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Theoretical Investigation about Inhibition Performance of Acyclovir (ACV) Molecule on Corrosion of Fe (1 1 0) Surface in Acidic Medium: DFT, MC, Toxicity and Solubility Analyses

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ABSTRACT

In the present paper, mechanistic insights for the corrosion inhibition efficiency of a drug, namely 2-amino-9-[(2-hydroxyethoxy) methyl]-6,9-dihydro-1H-purin-6-one (Acyclovir) for Fe (1 1 0) surface in acidic medium are reported by means of Density Functional Theory and Molecular Dynamic Simulation calculations. Intercalarily, some useful information about toxicity and solubility of the mentioned chemical system is presented. For Acyclovir, many popular global and local reactivity descriptors of Conceptual DFT were calculated for the studied molecule, and how these parameters affect the inhibition efficiency of the molecule was discussed in detail. The calculations of the parameters were done via B3lyp/SVP, CAM-B3lyp/TZVP and ωB97XD/Def2-TZVP calculation level in both gas phase and aqueous media. Adsorption behaviors of the mentioned molecule on Fe (1 1 0) surface was checked with the help of Monte Carlo (MC) simulation approach. The results of both DFT and MC approaches are in good agreement with the experimental results reported previously in the literature. Also, the reactivity of the molecule was evaluated in terms of well-known electronic structure principles such as Maximum Hardness and Minimum Electrophilicity Principles. In terms of toxicity, the ACV molecule having log IGC50 value of 0.91 mmol/L exhibits good solubility and the highly negative calculated adsorption energy value for the interaction between Fe (1 1 0) surface and ACV implies the good inhibition performance of this molecule.

Keywords: Acyclovir, DFT, MDS,Corrosion, Toxicity.

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Introduction

Corrosion can be simply defined as the wearing away and deterioration of metals by the influence of environmental conditions or by reaction with environmental components [1,2]. Corrosion is among the factors that negatively affect the costs of industrial investments and production activities. Safe and high-efficiency work can only be achieved by taking the necessary precautions against corrosion. Interest in experimental and theoretical studies involving the design and synthesis of cheap and effective inhibitor molecules for the protection of metals from corrosion is increasing day by day. It has been frequently reported that organic molecules containing electron-donating atoms such as nitrogen, sulfur, oxygen, conjugated pi bonds, and electron-donating functional groups interact strongly with metal surfaces because of electron transfer between inhibitor and metal and significantly prevent corrosion [3,4]. In this field, researchers, in parallel with experimental studies, present studies on the design and development of effective inhibitors with quantum chemical calculations and molecular dynamics simulation-based analyses to the literature [5,6].

Acyclovir (ACV), one of the purine derivatives, has been reported as a drug frequently used in the effective treatment of varicella zoster and herpes simplex infections. In addition to studies proving that purine derivatives exhibit high biological activity against various biological systems, studies proving that this group of molecules is an effective corrosion inhibitor are frequently encountered in the literature [7,8]. In the experimental study conducted by C. Verma et al. [9], acyclovir was reported to be a good inhibitor against the corrosion of mild steel in 1 M HCl solution. Another study penned by Abdallah and coworkers [10] tested the corrosion inhibition efficiency against Sabic iron corrosion of Acyclovir (ACV) and Omeprazole (OMP) drugs with required comparisons made through weight loss, electrochemical impedance and polarization measurements. In our previously published paper [11], we theoretically investigated the corrosion inhibition efficiency of omeprazole and tinidazole drugs presenting required mechanistic insights and with the help of B3lyp/SVP, CAM-B3lyp/TZVP and ωB97XD/Def2-TZVP computation levels of the theory. In a recent study including experimental and theoretical insights, Zhang and coworkers [12] analyzed the inhibitive performance of two purine derivatives (FAP and N-BAP) for mild steel corrosion and proved high inhibition efficiency of the mentioned molecules in acidic medium.

This study includes important explanations about the reactivity, toxicity and solubility of Acv, a purine derivative, while the interaction modes of the mentioned molecule with the Fe (110) surface will be given through MDS simulations. In the highlighting of the chemical reactivity, the popular parameters and principles of the Conceptual DFT will be considered. The main scope of this article is to present nontoxic and highly soluble nature of ACV molecule in addition its high inhibition performance against the corrosion of Fe (110) surface. Additionally, the results obtained will be compared with the results of previously published theoretical papers about the studied molecule.

