.160	0.094
S12	30.085	100.515	-0.359	-0.033	0.326	0.163	-0.196	0.118
S13	63.530	183.82	-0.651	-0.064	0.587	0.293	-0.357	0.218
S14	26.618	85.155	-0.230	-0.025	0.205	0.051	-0.128	0.080
S15	14.609	49.686	-0.126	-0.014	0.112	0.055	-0.070	0.044
S16	73.470	217.290	-0.633	-0.062	0.571	0.285	-0.348	0.212

The PM3 calculations yielded results generally consistent with those from the AM1 method, although some differences were evident in the numerical values of the calculated parameters. Examination of the electronic descriptors indicates that the investigated compounds respond differently to the influence of their substituent groups. In several cases, compounds with relatively higher HOMO energies exhibited greater electronic activity, whereas lower HOMO energies were associated with more stable electronic configurations. The calculated hardness (η) and electrophilicity index (ω) also varied among the studied structures, suggesting differences in their ability to accept electrons and participate in electronic interactions. Taken together,

the calculated parameters help clarify how molecular structure influences stability and reactivity.

Results Obtained Using the Hartree–Fock (HF) Method

To obtain a more detailed description of the electronic structure, the investigated compounds were further analyzed using the Hartree–Fock (HF) approach. The calculated electronic parameters derived from this method are summarized in Table 3.

Table 3. Electronic parameters calculated using the Hartree–Fock (HF) approach.

Comp	HOMO	LUMO	ΔE	W	μ	Ƞ
S1	-0.186	0.016	0.202	0.101	-0.084	0.035
S2	-0.165	0.012	0.177	0.089	-0.076	0.032
S3	-0.073	0.008	0.081	0.041	-0.032	0.012
S4	-0.169	0.019	0.188	0.094	-0.075	0.029
S5	-0.189	0.018	0.207	0.103	-0.085	0.035
S6	-0.100	0.010	0.110	0.055	-0.044	0.018
S7	-0.215	0.020	0.235	0.118	-0.097	0.040
S8	-0.133	0.019	0.152	0.076	-0.057	0.021
S9	-0.168	0.017	0.185	0.093	-0.075	0.030
S10	-0.126	0.019	0.145	0.073	-0.053	0.019
S11	-0.116	0.014	0.130	0.065	-0.051	0.020
S12	-0.164	0.019	0.183	0.092	-0.072	0.028
S13	-0.327	0.033	0.360	0.180	-0.147	0.060
S14	-0.141	0.014	0.155	0.077	-0.063	0.025
S15	-0.097	0.006	0.103	0.052	-0.045	0.020
S16	-0.303	0.032	0.335	0.167	-0.135	0.055

The electronic descriptors obtained from the Hartree–Fock calculations followed trends comparable to those observed with the AM1 and PM3 methods, while providing a more detailed representation of the molecular electronic structure. Differences in HOMO and LUMO energies among the investigated compounds

reflected variations in electron distribution and molecular behavior. Compounds characterized by lower HOMO energies together with relatively higher LUMO values generally exhibited greater electronic stability. Variations in chemical hardness (η) and electrophilicity index (ω) were also observed, indicating differences in molecular reactivity and electron-accepting ability. In general, compounds possessing higher values of these descriptors tended to show more stable electronic configurations and lower reactivity. Similar trends were evident in the calculated energy-gap values, further supporting the relationship between electronic structure and molecular stability.

Statistical Analysis

Simple Linear Regression Analysis

To evaluate the influence of the calculated electronic descriptors on electrical conductivity, simple linear regression models were fitted in SPSS. The statistical outcomes obtained from this analysis are summarized in the following tables.

Table (4). Results of the Simple Linear Regression Analysis Using the AM1 Method

Dep. Var	Indep Var	R	R^2	Std.Error	Const.	Value
Conductivity	HeatFormation	0.985	0.971	0.000	$-8.616E^{-11}$	$5.096E^{-11}$
	Total Energy	0.984	0.967	0.000	$-3.510E^{-11}$	$1.685E^{-11}$
	HOMO	0.994	0.988	0.000	$-6.362E^{-12}$	$-1.006E^{-8}$
	LUMO	0.979	0.959	0.000	$1.564E^{-10}$	$-1.788E^{-8}$
	ΔE	0.362	0.131	0.000	$2.377E^{-9}$	$-7.991E^{-9}$
	η	0.956	0.914	0.000	$3.103E^{-10}$	$3.509E^{-9}$
	μ	0.938	0.879	0.000	$1.372E^{-10}$	$-1.176E^{-8}$
	W	0.894	0.800	0.000	$3.017E^{-10}$	$6.806E^{-8}$

