

Theoretical Investigation of Corrosion Behaviors of Pyridazine Derivatives Using DFT

Yoğunluk Fonksiyonel Teorisi (DFT) Hesaplamaları Kullanılarak Piridazin Türevlerinin Korozyon Davranışlarının Teorik İncelenmesi

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ABSTRACT

Metal corrosion represents a significant challenge in industrial applications, leading to substantial economic losses and safety concerns. In this study, the corrosion inhibition performance of selected pyridazine derivatives was systematically investigated using Density Functional Theory (DFT). Despite the wide evaluation of heterocyclic inhibitors, a systematic structural comparison targeting the positional and substituent variations in pyridazine frameworks remains elusive. This study addresses this gap by rationally designing a novel series of multi-substituted pyridazine derivatives to maximize surface adsorption sites. Quantum chemical calculations were performed at the B3LYP/6-311G(d,p) level to evaluate frontier molecular orbitals (EHOMO, ELUMO), energy gap (ΔE), and global reactivity descriptors including electronegativity (χ), hardness (η), softness (S), electrophilicity index (ω), and fraction of electron transfer (ΔN). The results reveal a clear structure–reactivity relationship, where molecules with higher electron-donating ability and lower energy gaps exhibit enhanced inhibition performance. Among the studied compounds, compound 5 showed the highest inhibition potential due to its lowest ΔE and highest ΔN values. Molecular electrostatic potential (MEP) and density of states (DOS) analyses further support strong adsorption tendencies. The findings provide a comprehensive theoretical framework for understanding corrosion inhibition mechanisms of pyridazine derivatives and contribute to the rational design of efficient organic inhibitors. These findings provide useful theoretical support for corrosion inhibition applications in acidic media.

Keywords: Pyridazine derivatives, corrosion inhibition, density functional theory, quantum chemical descriptors, MEP, DOS

ÖZ

Metal korozyonu, endüstriyel uygulamalarda önemli bir zorluk teşkil etmekte olup, ciddi ekonomik kayıplara ve güvenlik endişelerine yol açmaktadır. Bu çalışmada, seçilen piridazin türevlerinin korozyon önleme performansı, Yoğunluk Fonksiyonel Teorisi (DFT) kullanılarak sistematik olarak incelenmiştir. Heterosiklik inhibitörlerin geniş çaplı değerlendirilmesine rağmen, piridazin iskeletlerindeki pozisyonel ve sübstitüent varyasyonlarını hedefleyen sistematik bir yapısal karşılaştırma hâlâ gerçekleştirilememiştir. Bu çalışma, yüzey adsorpsiyon bölgelerini en üst düzeye çıkarmak için rasyonel olarak tasarlanmış yeni bir çoklu sübstitüe piridazin türevleri serisi geliştirerek bu boşluğu ele almaktadır. Sınır moleküler orbitalleri (EHOMO, ELUMO), enerji aralığı (ΔE) ve elektronegatiflik (χ), sertlik (η), yumuşaklık (S), elektrofilitiklik indeksi (ω) ve elektron transfer oranı (ΔN) dahil olmak üzere küresel reaktivite tanımlayıcılarını değerlendirmek için B3LYP/6-311G(d,p) seviyesinde kuantum kimyasal hesaplamalar yapılmıştır. Sonuçlar, daha yüksek elektron verme yeteneğine ve daha düşük enerji aralıklarına sahip moleküllerin daha yüksek inhibisyon performansı sergilediği açık bir yapı-reaktivite ilişkisini ortaya koymaktadır. İncelenen bileşikler arasında, bileşik 5, en düşük ΔE ve en yüksek ΔN değerleri nedeniyle en yüksek inhibisyon potansiyelini göstermiştir. Moleküler elektrostatik potansiyel

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analizleri, güçlü adsorpsiyon eğilimlerini daha da desteklemektedir. Bulgular, piridazin türevlerinin korozyon önleme mekanizmalarını anlamak için kapsamlı bir teorik çerçeve sunmakta ve etkili organik inhibitörlerin rasyonel tasarımına katkıda bulunmaktadır. Bu bulgular, asidik ortamlarda korozyon önleme uygulamaları için faydalı teorik destek sağlamaktadır.

