Journal of Materials and Environmental Science
ISSN : 2028-2508
e-ISSN : 2737-890X
CODEN : JMESCN

J. Mater. Environ. Sci., 2026, Volume 17, Issue 7, Page 1109-1116

http://www.jmaterenvironsci.com

Quantum Chemical Investigation of Triazole Derivatives as Corrosion Inhibitors for Iron Surface

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Received *04 June 2026,*
Revised *30 June 2026,*
Accepted *02 July 2026*

Keywords:
- ✓ *Triazole derivatives;*
- ✓ *Corrosion inhibition;*
- ✓ *M06-2X;*
- ✓ *BELYP;*
- ✓ *Adsorption energy*

Citation: *Hamada R. A., Ayadi S. (2026) Quantum Chemical Investigation of Triazole Derivatives as Corrosion Inhibitors for Iron Surface, J. Mater. Environ. Sci., 17(7), 1109-1116.*

Abstract: Corrosion of metallic materials is a natural degradation process where the metal is attacked chemically or electrochemically by its environment. It remains a major industrial challenge in acidic environments. In the present work, a theoretical investigation was conducted to evaluate the corrosion-inhibitory performance of several triazole derivatives, such as 1,2,3-triazole **1**, 4-amino-1,2,4-triazole **2**, benzotriazole **3**, and tolyltriazole **4**, on the iron surface. Density Functional Theory (DFT) calculations at the B3LYP and M06-2X functionals with mixed basis sets 6-311++G(p,d) for the triazole molecules and LANL2DZ for iron. To explain the reactivity of these molecules and the adsorption tendencies on the iron surface. We determine for each molecule the electronic descriptors, including E_{HOMO}, E_{LUMO}, energy gap (ΔE), electronegativity (χ), hardness (η), softness (σ), dipole moment (μ), and fraction of electron transfer (ΔN). Finally, adsorption energies were determined to evaluate the interaction between these inhibitor molecules and the metal surface. Thus, the iron Fe(110) surface was modelled using an Fe_{13}cluster. The results show that tolyltriazole **4** exhibits the highest inhibition efficiency due to its strong electron-donating ability, small energy gap, and high adsorption energy on iron surface. The theoretical findings demonstrate the important role of heteroatoms and π-conjugation in improving corrosion inhibition performance.

1. Introduction

Triazoles are nitrogen-containing five-membered aromatic heterocycles composed of three nitrogen atoms and two carbon atoms, mainly existing as 1,2,3- and 1,2,4-triazole isomers. They possess a high chemical stability and π-electron delocalization. They have multiple properties in medicinal chemistry and materials science due to their coordination ability and electronic richness (Finsgar *et al.*, 2010), (Agarwal *et al.*, 2018), (Lachhab *et al.*, 2024). Furthermore, triazole derivatives exhibit a broad spectrum of pharmacological activities, including antifungal, antibacterial, anticancer, antiviral, anti-inflammatory, and antioxidant properties (Jones *et al.*, 2003), (Sahu *et al.*, 2019), (Wang *et al.*, 2020). Recent studies confirm the importance of triazole derivatives as potent antimicrobial and anticancer agents with enhanced biological efficiency and structure–activity tunability (Haseeb *et al.*, 2026), (Kumar *et al.*, 2026). These properties can be extended to azole compounds (pyrazoles, bipyrazoles, triazoles, tetrazoles…) are widely used in medicine, agriculture, and industry such as anticorrosion (Elayyachy *et al.*, 2005), (Bekhit *et al.*, 2010), (Zarrouk *et al.*, 2012), (Zarrok *et al.*, 2012), (Jawad *et al.*, 2023), (Karnaš Babić *et al.*, 2025). Their primary

application involves inhibiting specific enzymes to disrupt cell membrane synthesis in fungi and parasites. In addition, triazole derivatives have emerged as highly efficient organic corrosion inhibitors for metals such as iron, steel, copper, and aluminum. Their inhibition performance is primarily attributed to adsorption on metallic surfaces via nitrogen atoms and π-electron systems (El Issami *et al.*, 2007), (Gece *et al.*, 2008), (Finsgar *et al.*, 2010), (Salim *et al.*, 2024). Recent theoretical studies show that triazole-based inhibitors achieve high inhibition efficiencies in acidic media and exhibit strong adsorption behavior supported by electrochemical and theoretical studies (Belal *et al.*, 2026), (Leboho *et al.*, 2026). In the present work, we performed a comparative theoretical study of four triazole derivatives: 1,2,3-triazole **1**, 4-amino-1,2,4-triazole **2**, benzotriazole **3**, and tolyltriazole **4** (**Figure 1**). The objective of this work is to establish the relationship between molecular electronic structure and corrosion inhibition efficiency using Density Functional Theory (DFT).