Table (5). Results of the Simple Linear Regression Analysis Using the PM3 Method

Dep.Var	Indep Var	R	R^2	Std.Error	Const.	Value
Conductivity	HeatFormation	0.983	0.966	0.000	$1.741E^{-10}$	$4.637E^{-11}$
	Total Energy	0.984	0.967	0.000	$-3.510E^{-11}$	$1.685E^{-11}$
	HOMO	0.922	0.851	0.000	$1.895E^{-10}$	$-4.678E^{-9}$
	LUMO	0.799	0.638	0.000	$2.486E^{-10}$	$-4.141E^{-8}$
	ΔE	0.351	0.123	0.000	$2.264E^{-9}$	$-1.919E^{-9}$
	η	0.888	0.788	0.000	$3.929E^{-10}$	$9.296E^{-9}$
	μ	0.928	0.862	0.000	$1.351E^{-10}$	$-8.742E^{-9}$
	W	0.914	0.836	0.000	$2.394E^{-11}$	$1.488E^{-8}$

Table (6). Results of the Simple Linear Regression Analysis Using the Hartree–Fock (HF) Method

Dep.Var	Indep Var	R	R^2	Std.Error	Const.	Value
Conductivity	Total Energy	0.984	0.967	0.000	$-3.510E^{-11}$	$1.685E^{-11}$
	HOMO	0.955	0.913	0.000	$-5.316E^{-11}$	$-1.052E^{-8}$
	LUMO	0.873	0.762	0.000	$5.895E^{-11}$	$9.282E^{-8}$
	ΔE	0.400	0.160	0.000	$2.449E^{-9}$	$-4.018E^{-9}$
	η	0.955	0.912	0.000	$-6.971E^{-11}$	$1;.921E^{-8}$
	μ	0.954	0.910	0.000	$-2.606E^{-11}$	$-2.329E^{-8}$
	W	0.947	0.896	0.000	$3.291E^{-11}$	$5.532E^{-8}$

The regression analysis revealed that electrical conductivity was closely related to a number of the calculated electronic parameters. The high values of both R and R^2 indicate that these parameters account for a substantial proportion of the observed variation in conductivity. Among the investigated variables, HOMO energy and heat of formation exhibited the strongest influence on the predictive models. The results

suggest that conductivity is strongly influenced by the electronic properties of the investigated Schiff base compounds.

Correlation Matrix

A correlation matrix was constructed to examine the relationships among the electronic descriptors and their association with electrical conductivity. The resulting correlation coefficients are summarized in the following tables.

Table (7). Correlation matrix of electronic descriptors derived from the AM1 calculations.

Par.	Conductivity	HeatFormation	TotalEnergy	HOMO	LUMO	ΔE	η	μ	W
Conductuvity	1								
HeatFormation	0.971	1							
Total Energy	0.967	0.997	1						
HOMO	0.988	0.966	0.960	1					
LUMO	0.959	0.940	0.931	0.979	1				
ΔE	0.131	0.138	0.135	0.213	0.112	1			
η	0.914	0.894	0.887	0.915	0.844	0.148	1		
μ	0.879	0.848	0.846	0.891	0.880	0.137	0.823	1	
W	0.800	0.796	0.787	0.832	0.894	0.107	0.594	0.744	1

Table (8). Correlation matrix of electronic descriptors derived from the PM3 calculations.

Par.	Conductivity	Heat Formation	TotalEnergy	HOMO	LUMO	ΔE	η	μ	W
Conductivity	1								
HeatFormation	0.966	1							
Total Energy	0.967	0.946	1						
HOMO	0.851	0.879	0.960	1					
LUMO	0.638	0.674	0.931	0.599	1				
ΔE	0.123	0.135	0.137	0.246	0.157	1			
η	0.788	0.816	0.887	0.967	0.531	0.322	1		
μ	0.862	0.892	0.846	0.997	0.655	0.246	0.958	1	
W	0.836	0.876	0.787	0.928	0.831	0.256	0.875	0.954	1

Table (9). Correlation matrix of electronic descriptors derived from the HF calculations.