Computational Details and Equations Used in DFT Studies

In the present study, all computational studies were performed with the help of Density Functional Theory (DFT) methods having GD3 corrections. The optimizations of the structures were made through B3LYP [24], CAM-B3LYP and ωB97XD methods and valance polarization (SVP), triple-ζ valance polarization (TZVP) and valance triple-ζ polarization (def2-TZVP) basis sets. In such studies, basis sets and functionals that provide more accurate results with the approaches they contain should be used to reliably analyze the reactivity of the studied molecule. The reason of the selecting of three different calculation level showing this property is to compare the results obtained via different levels of the calculation. To see the solvent effect, polarizable continuum model (PCM) [30] was preferred. In the solvent-based calculations, the dielectric constant of ε = 78.36 and a refractive index of n = 1.33 were used. Geometry optimizations were performed using equilibrium solvation for the respective state (S_0). To check the stability of the optimized structures, frequency computations were made. All calculations were made via the Gaussian09 program suite. Conceptual Density Functional Theory (CDFT) is one of the most popular theoretical tools selected for corrosion inhibition studies. This theory presents the following mathematical relations for the parameters like chemical potential (μ), electronegativity (χ), hardness (η) and softness (σ) [13].

$$\mu = -\chi = \left[\frac{\partial E}{\partial N}\right]_{v(r)} \tag{1}$$

$$\eta = \left[\frac{\partial^2 E}{\partial N^2}\right]_{v(r)} \tag{2}$$

$$\sigma = 1/\eta \tag{3}$$

By means of the finite differences method, the aforegiven mathematical relations including the total electronic energy (E) and total number of the electrons (N) of the studied chemical systems turn into ionization energy (I) and electron affinity (A) based equations as [14].

$$\mu = -\chi = -\left(\frac{I+A}{2}\right) \tag{4}$$

$$\eta = I - A \tag{5}$$

Electrophilicity index (ω) is one of the most used parameters to highlight the organic reaction mechanisms. Parr's electrophilicity index [15] (or first electrophilicity index) (ω_1), second electrophilicity index (ω_2) and net electrophilicity ($\omega^{\pm}$) of a molecular chemical system are calculated as [16,17]:

$$\omega_1 \equiv \frac{\chi^2}{2\eta} \tag{6}$$

$$\omega_2 = I.A/I - A \tag{7}$$

$$\Delta\omega^{\pm} = \omega^{+} - (-\omega^{-}) = \omega^{+} + \omega^{-} \tag{8}$$

In this study, to predict the ionization energy and electron affinity of Acv molecule, we considered Koopmans Theorem [18] giving the relations $I=-E_{HOMO}$ and $A=-E_{LUMO}$, where E_{HOMO} and E_{LUMO} are the energies of HOMO and LUMO orbitals, respectively.

The Fukui function at a point, r, in the space around the molecule is mathematically presented as the first derivative with respect to the number of electron density at a constant external potential.

$$f(r) = \left(\frac{\partial \rho(r)}{\partial N}\right)_{v} = \left(\frac{\partial \mu}{\partial v(r)}\right)_{N} \tag{9}$$

Using Eq. 9, one can write the Fukui indices for nucleophilic (+) and electrophilic (-) attacks as:

$$f^{+}(r) = \left(\frac{\partial \rho(r)}{\partial N}\right)_{v}^{+} \tag{10}$$

$$f^{-}(r) = \left(\frac{\partial \rho(r)}{\partial N}\right)_{v}^{-} \tag{11}$$

As is known, Fukui functions [19] are often preferred in the analysis of which regions or atoms a molecule uses for nucleophilic, electrophilic and radical attacks when interacting with another system. The Fukui functions for nucleophilic, electrophilic and radical attacks are calculated as follows, respectively, where q_k represents the charge on atom k in the molecule.

$$f_k^{+} = q_k(N+1) - q_k(N) \quad (12)$$

$$f_k^{-} = q_k(N) - q_k(N-1) \quad (13)$$

$$f_k^{0} = [q_k(N+1) - q_k(N-1)]\ /2 \quad (14)$$

It should be noted that in the calculations of Fukui functions, we used Mulliken charges on atoms considering the published papers in literature.