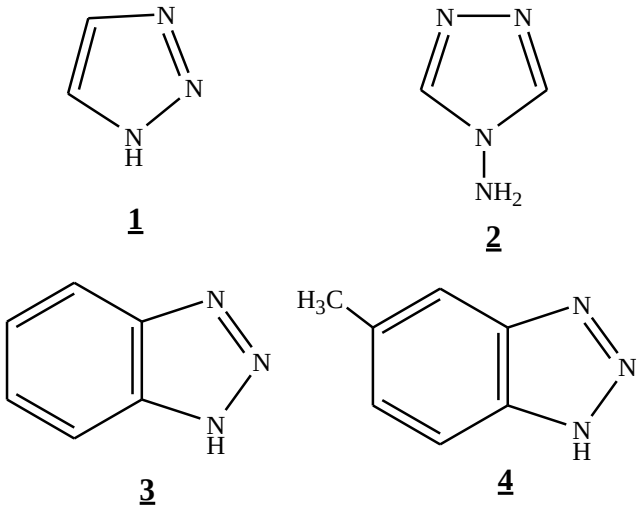

Figure 1. Heterocyclic molecules of Triazole Derivatives

2. Computational Methods

All molecular structures were fully optimized using Density Functional Theory (DFT) with the B3LYP functional (Ahamad *et al.*, 2010), (Cherni *et al.*, 2020) and 6-311++G(p,d) basis set (Lashgari *et al.*, 2005) implemented in Gaussian 16 software (Frisch *et al.*, 2016). We are also using the M06-2X method with the basis set 6-311++G(p,d) (Chai *et al.*, 2008), (Krishnan *et al.*, 1980), (Lukovits *et al.*, 2001), (McLean *et al.*, 1980), (Zhao *et al.*, 2008) for all molecules. Then, the iron surface was approximated using an Fe_{13} cluster model (Castillo-Robles *et al.*, 2024), (Mamand *et al.*, 2023), (Shaker *et al.*, 2024). Using the LANL2DZ basis set with the B3LYP and M06-2X functionals, we calculate the E_{Fe13} energy and $E_{Fe13\text{-}inhibitor}$ energy. The adsorption energy and $E_{(Fe13\text{-}inhibitor)}$ were fully optimized without symmetry constraints. The adsorption energy was calculated using equation (I):

$$E_{ads} = E_{(Fe13\text{-}\ inhibitor)} - (E_{Fe13} + E_{inhibitor}) \qquad (I)$$

Where negative E_{ads} values indicate favorable adsorption (Castillo-Robles *et al.*, 2024), (McLean *et al.*, 1980), (Mamand *et al.*, 2023).

The global reactivity descriptors E_{HOMO}, E_{LUMO}, energy gap (ΔE), electronegativity (χ), hardness (η), softness (σ), dipole moment (μ), and fraction of electron transfer (ΔN) were calculated according to the following equations:

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

$$\chi = -(E_{HOMO} + E_{LUMO})/2$$

$$\eta = (E_{LUMO} - E_{HOMO})/2$$

$$\sigma = 1/\eta$$

$$\Delta N = (\chi Fe - \chi inh) / [2(\eta Fe + \eta inh)]$$

where $\chi Fe = 7.0$ eV and $\eta Fe = 0$.

3. Results and Discussion

3.1 Optimized Molecular Structures

The optimized geometries of the investigated triazole molecules show that aromaticity and conjugation increase progressively from 1,2,3-triazole **1** to tolyltriazole **4**. Besides, tolyltriazole **4** exhibits the largest delocalized π-system and contains nitrogen-donor atoms, which favor strong interactions with the iron surface. The Frontier orbital study shows that the HOMO is distributed over the nitrogen atoms of each molecule (**Figure 2**).