Anahtar Kelimeler: Piridazin türevleri, korozyon inhibisyonu, yoğunluk fonksiyonel teorisi, kuantum kimyasal tanımlayıcılar, MEP, DOS

INTRODUCTION

Corrosion of metallic materials in acidic environments remains a major challenge in industrial processes such as acid cleaning, pickling, and descaling.¹ This degradation leads to significant economic losses and operational risks. Among various mitigation strategies, the use of organic corrosion inhibitors is widely recognized as one of the most effective and economical approaches.²

Organic inhibitors primarily function through adsorption onto metal surfaces, forming a protective barrier that suppresses metal dissolution. Their efficiency is strongly influenced by molecular structure, particularly the presence of heteroatoms and π -electron systems that facilitate interaction with metal d-orbitals.^{2,3} In this context, nitrogen-containing heterocyclic compounds have attracted considerable attention due to their strong adsorption capability and relatively low environmental impact.⁴ Heterocyclic compounds containing nitrogen atoms, such as pyridazine, pyrimidine, and their derivatives, have attracted significant attention in recent years due to their outstanding corrosion inhibition performance in acidic media.^{5,6} Theoretical tools, particularly Density Functional Theory (DFT), have become crucial in predicting the inhibition efficiency and explaining the adsorption mechanism at an atomic level.⁷⁻⁹ Recently, several theoretical frameworks have been reported to assess the global and local reactivity parameters of organic networks.⁹⁻¹²

Pyridazine derivatives, characterized by a six-membered aromatic ring containing two nitrogen atoms, exhibit notable electron-donating and electron-accepting properties. These features make them promising candidates for corrosion inhibition, as they can effectively interact with metal surfaces through donor–acceptor mechanisms.¹³

Density Functional Theory (DFT) has emerged as a powerful tool for predicting corrosion inhibition performance by providing molecular-level insights into electronic structure and reactivity. Key parameters such as the energies of the highest occupied molecular

orbital (E_{HOMO}), lowest unoccupied molecular orbital (E_{LUMO}), and the energy gap (ΔE) are widely used to evaluate molecular reactivity and adsorption behavior. In addition, global reactivity descriptors—including ionization potential (I), electron affinity (A), global hardness (η), softness (S), electronegativity (χ), electrophilicity index (ω), and fraction of electron transfer (ΔN)—offer a quantitative framework for understanding charge transfer interactions between inhibitor molecules and metal surfaces.¹⁴⁻¹⁹

Although numerous DFT-based studies on corrosion inhibitors have been reported, systematic investigations focusing specifically on pyridazine derivatives remain limited. Therefore, in the present study, a series of pyridazine-based compounds (Sigma-Aldrich) methyl pyridazine-4-carboxylate (**1**), 3,6-dichloro-4-(trifluoromethyl)pyridazine (**2**), 6-hydrazinoimidazo [1,2-b] pyridazine (**3**), 6-chloro[1,2,4]triazolo [4,3-b] pyridazine (**4**), and 6-chloro-2-chloromethylimidazo [1,2-b] pyridazine (**5**) (Figure 1) were systematically investigated using DFT calculations.

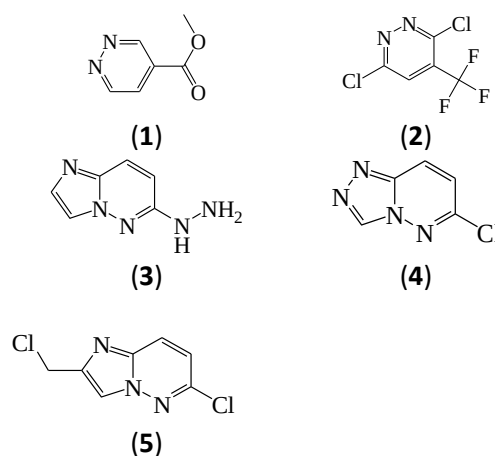


Figure 1. Pyridazine compounds

Unlike many previous studies that rely on a limited number of descriptors, this work employs a comprehensive set of frontier molecular orbital parameters and global reactivity descriptors, together with molecular electrostatic potential (MEP) analysis, to establish a more reliable structure–inhibition relationship. To the best of our knowledge, this is the

first comprehensive DFT study comparing substituted pyridazine derivatives in terms of corrosion inhibition performance using a multi-descriptor approach. This integrated theoretical approach provides deeper insight into the corrosion inhibition mechanism of pyridazine derivatives and contributes to the rational design of efficient organic inhibitors.