Monte Carlo (MC) Simulation

Using Monte Carlo Simulation approach, adsorption behavior of Acv molecule on Fe (110) was checked. The mode of the interaction between Acv and Fe (110) surface was analyzed with the help of adsorption locator module of Materials Studio 2017 software [20]. Optimization of the adsorption system designed was done with Forcite module through COMPASS force field. There were three dimensions to the slab model: 19.859 Å × 19.859 Å x 14.187 with an enclosed addition of a 30 Å edge creating (12x12) supercell. In the calculation process, an inhibitor molecule, 180 water molecules, $4H_3O^+$ and 4 Cl^- ions were used. Calculations were performed at 298 Kelvin temperature (NVT) canonical ensemble with a simulation duration of 600 ps (1 fs time step). In the light of the analysis, the most stable adsorption mode of the inhibitor on Fe (110) surface and how high the adsorption energy for the interaction were determined.

Environmental Toxicity and Solubility Prediction of Acyclovir Molecule

Toxicity and solubility of the Acv molecule that its structure is given in Fig. 1 were estimated with the help of the chemical databases given in modeling environment website [21].

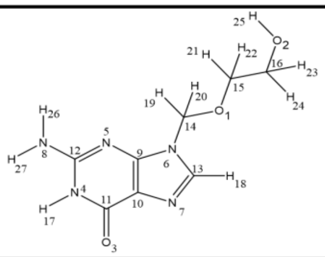
Abbreviation	Structures	Nomenclature
ACV		Acyclovir

Figure 1. Molecular structure, name and abbreviations of studied inhibitor

Results and Discussion

Toxicity and Solubility Analysis

Toxicity and solubility results obtained for ACV molecule are given in Table 1. From the values given in this table, Log (IGC50) is known as the toxic potency of the molecules to provide 50% inhibitory growth of species. This value is generally reported for like Tetrahymena pyriformis or Daphnia magna. Log P values presented for molecules imply their lipophilic character. The more negative the Log P value is, the more soluble the molecule is in water. According to calculated Log P value for ACV molecule, it can be said that this molecule has good solubility in water media. It should be noted that in the paper mentioned in the introduction part, Abdallah and coworkers experimentally studied the efficiency of ACV in hydrochloric acid solution at the concentration range between 100 ppm and 500 ppm. The IGC50 value determined for Acv molecule is less than the concentration used in experimental analysis. If so, we can say that ACV is an environmentally friendly compound at the studied concentration range

Table 1. Predicted toxicity and solubility values for ACV molecule

Inhibitor Molecule	Log (IGC50) (mmol/L)	Log P (mol/L)
ACV	0.91	-2.1

DFT Calculations

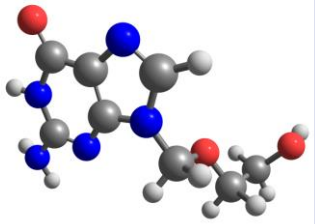
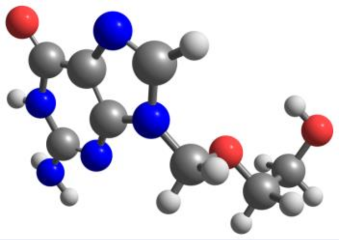
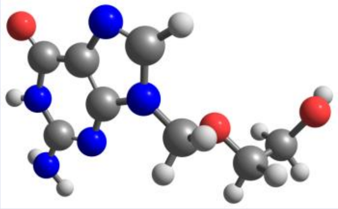
Comp	B3LYP/SVP	CAM-B3LYP/TZVP	wB97XD/def2TZVP
ACV			

Figure 2. Optimized geometries obtained in different calculation levels for ACV molecule

Figure 2. includes optimized geometries obtained at different calculation levels for ACV molecule while calculated reactivity descriptors for ACV molecule in both gas phase and aqueous phase are presented in Table 2. Chemical reactivity descriptors such as frontier orbital energies, hardness, electronegativity, first electrophilicity index, second electrophilicity index, electrodonating/accepting powers, dipole moment and polarizability obtained via Density Functional Theory calculations are widely used in the estimation of the

corrosion inhibition efficiency of the molecules [22]. HOMO and LUMO orbital energies used in chemical reactivity analysis in Molecular Orbital Theory (MOT) reflect the corrosion inhibition performances also of the molecules. The molecules with higher HOMO energies are good corrosion inhibitors because such molecules are effective electron donors. Chemical hardness concept [23] introduced by R.G. Pearson is a measure of the resistance against polarization of chemical systems. According to Maximum Hardness Principle [24], this quantity reflects the stability of the molecules. Hard molecules exhibiting high stability cannot give the electrons easily to metal surfaces and are not good corrosion inhibitors. If so, it should be noted that good corrosion inhibitors should be soft molecules with high reactivity. Considering electronegativity, it can be said that effective corrosion inhibitors should have low electronegativity.