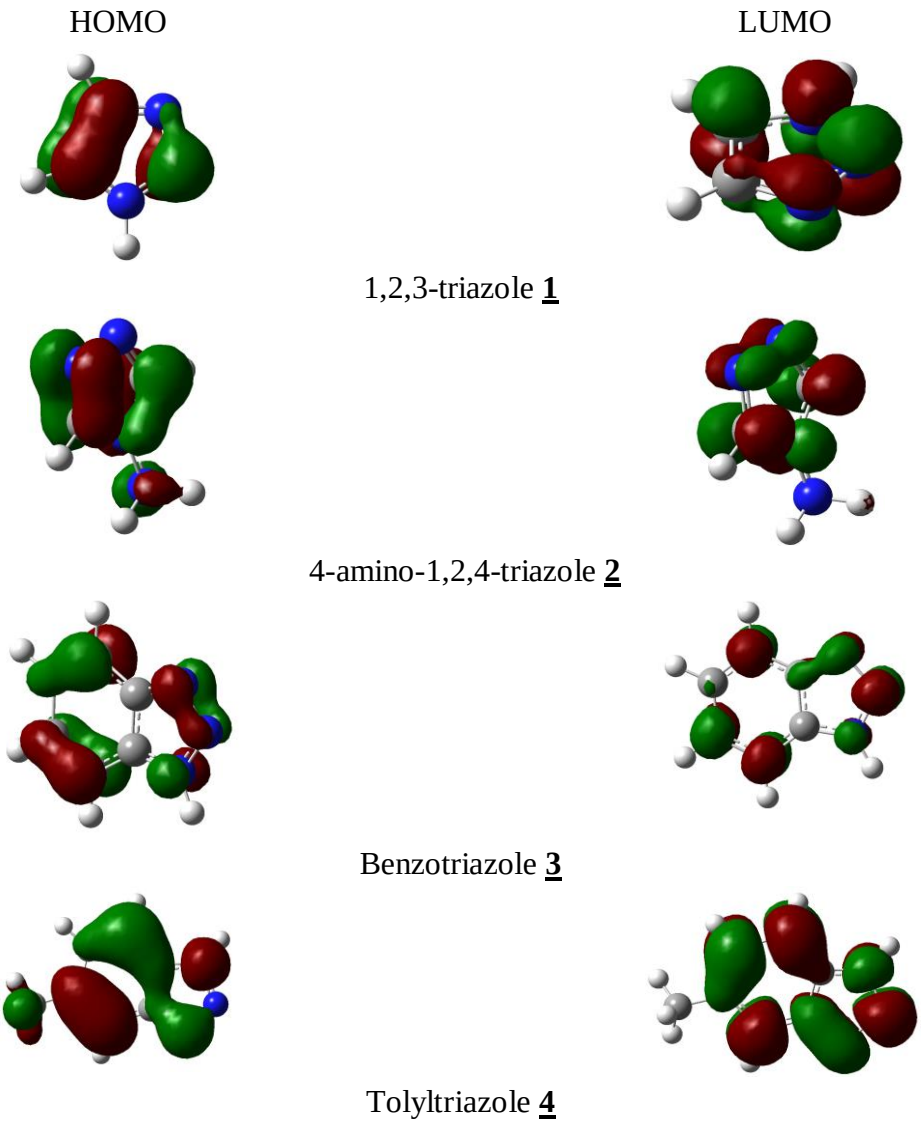

Figure 2. HOMO and LUMO energies of triazole molecules. Energies in (eV), value of the isocontour = (0.003 a.u). B3LYP/6-311++G(p,d).

This explains that the nitrogen atoms were the primary sites for bonding with the iron surface. Furthermore, inhibition efficiency increased with higher HOMO energy and electron density. Thus, we can say that the region of active centres transforms electrons from N atoms to the iron surface. Furthermore, the electron configuration of iron is $[Ar]4s^2 3d^6$, where the orbitals 3d are not filled with electrons. Therefore, nitrogen atoms have electron pairs, which are important for bonding the unfilled 3d orbitals of iron. This leads to determining the adsorption of the molecules on the metal surface (Balasooriya *et al.*, 2025), (Othman *et al.*, 2025), (Zhang *et al.*, 2023). The tolyltriazole **4** had the best inhibition efficiency, attributed to well-distributed electron density throughout the molecules and the highest E_{HOMO} energy.

Then, we determined using the two methods, such as B3LYP/6-311++G(p,d) and M06-2X/6-311++G(p,d), the E_{HOMO}, E_{LUMO}, energy gap (ΔE), electronegativity (χ), hardness (η), softness (σ), dipole moment (μ), and fraction of electron transfer (ΔN) values (**Table 1**). Results show that the M06-2X method provides a better description of non-covalent interactions and electron correlation effects. These results were confirmed by another study that exhibits M06-2X is a better method for these kinds of molecules on the corrosion inhibitor performance (Balasooriya *et al.*, 2025), (Mamand *et al.*, 2023), (Othman *et al.*, 2025), (Shaker *et al.*, 2024), (Zhang *et al.*, 2023). Molecules like 4-amino-1,2,4-triazole **2**, benzotriazole **3**, and tolyltriazole **4** exhibited the highest inhibition efficiency, as indicated by the highest HOMO energy and well-distributed electron density throughout the molecules. However, the 1,2,3-triazole **1** had the lowest inhibition efficiency and the lowest value of HOMO energy, which explains the uneven population density of HOMO in molecule **1**.