METHODS

All quantum chemical calculations in this study were systematically performed in the gas phase using Density Functional Theory (DFT) as implemented in Gaussian16²⁰ to evaluate the intrinsic electronic and structural properties of the isolated pyridazine molecules prior to surface interaction. software package. All quantum chemical calculations and high-performance computing tasks were executed on Intel Xeon processor-based workstations utilizing the advanced computational infrastructure of the Turkish National Science e-Infrastructure (TRUBA). The molecular structures of the selected pyridazine derivatives were fully optimized using the Becke three-parameter hybrid functional combined with the Lee–Yang–Parr correlation functional (B3LYP) and the 6-311G(d,p) basis set.²¹ This level of theory is widely accepted in corrosion inhibition studies due to its reliability in describing the electronic and structural properties of organic molecules.

Geometry optimizations were carried out without imposing any symmetry constraints to ensure convergence to the lowest-energy configurations. Frequency calculations were subsequently performed at the same level of theory to confirm that the optimized structures corresponded to true minima on the potential energy surface, as evidenced by the absence of imaginary frequencies. The optimized geometries were used to obtain structural parameters such as bond lengths, bond angles, and dihedral angles, along with total electronic energies.

For molecules exhibiting conformational flexibility, initial conformer geometries were generated to identify the most stable low-energy structures. Although extensive conformational scanning can be computationally demanding for large molecules, preliminary optimization ensured that the global minimum conformer was selected for subsequent electronic structure analysis.

The corrosion inhibition performance of the investigated pyridazine derivatives was evaluated using frontier molecular orbital theory and global reactivity descriptors. The energies of the Highest Occupied

Molecular Orbital (E_{HOMO}) and the Lowest Unoccupied Molecular Orbital (E_{LUMO}) were obtained directly from the optimized molecular structures. The energy gap (ΔE), which reflects molecular reactivity and stability, was calculated as the difference between E_{LUMO} and E_{HOMO} :

$$\Delta E = E_{\text{LUMO}} - E_{\text{HOMO}}$$

Based on Koopmans' theorem, the ionization potential (I) and electron affinity (A) were estimated using the following expressions²²:

$$I = -E_{\text{HOMO}}$$

$$A = -E_{\text{LUMO}}$$

The global hardness (η) and global softness (S), which describe resistance to charge transfer and molecular reactivity, respectively, were calculated as^{23,24}:

$$\eta = \left(\frac{E_{\text{LUMO}} - E_{\text{HOMO}}}{2} \right) = \left(\frac{I - A}{2} \right)$$

$$S = \left(\frac{1}{2\eta} \right)$$

The electronegativity (χ) and chemical potential (μ) were determined according to^{25,26}:

$$\chi = -\mu = \left(\frac{-E_{\text{HOMO}} - E_{\text{LUMO}}}{2} \right) = \left(\frac{I + A}{2} \right)$$

$$\mu = -\chi = \left(\frac{\partial E}{\partial N} \right)_{g(r)}$$

The global electrophilicity index (ω), which indicates the tendency of a molecule to accept electrons, was calculated using²⁷:

$$\omega = \frac{\mu^2}{2\eta} = \frac{\chi^2}{2\eta}$$

The fraction of electrons transferred (ΔN) from the inhibitor molecule to the metal surface was estimated using the following relation:

$$\Delta N = \frac{\chi_{\text{M}} - \chi_{\text{inh}}}{2(\eta_{\text{M}} + \eta_{\text{inh}})},$$

where χ_{metal} and η_{metal} denote the electronegativity and global hardness of the metal surface, respectively, and χ_{inh} and η_{inh} correspond to those of the inhibitor

molecule. For iron surfaces, commonly reported literature values of $\chi_{\text{Fe}} = 7.0$ eV and $\eta_{\text{Fe}} = 0$ eV were employed.²⁸