Table 2. Calculated reactivity descriptors for ACV molecule in both gas phase and aqueous phase

	B3LYP/SVP		CAM-B3LYP/TZVP		ωB97XD/Def2-TZVP	
Parameter	**Gas**	**Water**	**Gas**	**Water**	**Gas**	**Water**
E_{HOMO} (eV)	-5.656	-5.826	-7.472	-7.518	-7.792	-7.976
E_{LUMO} (eV)	-0.244	-0.340	0.681	0.636	1.567	1.330
I	5.656	5.826	7.472	7.518	7.792	7.976
A	0.244	0.340	-0.681	-0.636	-1.567	-1.330
χ	2.950	3.083	4.077	4.077	4.680	4.653
η	5.412	5.486	6.791	6.882	6.225	6.646
ω_1	0.804	0.866	1.224	1.208	1.759	1.629
ω_2	0.255	0.361	0.749	0.695	1.961	1.596
ω^-	3.421	3.617	4.910	4.884	6.247	6.000
ω^+	0.471	0.534	0.833	0.807	1.567	1.347
Net electrophilicity	3.892	4.151	5.743	5.691	7.814	7.347
Polarizability (α.u)	128.466	163.444	136.252	177.917	139.921	183.825
Dipole moment (Debye)	11.421	7.848	10.931	8.220	12.127	11.421

Especially, the electronegativity and chemical hardness values determined for ACV molecule in B3LYP/SVP level is smaller than the data obtained via CAM-B3LYP/TZVP and ωB97XD/Def2-TZVP levels. Polarizability is a property minimized in stable states [25]. If so, a good corrosion inhibitor should have high polarizability. Noting that the dipole moment is a measure of the polarizability of molecules, some researchers proved that the molecules with high dipole moment are good corrosion inhibitors. Both calculated polarizability and calculated dipole moment support that ACV is an effective corrosion inhibitor as reported by Abdallah and coworkers [10].

As given in computational details section, net electrophilicity is the sum of electrodonating power (ω^-) and electroaccepting power (ω^+) of the molecules. For the calculating of ω^- and ω^+, we used the following equations derived by Gazquez and coworkers [26].

$$\omega^- = (3I + A)^2/(16(I - A)) \tag{15}$$

$$\omega^+ = (I + 3A)^2/(16(I - A)) \tag{16}$$

Electrodonating power reflects the electron donating ability of the chemical systems. It is noteworthy that the calculated values of this parameter for the Acv molecule at various computational levels are quite high.

Fukui indices can provide insight into the anti-corrosion mechanism of a compound. For example, a high positive Fukui index value (f^+) in a reactive region of a molecule indicates that the frontier electron density in that region is high, thus the potential for nucleophilic attack is high. Knowing the reactive sites can help determine which sites are most effective in inhibiting the corrosion process.

Acyclovir compound has 27 reactive sites, which are labelled from 1O to 27H. The Fukui indices of the acyclovir compound were calculated in the gas phase and in water at different calculation levels and are presented in Tables 3-5.

Table 3 shows the order of reactive sites, as determined by the Fukui indices, for the Acyclovir compound using DFT/B3LYP/SVP method both in the gas and in water. The most reactive site for nucleophilic attack is the 2O atom in the gas phase. For electrophilic attacks, the most reactive site is the 26H atom. In water, the most reactive site is the 12C for nucleophilic attack and is the 13C for electrophilic attack.