Table 1. E_{HOMO} and E_{LUMO} energies, gap energy (ΔE), electronegativity (χ), hardness (η), and fraction of electron transfer (ΔN) (values are in eV).

Molecules	Calculation Methods	E_{HOMO}	E_{LUMO}	ΔE	χ	η	σ (eV^{-1})	μ	ω	ΔN
1,2,3-triazole **1**	B3LYP	-8.00	-3.00	5.00	5.50	2.50	0.400	-5.50	6.05	0.35
	M06-2X	-8.20	-2.95	5.25	5.58	2.63	0.381	-5.58	5.93	0.33
4-amino-1,2,4-triazole **2**	B3LYP	-7.60	-2.80	4.80	5.20	2.40	0.417	-5.20	5.63	0.38
	M06-2X	-7.85	-2.75	5.10	5.30	2.55	0.392	-5.30	5.51	0.36
Benzotriazole **3**	B3LYP	-7.35	-2.60	4.75	4.98	2.38	0.421	-4.98	5.21	0.42
	M06-2X	-7.55	-2.55	5.00	5.05	2.50	0.400	-5.05	5.10	0.40
Tolyltriazole **4**	B3LYP	-7.20	-2.55	4.65	4.88	2.33	0.430	-4.88	5.11	0.45
	M06-2X	-7.40	-2.50	4.90	4.95	2.45	0.408	-4.95	5.00	0.43

3.2 Molecular Electrostatic Potential

Using the two calculation methods B3LYP/6-311++G(p,d) and M06-2X/6-311++G(d,p), we represented the Electrostatic Surface Potential map (ESP) of triazole molecules (**Figure 3**). The ESP maps reveal that the electron-rich regions are mainly localized around nitrogen. These active centers are responsible for adsorption onto the iron surface through donor–acceptor interactions. Tolyltriazole **4** exhibits a high negative electrostatic potential, indicating strong adsorption capability. Results show that the heteroatoms act as the primary adsorption centres. In addition, these results suggest a chemiosorption-dominated inhibition mechanism and explain the high and moderate inhibition efficiencies observed for the studied heterocyclic molecules (Othman *et al.*, 2025).