Par.	Conductivity	Total Energy	HOMO	LUMO	ΔE	η	μ	W
Conductivity	1							
Total Energy	0.967	1						
HOMO	0.913	0.860	1					
LUMO	0.762	0.776	0.831	1				
ΔE	0.160	0.145	0.116	0.222	1			
η	0.912	0.865	0.998	0.859	0.127	1		
μ	0.910	0.850	0.998	0.794	0.104	0.993	1	
W	0.896	0.826	0.984	0.726	0.084	0.973	0.994	1

The calculated correlation coefficients revealed clear relationships among the variables studied. In general, relatively high correlation coefficients were obtained, reflecting meaningful statistical associations among the calculated descriptors. Total

energy, in particular, showed strong relationships with several of the remaining parameters, suggesting its important contribution to molecular stability. Because several variables were correlated, multiple regression analysis was used to assess their combined contribution to conductivity.

Multiple Regression Analysis (Two-Variable and Three-Variable Models)

Multiple regression models were developed to identify the combination of electronic descriptors that provides the most reliable prediction of electrical conductivity. The statistical parameters obtained from these models are summarized in the following tables.

Table (10). Binary Statistical Correlation Analysis Using the AM1 Method

dep Var	Indep Var	Const.	R	R^2	Std.Error	Factor 1	Factor 2
	HeatFormation HOMO	$-3.710E^{-11}$	0.950	0.990	0.000	$1.262E^{-11}$	$-7.631E^{-9}$
	Total Energy HOMO	$-2.584E^{-11}$	0.995	0.991	0.000	$4.038E^{-12}$	$-7.721E^{-9}$
	HOMO LUMO	$-2.974E^{-11}$	0.995	0.989	0.000	$-1.198E^{-8}$	$3.506E^{-9}$

Table (11). Ternary Binary Statistical Correlation Analysis Using the AM1 Method

dep Var	Indep Var	Const.	R	R^2	Std.Error	Factor 1	Factor 2	Factor 3
Conductivity	HeatFormation Total Energy HOMO	$-2.342E^{-11}$	0.995	0.991	0.000	$-2.403E^{-12}$	$4.751E^{-12}$	$-7.771E^{-9}$

The regression models developed in this study exhibited high coefficients of determination (R^2), indicating a strong agreement between the predicted and experimental conductivity values. Among the tested models, those incorporating HOMO energy along with heat of formation yielded the most accurate predictions, underscoring the contribution of these descriptors to charge-transport behavior.

The obtained results showed that conductivity depends on the combined effect of several electronic parameters rather than a single descriptor. Instead, the combined effect of several descriptors offers a more realistic representation of the relationship between molecular electronic structure and conductivity.

The PM3 and HF calculations yielded results generally consistent with those from the AM1 method. The consistency observed among the three computational approaches supports the reliability of the statistical models used in this work.

Based on the correlation and regression analyses, HOMO energy and heat of formation emerged as the most influential variables affecting conductivity. Total energy showed a secondary contribution, followed by LUMO energy, while the remaining descriptors exhibited comparatively smaller effects on the predictive models.

The regression equation describing the relationship between conductivity and the selected AM1 descriptors is given below:

Conductivity = $-3.758 \times 10^{-11} - 7.643 \times 10^{-9}$ (Heat Formation) + 1.205×10^{-11} (HOMO)

The calculated AM1 parameters were subsequently used to establish the relationship between theoretical predictions and the experimentally measured conductivity values, as illustrated in Figure 2.