Table 1. Fukui indices of reactive sites of the *Acyclovir* compound by using DFT/B3LYP/SVP method in both gas and in solvent (water). See figure 1 for numbering.

compound		**B3LYP/SVP**			**B3LYP/SVP**	
ACV		***Gas***			***Water***	
	f^+	f^-	f^0	f^+	f^-	f^0
1O	-0.001	-0.007	-0.004	0.003	0.000	0.001
2O	0.118	0.068	0.093	0.100	0.103	0.102
3O	0.003	-0.005	-0.001	0.001	0.001	0.001
4N	-0.002	0.006	0.002	-0.008	-0.007	-0.007
5N	0.049	0.030	0.039	0.048	0.043	0.045
6N	0.079	0.013	0.046	0.092	0.021	0.057
7N	-0.002	0.011	0.004	-0.005	0.024	0.009
8N	0.064	0.016	0.040	0.078	0.030	0.054
9C	0.058	0.068	0.063	0.074	0.148	0.111
10C	-0.008	-0.017	-0.012	0.002	0.009	0.005
11C	0.064	0.038	0.051	0.093	0.023	0.058
12C	0.107	0.065	0.086	0.121	0.059	0.090
13C	0.075	0.052	0.064	0.096	0.190	0.143
14C	-0.028	-0.043	-0.036	-0.005	-0.006	-0.005
15C	0.053	0.104	0.078	0.074	0.107	0.090
16C	-0.001	-0.029	-0.015	0.000	-0.001	0.000
17H	0.026	0.043	0.034	0.024	0.033	0.028
18H	0.038	0.069	0.054	0.022	0.027	0.025
19H	0.078	0.067	0.073	0.058	0.045	0.052
20H	0.020	0.047	0.034	0.007	0.009	0.008
21H	0.025	0.047	0.036	0.007	0.011	0.009
22H	0.047	0.050	0.049	0.036	0.059	0.047
23H	0.028	0.061	0.045	0.004	0.005	0.004
24H	0.005	0.022	0.014	0.003	0.004	0.003
25H	0.044	0.057	0.050	0.038	0.033	0.036
26H	0.047	0.105	0.076	0.037	0.030	0.033
27H	0.013	0.060	0.037	0.001	0.002	0.001

According to Table 4, the most reactive site is the 11C atom with a positive Fukui index value of 0.131, followed by the 2O atom with value of 0.126. The least reactive sites are 14C and 1O atoms, both with negative values indicating electrophilic character. In water, the most reactive site is the 11C atom for nucleophilic attack and are the 2O and 13C atoms for electrophilic attack.

Table 4. Fukui indices of reactive sites of compound Acyclovir by using DFT/ CAM-B3LYP/TZVP method both in the gas phase and in water.

Compound		**CAM-B3LYP/TZVP**			**CAM-B3LYP/TZVP**	
ACV		***Gas***			***Water***	
	f^+	f^-	f^0	f^+	f^-	f^0
1O	-0.003	-0.006	-0.004	0.004	-0.001	-0.280
2O	0.126	0.074	0.100	0.110	0.130	-0.412
3O	0.024	0.024	0.024	0.002	0.002	-0.432
4N	0.002	0.001	0.001	0.010	-0.002	-0.048
5N	0.038	0.012	0.025	0.049	0.050	-0.106
6N	0.084	0.010	0.047	0.103	0.038	-0.160
7N	0.007	0.025	0.016	0.011	0.025	-0.264
8N	0.072	0.028	0.050	0.091	0.022	-0.336
9C	0.037	0.079	0.058	0.039	0.109	-0.086
10C	0.021	0.000	0.011	0.013	0.027	-0.037
11C	0.131	0.100	0.116	0.181	0.060	-0.045
12C	0.111	0.075	0.093	0.118	0.085	-0.016
13C	0.048	0.050	0.049	0.048	0.248	0.018
14C	-0.040	-0.045	-0.042	-0.004	-0.005	-0.120
15C	0.038	0.110	0.074	0.046	0.048	0.239
16C	-0.003	-0.004	-0.003	-0.001	-0.002	-0.084
17H	0.014	0.037	0.025	0.016	0.017	0.153
18H	0.029	0.052	0.041	0.014	0.014	0.154
19H	0.071	0.070	0.070	0.042	0.032	0.174
20H	0.019	0.023	0.021	0.006	0.006	0.135
21H	0.027	0.037	0.032	0.006	0.007	0.132
22H	0.045	0.054	0.050	0.029	0.045	0.290
23H	0.027	0.030	0.028	0.003	0.003	0.136
24H	0.005	0.006	0.006	0.002	0.003	0.128
25H	0.038	0.057	0.048	0.030	0.020	0.287
26H	0.042	0.109	0.075	0.029	0.016	0.286
27H	-0.011	-0.008	-0.009	0.000	0.002	0.293

According to Table 5, the most reactive site is the 2O atom with a positive Fukui index value of 0.134, followed by the 11C atom with value of 0.121 in the gas phase. In water, the most reactive site is the 11C atom for nucleophilic attack with a positive Fukui index value of 0.169 followed by the 2O atom with value of 0.117 and are the 2O and 13C atoms for electrophilic attack.