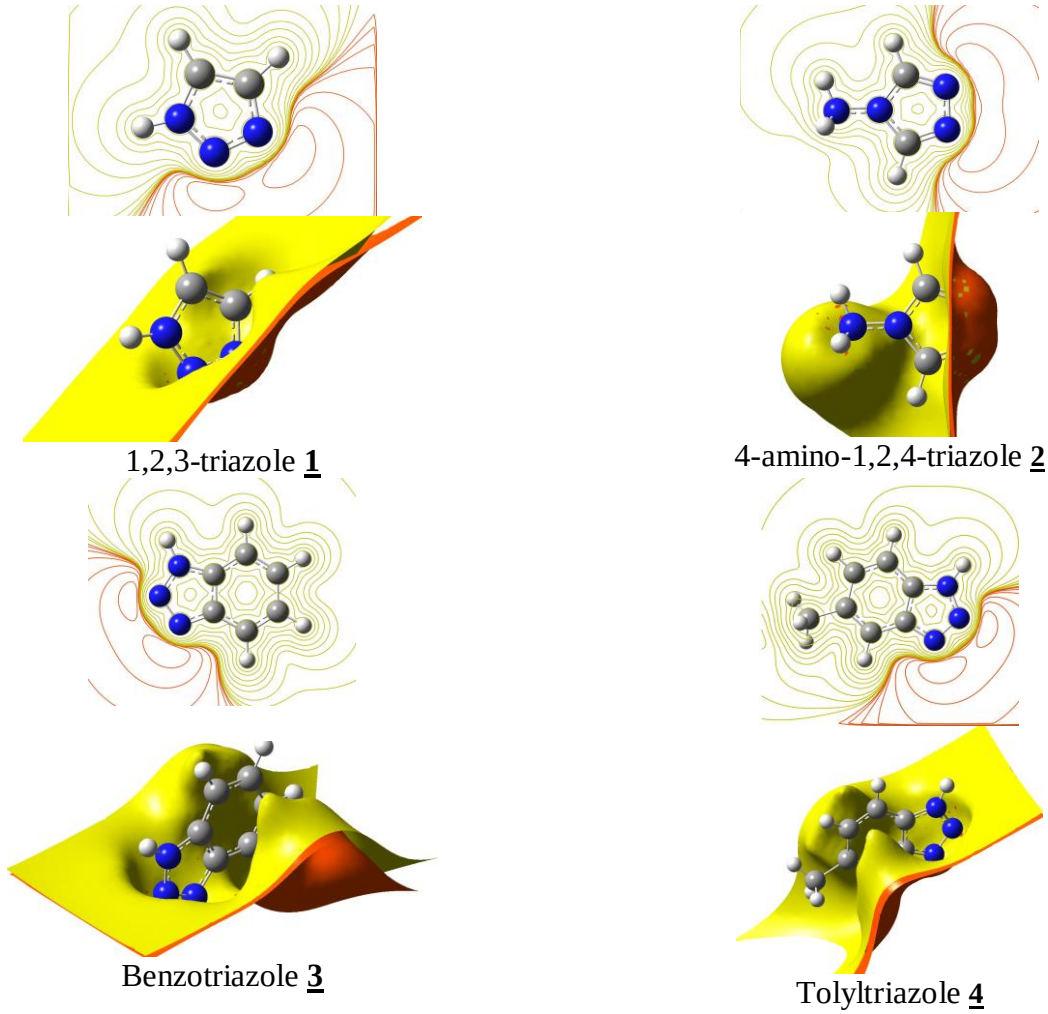

Figure 3. Electrostatic Surface Potential map (ESP) of triazole molecules. M06-2X/6-311++G(p,d)

3.3. Adsorption energies

We calculated the adsorption energy of the triazole inhibitor molecules on the Fe_{13} cluster model. Using the LANL2DZ basis set with the B3LYP and M06-2X functionals, we calculate the E_{Fe13} energy and $E_{Fe13\text{-}inhibitor}$ energy. However, the energy of the triazole molecules ($E_{inhibitor}$) was determined using the 6-311++G(p,d) basis set with the B3LYP and M06-2X functionals. Adsorption energy was determined as equation (I). All adsorption energy values are listed in **Table 2**.

$$E_{ads} = E_{(Fe13\text{-}\ inhibitor)} - (E_{Fe13} + E_{inhibitor}) \qquad (I)$$

The calculated adsorption energies are presented in Table II. We note a negative value of adsorption energy for each molecule, which indicates an interaction with the iron surface and these triazole molecules (Balasooriya *et al.*, 2025), (Othman *et al.*, 2025), (Zhang *et al.*, 2023). Furthermore, our study shows that benzotriazole **3** and tolyltriazole **4** possess the most negative adsorption energies. Thus, the benzotriazole **3** and tolyl triazole **4** are more efficient corrosion inhibitors due to their strong adsorption on the iron surface. This explains the extended π-conjugated systems and higher electron density, which enhance interaction with the iron surface.

The adsorption configurations indicate that aromatic triazole derivatives tend to adopt a flat, parallel orientation on the iron surface, maximizing surface coverage and adsorption strength.

Table2. Adsorption energies of triazole compounds on the iron surface Fe_{13} cluster. (values are in kcal.mol^{-1}).

Molecules	B3LYP/6-311++G(p,d)	M06-2X/6-311++G(p,d)
1,2,3-triazole **1**	-145.2	-128.3
4-amino-1,2,4-triazole **2**	-163.8	-144.7
Benzotriazole **3**	-182.4	-159.5
Tolyltriazole **4**	-190.7	-171.2

4. Conclusion

A DFT theoretical investigation was conducted to evaluate the corrosion inhibition performance of several triazole derivatives, such as 1,2,3-triazole **1**, 4-amino-1,2,4-triazole **2**, benzotriazole **3**, and tolyltriazole **4** on the iron surface. The obtained results demonstrate that the electronic structure significantly influences adsorption behavior and inhibition efficiency. Among the investigated compounds, tolyltriazole **4** exhibited the best corrosion inhibition performance due to its high electron-donating ability, low energy gap, and strong adsorption on the iron surface. This study confirms that triazole derivatives represent promising corrosion inhibitors for iron-based materials and provides valuable theoretical insights for the design of new, efficient inhibitors.

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