The back-donation energy ($\Delta E_{\text{back-donation}}$), which reflects the ability of the inhibitor molecule to accept electron density from the metal surface,^{29,30} was calculated as:

$$\Delta E_{\text{back donation}} = -\frac{\eta}{4}$$

Additionally, Molecular Electrostatic Potential (MEP) maps were generated to visualize the charge distribution within the molecules and to identify electrophilic and nucleophilic regions responsible for adsorption onto metal surfaces. All calculated quantum chemical parameters were systematically analyzed to establish structure–activity relationships and to predict the corrosion inhibition efficiencies of the selected pyridazine derivatives.

RESULTS

Fully geometric optimizations of all molecules, HOMO-LUMO diagrams (Figure 2), molecular electrostatic potential maps (MEPs) (Figure 3) and corrosion inhibition parameters (Table 1) were calculated with DFT and B3LYP (d, p) base set in Gaussian16 program. This computational approach has been widely used to investigate the relationship between electronic structure and corrosion inhibition efficiency.

Frontier molecular orbital analysis provides critical insight into the corrosion inhibition mechanism by revealing the electron donation and acceptance behavior of inhibitor molecules.³¹ The spatial distribution of the Highest Occupied Molecular Orbital (HOMO) reflects the regions responsible for electron donation to the metal surface, while the Lowest Unoccupied Molecular Orbital (LUMO) indicates the sites capable of accepting electrons through back-donation interactions (Figure 2).

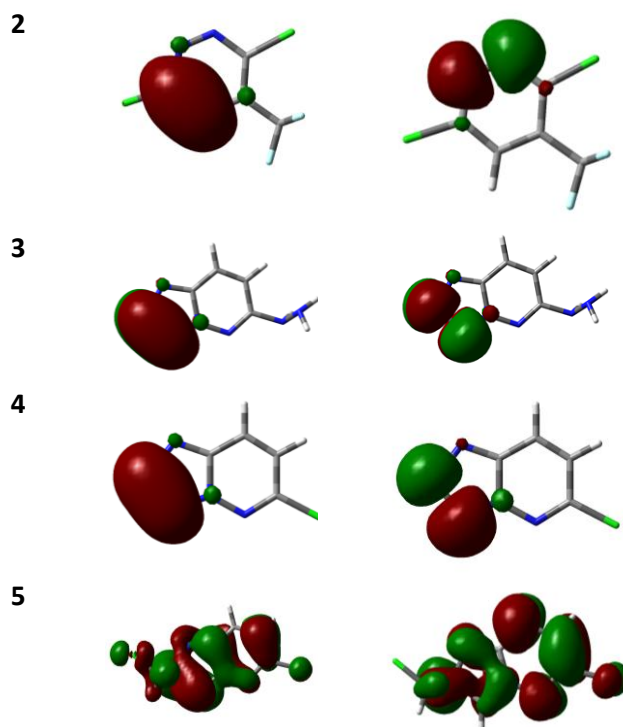


Figure 2. Frontier molecular orbital (FMO) analysis of compounds.