Table 5. Fukui indices of reactive sites of compound Acyclovir by using DFT/ωB97XD/def2-TZVP method both in the gas phase and in water.

Compound ACV	**ωB97XD/def2-TZVP** ***Gas***			**ωB97XD/def2-TZVP** ***Water***		
	f^{+}	f^{-}	f^{0}	f^{+}	f^{-}	f^{0}
1O	-0.003	-0.004	-0.003	0.004	0.000	0.002
2O	0.134	0.086	0.110	0.117	0.152	0.135
3O	0.000	0.000	0.000	0.001	0.001	0.001
4N	0.014	0.021	0.018	0.020	0.005	0.012
5N	0.055	0.010	0.033	0.062	0.048	0.055
6N	0.084	0.009	0.046	0.102	0.040	0.071
7N	0.014	0.049	0.031	0.020	0.038	0.029
8N	0.078	0.041	0.059	0.097	0.022	0.059
9C	0.050	0.084	0.067	0.060	0.091	0.075
10C	-0.003	-0.014	-0.008	-0.002	0.010	0.004
11C	0.121	0.111	0.116	0.169	0.066	0.118
12C	0.103	0.065	0.084	0.110	0.099	0.104
13C	0.037	0.033	0.035	0.037	0.243	0.140
14C	-0.029	-0.030	-0.030	-0.005	-0.006	-0.005
15C	0.027	0.095	0.061	0.036	0.036	0.036
16C	-0.008	-0.008	-0.008	-0.002	-0.002	-0.002
17H	0.019	0.035	0.027	0.018	0.018	0.018
18H	0.035	0.055	0.045	0.017	0.016	0.017
19H	0.068	0.065	0.066	0.039	0.029	0.034
20H	0.017	0.018	0.018	0.006	0.006	0.006
21H	0.025	0.031	0.028	0.006	0.007	0.006
22H	0.044	0.055	0.049	0.026	0.042	0.034
23H	0.026	0.028	0.027	0.003	0.003	0.003
24H	0.003	0.003	0.003	0.002	0.002	0.002
25H	0.036	0.053	0.045	0.028	0.018	0.023
26H	0.042	0.100	0.071	0.028	0.015	0.021
27H	0.011	0.012	0.011	0.001	0.001	0.001

It is worth nothing that the relative reactivity of the atomic sites can be significantly affected by the solvent environment, as seen in the differences between in the gas phase and in water results. The results show that the order of reactive sites varies depending on the method and solvent used.

Monte Carlo Simulation Results

To test the corrosion inhibition efficiency of Acv molecule against the corrosion of Fe (110) surface, in addition to DFT calculations, we made a Monte Carlo Simulation based analysis also [27,28]. Then, we checked whether the results of MC simulation based analysis are in good agreement with experimental data. As a result of the calculations made, the most stable (low energy) adsorption mode was determined for Fe (110)-Acv interaction. Fig. 3 visually presents the most stable low energy configuration for the adsorption of Acv on Fe (110) surface. In this figure, the top and side views of the most stable adsorption mode are seen.