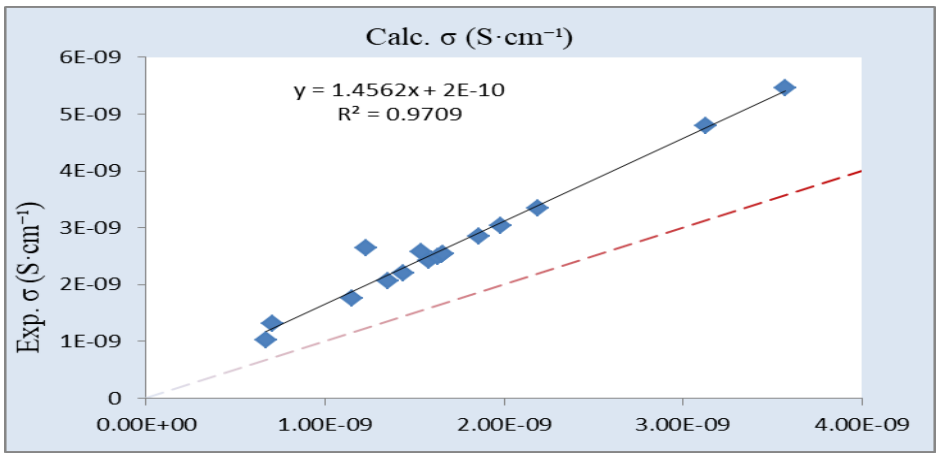


Figure 2 shows a clear linear association between the experimentally measured conductivity values and those predicted from the AM1-based model.

The relatively high coefficient of determination ($R^2 = 0.9709$) indicates that the model successfully accounts for most of the variation observed in the experimental data. The predicted conductivity values were in good agreement with the experimental measurements, indicating the suitability of the selected electronic descriptors. In particular, HOMO energy and heat of formation appear to play a significant role in influencing conductivity within the investigated Schiff base compounds.

References

1- Baruah, M. J., Dutta, R., Zaki, M. E. A., & Bania, K. K. (2024). Heterogeneous iron-based catalysts for organic transformation reactions: A brief overview. Molecules, 29(13), 3177.
2- Malav, R., & Ray, S. (2025). Recent advances in the synthesis and versatile applications of transition metal complexes featuring Schiff base ligands. RSC Advances, 15, 22889–22914.
3- Alammari, S., Aroua, L. M., & Alminderej, F. (2025). Schiff bases performance and challenge: Chemical synthesis and current state of biological activities. Egyptian Journal of Chemistry, 68(8), 425–449.
4- Zhuo, Y. (2024). Computational chemistry review article. Applied and Computational Engineering, 61, 262–273.
5- Schilter, O., Schwaller, P., & Laino, T. (2024). Balancing computational chemistry's potential with its environmental impact. Green Chemistry, 26, 8669–8679.
6- Zeki, N. M., Othman, K. M. Z., & Mustafa, Y. F. (2025). Computational Chemistry: A game-changer in the drug discovery field. Applied Chemical Engineering, 8(1), ACE-5601.
7- AL-Dahlaki, M. H., & Mohammed, A. H. (2024). Quantum mechanics/molecular mechanics (QM/MM) methods in drug design: a comprehensive review of development and applications. International Journal of Advanced Chemistry, 12(2), 86-92.
8- Barbatti, M. (2025). When theory came first: A review of theoretical chemical predictions ahead of experiments. Pure and Applied Chemistry, 97(9), 1115–1134.
9- Leghari, Q. A., Masihullah, W., Iqtadar, R., Mushtaque, S., Ali, S. T., & Wajdi, M. (2025). Computational chemistry in drug discovery: Insights and innovations — A review. Frontier in Medical & Health Research, 3(2).9.
10- Ponte-Cordova, J. J., Luna-Martinez, J. F., Mohammed-Noriega, N., and Miranda-Valdez, E. Y. (2024). Electrical conductivity mechanisms in ethylcellulose films under the influence of continuous and alternating electric fields. Polymers, 16(5), 628.
11- Pal, S., Srivastava, V., Avasare, V., & Maruani, J. (Eds.). (2025). Theoretical methods, algorithms, and applications of quantum systems in chemistry, physics. and biology, (1st ed., pp. 1–341).
12- Zaklika, J., Ordon, P., & Komorowski, L. (2024). Hyperhardness and hypersoftness of atoms and their ions. Journal of Molecular Modeling, 30(10), 344.
13- Ruvalcaba, R., Liu, Z., Nugraha, M. I., Harrison, G., Yang, Y.-Y., Thaler, M., Marsh, A. V., Zeilerbauer, M., Aivalioti, C., Aguileta-Vazquez, R. R., Tsetseris, L., Patera, L. L., Zahl, P., Heeney, M., & Anthopoulos, T. D. (2025). On-surface reactions of electronically active self-assembled monolayers for electrode work function tuning. ACS Materials Letters, 7(7), 1421–1430. 14.
14- Sabry, N. M., Badry, R., Abdel-Gawad, F. K., Elhaes, H., & Ibrahim, M. A. (2025). In vitro, in silico, and DFT evaluation of antimicrobial imidazole derivatives with insights into mechanism of action. Scientific Reports, 15, Article 24847.