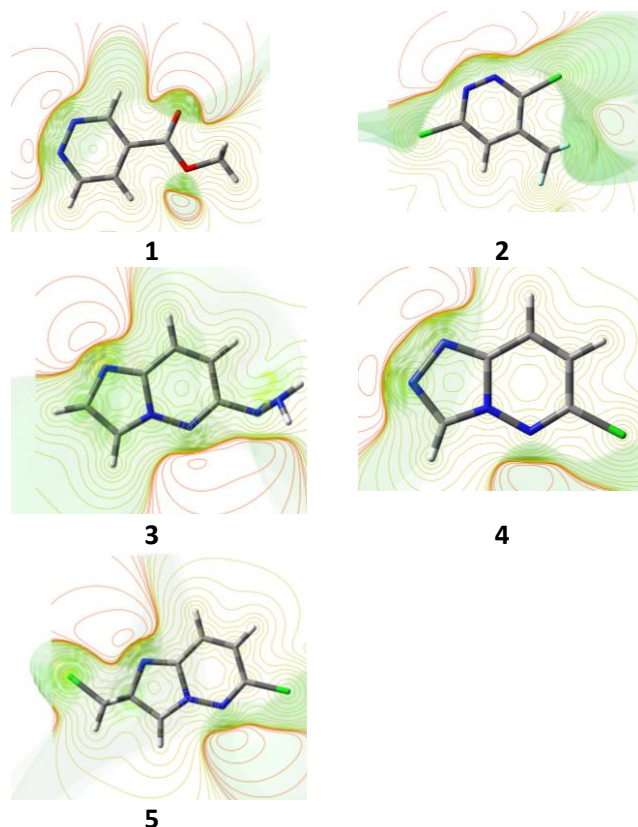
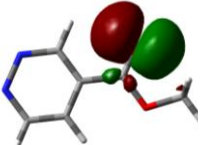
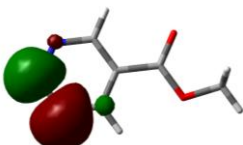


Figure 3. The MEPs of all compounds.

Comp.	HOMO	LUMO
1		

The HOMO of compound **1** is mainly localized over the pyridazine ring and associated heteroatoms, indicating that electron donation primarily originates from the aromatic π -system and nitrogen atoms. The LUMO is moderately distributed over the molecular framework, suggesting limited back-donation capability. This orbital distribution corresponds to moderate adsorption strength and is consistent with its intermediate inhibition efficiency. The HOMO density is relatively localized and less pronounced compared to the other compounds, indicating a weaker electron-donating ability. The LUMO is mainly concentrated on electron-withdrawing substituent regions, which restricts effective orbital overlap with the metal surface (Figure 4).

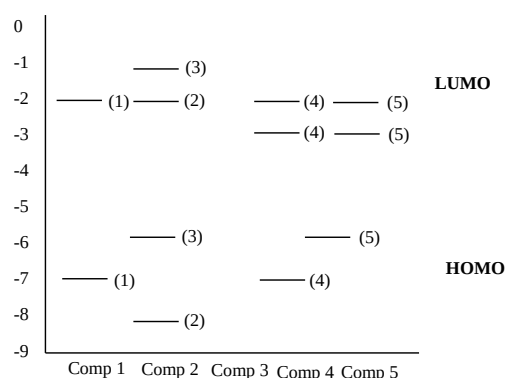


Figure 4. HOMO-LUMO energy level.

These features explain the lowest inhibition performance observed for compound **2**. The HOMO of compound **3** is widely delocalized over the heterocyclic ring system and adjacent functional groups, providing multiple active centers for electron donation. The LUMO distribution overlaps significantly with the conjugated framework, facilitating efficient back-donation. This favorable HOMO–LUMO arrangement supports strong inhibitor–metal interaction, in agreement with its high ΔN value and good inhibition efficiency. In compound **4**, the HOMO is localized around the heteroatoms and the fused ring system, while the LUMO is partially delocalized over the molecular backbone. Although this distribution allows for donor–acceptor interactions, the extent of delocalization is less pronounced than in compounds **3** and **5**. Consequently, compound **4** exhibits moderate corrosion inhibition behavior. Compound **5** displays the most favorable orbital characteristics among the investigated molecules. The HOMO is highly delocalized over the pyridazine ring and substituent groups, indicating strong electron-donating capability. Simultaneously, the LUMO is well distributed over the same regions, promoting efficient back-donation from

the metal surface. This strong spatial overlap between HOMO and LUMO orbitals facilitates robust adsorption and explains the superior inhibition efficiency of compound **5**. The HOMO–LUMO distributions correlate well with the calculated global reactivity descriptors and MEP analysis. The observed high EHOMO and low energy gap (ΔE) values for the investigated multi-substituted pyridazine molecules indicate a strong tendency to donate electrons to the vacant d-orbitals of the metal surface, which aligns perfectly with recent literature reports on diazine-based corrosion inhibitors.^{32,33}

In summary, compound **2** is the most stable (hard) according to HOMO-LUMO values. In this compound, the HOMO-LUMO distance is the widest ($\Delta E=7.12$ eV), therefore electron transfer ($\Delta N=0.224$) is the most difficult. Compound **5** is the most reactive (soft). The gap is the narrowest ($\Delta E=3.95$ eV) and its ΔN value (0.611) is the highest. This compound reacts most readily.