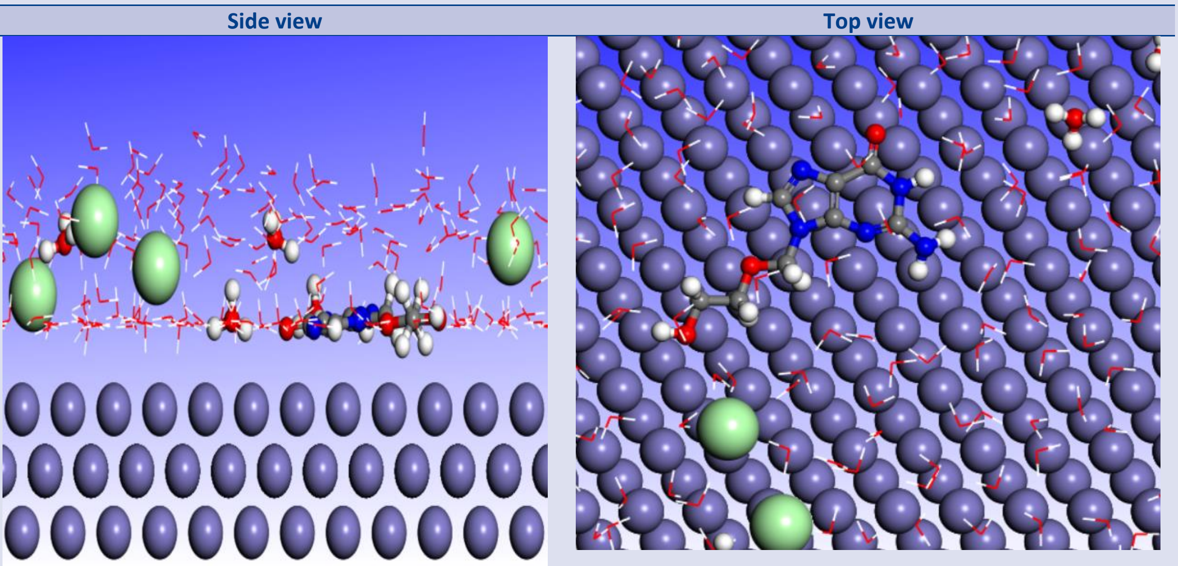


Figure 3. The most stable /low energy configuration for the adsorption of Acv on Fe (110) surface

With the help of Monte Carlo Simulations based calculations, in addition to the most stable adsorption mode of the inhibitor, the power of the interaction between metal surface and inhibitor can be also determined via adsorption energy prediction. As can be seen from Fig 3 that inhibitor has an orientation parallel to the metal surface. In this way, the surface interacts more strongly with the heteroatoms in its structure. Adsorption energy (Eads) is a parameter reflecting the power of the interaction between metal and inhibitor and corrosion inhibition efficiency of the studied molecule. The more negative the calculated adsorption energy for the metal-inhibitor interaction, the more effective the inhibitor is in protecting the considered surface from corrosion. In the acidic medium designed via Monte Carlo method, the adsorption energy value calculated for Fe (110)-ACV interaction is -3352.92 kcal/mol. This value is the proof that Acv is an effective inhibitor against steel corrosion. Additionally, it implies that adsorption is chemical as compatible with previously published experimental study. In a recent paper, Anadebe and coworkers [29] analyzed the corrosion inhibition mechanism of ACV molecule on Fe (110) using computational model based on DFT, RDF and MD simulation. Our study includes toxicity analysis and solubility study also for same molecule. Quantum chemical parameters calculated at B3LYP/SVP calculation level in this paper are in good agreement with the values presented by Anadebe and coworkers.

Conclusions

Density Functional Theory based calculations illuminate the reactive or stable behaviors of the molecules while Monte Carlo Simulation based analyses effectively explain the natures of the interactions between metal surfaces and corrosion inhibitors. While the strength of inhibitor-metal interactions can be easily analyzed in Monte Carlo Simulation based analyses the orientation of the inhibitor molecule in these interactions can also be easily explained. This paper includes Density Functional Theory (DFT) calculations to highlight the chemical reactivity of Acv molecule. In addition, adsorption behaviors of the molecule on Fe (110) surface were explained in the light of Monte Carlo Simulations. Regarding to the corrosion inhibition performance of the Acv molecule with high solubility and non-toxic nature, the following conclusions can be given.

1. Studied molecule is effective corrosion inhibitor against the corrosion of mild steel in acidic medium
2. Theoretically predicted reactivity descriptors at different calculation levels are in good agreement with experimental observations.
3. The presented data here will provide important clues to experimental corrosion scientists in terms of the design of new and effective purine derivatives.
4. The studied molecules exhibit nontoxic nature and high solubility in aqueous media as expected from good corrosion inhibitor.
5. The heteroatoms of the studied inhibitor molecule are positioned parallel to the metal surface to maximize their interaction with the surface.

Conflict of Interest

We declare that we have no conflicts of interest related to this study. We have no personal or financial relationships that could influence our work.

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