Molecules exhibiting broader HOMO delocalization and better HOMO–LUMO overlap show lower energy gaps, higher global softness, and larger electron transfer fractions (ΔN), which collectively enhance adsorption strength and corrosion inhibition performance.³⁴

The calculated quantum chemical descriptors reveal a clear structure–inhibition relationship among the investigated pyridazine derivatives. As shown in Table 1, compound **5** exhibits the highest corrosion inhibition potential, which can be attributed to its highest HOMO energy (−6.56 eV), lowest energy gap (3.95 eV), and maximum fraction of electron transfer ($\Delta N = 0.611$). These parameters indicate a strong tendency for electron donation to the iron surface and enhanced chemical reactivity, favoring chemisorption as the dominant inhibition mechanism.

Table 1. Frontier molecular orbital (FMO) parameters (eV) and reactivity descriptors of compounds **1–5**

Comp.	1	2	3	4	5
E_{HOMO}	−7.8996	−8.9636	−6.8547	−8.4439	−6.5608
E_{LUMO}	−1.1211	−1.8449	−0.5361	−2.4681	−2.6096
ΔE	6.7785	7.1187	6.3186	5.9758	3.9512
I	7.8996	8.9636	6.8547	8.4439	6.5608
A	1.1211	1.8449	0.5361	2.4681	2.6096
χ	4.5104	5.4043	3.6954	5.4560	4.5852
η	3.3893	3.5594	3.1593	2.9879	1.9756
S	0.1475	0.1404	0.1583	0.1673	0.2531
ω	3.0000	4.1000	2.1600	4.9800	5.3200
ΔN	0.3670	0.2240	0.5230	0.2580	0.6110
ΔE_{back}	−0.8470	−0.8900	−0.7900	−0.7470	−0.4940

Compound **3** also demonstrates notable inhibition performance, characterized by a relatively high HOMO energy and a large ΔN value (0.523), suggesting efficient charge transfer from the inhibitor molecule to the metal surface. In contrast, compounds **1** and **4** exhibit moderate inhibition efficiencies. Although compound **4** shows a smaller energy gap than compound **1**, its lower ΔN value indicates a weaker electron-donating ability toward the metal surface, resulting in reduced inhibition effectiveness.

Compound **2** displays the lowest inhibition performance among the studied molecules. Its highly negative HOMO energy and the largest HOMO–LUMO gap (7.12 eV) reflect low molecular reactivity and limited charge transfer capability. Additionally, the smallest ΔN value (0.224) suggests weak adsorption interaction with the iron surface.

The relationship between the electrophilicity index (ω) and the global reactivity descriptors, namely chemical hardness (η) and global softness (S), was systematically analyzed to elucidate the electronic factors governing the inhibition behavior of the investigated compounds. According to conceptual density functional theory, the electrophilicity index is defined as $\omega = \frac{\mu^2}{2\eta} = \frac{\chi^2}{2\eta}$, which inherently suggests an inverse dependence of ω on η and a direct dependence on S (where $S = \left(\frac{1}{2\eta}\right)$).

As illustrated by the ω – η correlation, an inverse trend is observed, indicating that compounds with lower chemical hardness exhibit higher electrophilicity. This behavior reflects an enhanced ability of softer molecules to undergo charge redistribution upon interaction with the metal surface. In particular, the compound exhibiting the lowest η value also shows the highest ω value, highlighting its increased reactivity and stronger tendency to accept electronic charge.

Conversely, the ω – S correlation demonstrates a positive relationship between the electrophilicity index and global softness. The increase in ω with increasing S confirms that molecular softness plays a crucial role in enhancing the electrophilic character of the inhibitors. Softer molecules, characterized by higher S values, facilitate charge transfer interactions more effectively, thereby promoting stronger adsorption onto the metal surface.³⁵

Overall, these correlations are fully consistent with the principles of conceptual DFT and clearly indicate that molecules with high electrophilicity and softness, combined with low chemical hardness, are more

favorable for charge transfer interactions. Consequently, such electronic characteristics are expected to contribute significantly to improved inhibition performance.³⁵

Molecular electrostatic potential (MEP) maps (Figure 3) were used to visualize the charge distribution and to identify the most probable adsorption sites of the investigated pyridazine derivatives on iron surfaces. In the MEP representations, regions of negative electrostatic potential (red–yellow) correspond to electron-rich centers capable of donating electrons to the vacant d-orbitals of the metal, whereas positive regions (blue) indicate electron-deficient sites.

The MEP map shows moderate negative potential regions mainly localized around the pyridazine nitrogen atoms and the conjugated ring system. The negative potential is relatively localized rather than broadly delocalized, indicating moderate electron-donating capability, consistent with its intermediate inhibition performance for compound **1**. Compared to the other molecules, compound **2** exhibits less intense and more localized negative potential regions. The predominance of electron-withdrawing substituents reduces the overall electron density available for donation. This MEP pattern supports weaker adsorption tendency and correlates well with its lowest inhibition efficiency among the studied compounds.

The MEP surface of compound **3** displays pronounced negative potential regions distributed over the heterocyclic nitrogen atoms and adjacent π -systems. The relatively broader distribution of electron-rich regions suggests enhanced charge donation and stronger surface interaction, in agreement with its high ΔN value and good inhibition performance.

For compound **4**, negative electrostatic potential regions are present around the heteroatoms; however, their intensity and spatial extension are moderate compared to compounds **3** and **5**. This indicates a balanced but not dominant electron-donating behavior, explaining its moderate inhibition efficiency. Compound **5** exhibits the most intense and widely distributed negative electrostatic potential regions among all investigated molecules. The strong delocalization of electron density over the pyridazine ring and substituent groups provides multiple active adsorption centers, favoring strong chemisorption on the iron surface. This MEP behavior is fully consistent with its lowest energy gap, highest global softness, and largest fraction of electron transfer, confirming compound **5** as the most efficient corrosion inhibitor in this series.

The qualitative MEP trends closely correlate with the frontier molecular orbital and global reactivity descriptor analyses. Molecules displaying stronger and more delocalized negative MEP regions also show higher EHOMO values, lower ΔE , and larger ΔN values, indicating enhanced electron donation to the metal surface. Conversely, weak or localized negative potential regions correspond to reduced charge transfer capability and lower inhibition efficiency.

Overall, the MEP analysis supports a mixed adsorption mechanism, where electrostatic interactions (physisorption) facilitate initial adsorption, followed by coordinate bond formation (chemisorption) between electron-rich sites of the inhibitor molecules and iron d-orbitals. The combined MEP and DFT descriptor results reinforce the inhibition efficiency order: **5** > **3** > **1** > **4** > **2**. Similar theoretical parameters indicating that enhanced surface coverage and high electron-donating capability lead to superior protection in aggressive acid environments have been widely demonstrated in recent computational studies.^{36,37}

The electronic structure of compound **5** was further analyzed by means of density of states (DOS)³⁸ calculations in order to gain deeper insight into its reactivity and inhibition behavior. The DOS spectrum reveals the distribution of electronic states as a function of energy and provides valuable information regarding the contribution of molecular orbitals near the Fermi level (Figure 5).

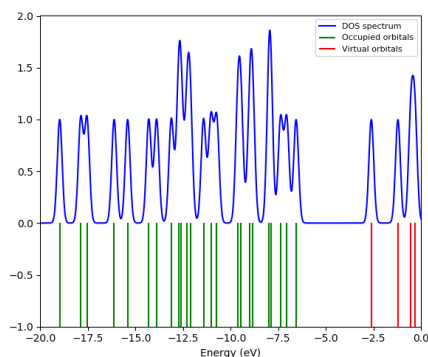


Figure 5. Density of states (DOS) spectrum of compound **5**.

As shown in the DOS profile, a significant contribution of electronic states is observed in the vicinity of the Fermi level. This feature indicates an enhanced availability of frontier orbitals capable of participating in charge transfer interactions. In particular, the pronounced density near the Fermi energy suggests that compound **5** can effectively interact with the metal surface through electron

donation and back-donation mechanisms, which are essential for strong adsorption.

The dominant contribution of the frontier molecular orbitals around the Fermi level is mainly associated with the heteroatom-containing functional groups of the molecule. These regions act as active adsorption centers, facilitating electron exchange between the inhibitor and the metal surface. The overlap of occupied and unoccupied states near the Fermi level further supports the high reactivity of compound **5** and its tendency to form stable adsorption configurations.

Moreover, the relatively narrow energy gap between the occupied and unoccupied states observed in the DOS spectrum is consistent with the low HOMO–LUMO energy gap obtained from quantum chemical calculations. This reduced gap reflects higher molecular polarizability and softness, which correlates well with the high electrophilicity index (ω) and global softness (S) values previously discussed. Consequently, the DOS results reinforce the conclusion that compound **5** exhibits superior charge transfer capability.

Overall, the DOS analysis clearly confirms that compound **5** possesses favorable electronic characteristics for corrosion inhibition. The high density of states around the Fermi level, combined with its enhanced electrophilic nature and molecular softness, indicates strong metal–inhibitor interactions and supports its superior inhibition performance compared to the other investigated compounds.

The relationship between the density of states (DOS) features and the inhibition efficiency provides direct insight into the electronic origin of the corrosion inhibition performance. Higher inhibition efficiency is generally associated with an increased density of electronic states in the vicinity of the Fermi level, as this facilitates efficient charge transfer interactions between the inhibitor and the metal surface. In this context, compound **5**, which exhibits a pronounced DOS near the Fermi energy, demonstrates an enhanced ability to donate and accept electrons, leading to stronger adsorption and higher surface coverage. The elevated DOS around the Fermi level promotes both electron donation from the inhibitor to the vacant metal d-orbitals and back-donation from the metal to the antibonding orbitals of the inhibitor. This synergistic charge transfer mechanism stabilizes the adsorbed layer and directly contributes to an increase in inhibition efficiency. Furthermore, the reduced energy gap reflected in the DOS profile supports greater molecular polarizability and softness, which are known

to enhance adsorption strength and inhibition performance.

Overall, the DOS results clearly indicate that compounds with higher electronic density near the Fermi level are capable of forming more stable and effective adsorption films on the metal surface, thereby exhibiting higher inhibition efficiency. This direct correlation between DOS features and inhibition efficiency confirms that the superior inhibition performance of compound **5** originates from its favorable electronic structure and enhanced charge transfer capability.

Although purely theoretical descriptors possess inherent limitations in replication of complex electrochemical environments, they serve as highly reliable screening and predictive tools to establish baseline structure-inhibition relationships before rigorous experimental validation.

DISCUSSION

This study provides a systematic DFT-based investigation of pyridazine derivatives as corrosion inhibitors. The results demonstrate that inhibition efficiency is strongly influenced by electronic properties such as HOMO energy, energy gap, and electron transfer capability.

Among the studied compounds, compound **5** exhibits superior inhibition performance due to its favorable electronic structure, including high softness and strong charge transfer ability. The combined analysis of frontier orbitals, global descriptors, MEP, and DOS confirms that multiple electronic factors collectively determine inhibition behavior.

Importantly, the findings highlight that no single descriptor is sufficient to predict inhibition efficiency, and a multi-parameter approach is necessary. This work provides a theoretical basis for the rational design of effective corrosion inhibitors and offers guidance for future experimental validation studies.

In conclusion, although purely theoretical quantum chemical descriptors possess inherent limitations in fully replicating complex electrochemical and dynamic industrial environments, the framework established in this study proves that DFT calculations serve as highly reliable, cost-effective screening and predictive tools to establish baseline structure-inhibition relationships before undergoing rigorous experimental validation.

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Taraması, Yazıyı Yazan, Eleştirel İnceleme; Begum Cagla Akbas: Fikir, Tasarım, Denetleme, Kaynaklar, Veri Toplanması ve/veya İşlemesi, Analiz ve/veya Yorum, Literatür Taraması, Yazıyı Yazan, Eleştirel İnceleme.

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