



Original Article

Theoretical properties of Thiazepine and its derivatives on inhibition of Aluminium *Al (110)* surface.

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ABSTRACT

In this work, corrosion inhibition of Aluminium was evaluated theoretically through quantum functions. The studied molecules thiazepine and its derivatives were optimized and simulated with local density function B3LYP using DFT-D under restricted spin polarization DNP basis to obtain the stable geometry of the thiazepine structures. the Fukui density functions were evaluated to determine the frontier molecular orbitals (FMO) of the compounds. The number of adsorption sites (physisorption) was the mode of interaction with the heteroatoms such as Chlorine, Nitrogen, Sulphur oxygen and methylene (-CH₂-) functional groups serving as the focal point for the selectivity of the donation and acceptance of electrons between the metal and the pyrimidine molecules as ($\omega+$) electron accepting power and ($\omega-$) electron donating power complement each other. The adsorption efficiency of the molecules as obtained by the simulated molecules was in the order PTA>CTA>ATP>TZP. Selectivity of the molecules was observed as the thiazepine molecules donate electrons more to p-orbital of the *Al (110)* surface.

1. Introduction

Metals like Aluminum, despite been essential material in construction of essential materials at home face the dangers of been susceptible in an aqueous environment that have pH greater than 7 or less than the neutral scale of the pH metal (alkaline and acid) [1]. Aluminum is an amphoteric material which can react in both alkalinity and acidic environment [2]. Aluminum despite forming a salve protection by forming a protective layer with the oxygen molecule, become more exposed to the environment when the temperature of the system or the concentration of the medium is unfavorable [3,4]. Though it shows no sign of reaction in hydrogen water at what so ever pH [5]. This attack on the surface of metal is called corrosion which destroyed the physical properties of the metal such as ductility, malleability, conductivity and even the lustrous nature of the metal [6].

Corrosion is defined as the deterioration of a material properties due to its interaction with its environment. It can also be known as oxidation of pure metallic materials which reduce to its impure form [7,8,9]. These failures mostly lead to the collapse of important bridges, oil pipes, refineries, buildings among others [8]. Of recent, the industrial activities such as pickling, chemical cleaning and processing of oil wells has been reported by leading numbers of scientist to be the potential source of corrosion which bring about the surface wearing of the metals [10]. The use of mechanical inhibitors such as coating the surface with other metals was approached by early scientist by galvanizing the surface of interested metals. today, the attention has been shifted to the green environment which provide enough biodegradable materials which

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can enable the prevention of corrosion of the metal surfaces [11]. The presence of unpaired electrons or unstable bonds (π -bonds) among methylene ($-\text{CH}_2-$) and some heteroatom such as Nitrogen, Sulphur, Oxygen among others brings a convincing inhibition of these metals [12].

Theoretical studies using computational method recently conducted to model electronic, structural and molecular properties of compounds that have been established to be promising corrosion inhibitors revealed that these compounds are either in nature inorganic, organic or condensed matter [13-14]. The inhibition efficiency of inhibitor molecules was found to be strongly correlated with their molecular/electronic properties. The adoption of traditional measures in tackling the level of corrosion, such as weight loss method, potentiodynamic polarization and electrochemical impedance spectroscopy to perform this drill is time consuming and cost unfriendly, therefore theoretical techniques which overcome these lapses are strongly recommended [1-2]. Quantum chemical calculations are used to determine the interaction between the inhibitor molecules and metal surface [4]. The use of theoretical parameters allows the characterization of molecular structures of inhibitors and suggests a mechanism for their interaction with metal surface [15]. Molecular dynamic simulation is an excellent method that provides the actual interaction and adsorption energy between the inhibitor molecule and metal surface [16-17].

In this research Thiazepine derivatives were tested on the surface of Aluminum to compare their inhibitive potential through Theoretical Computational method using Density Functional Theory (DFT) and Forcite quench dynamics methods to simulate the molecular and electronic properties on Al (110).

The molecules [1,2] thiazepine (TZP), 6-Aziridin-1-yl-[1,2] thiazepine (ATP), (4-phenyl-3,4-dihydro-2H-[1,4] thiazepine-7-ylidene)-vinyl-amine (PTA) and 4-chlorophenyl-(1-phenyl-1,2,3,6,7,8-hexahydro-cyclopent[1,4]thiazepine-5-ylidene)-amine (CTA) are as presented in Figure 1.

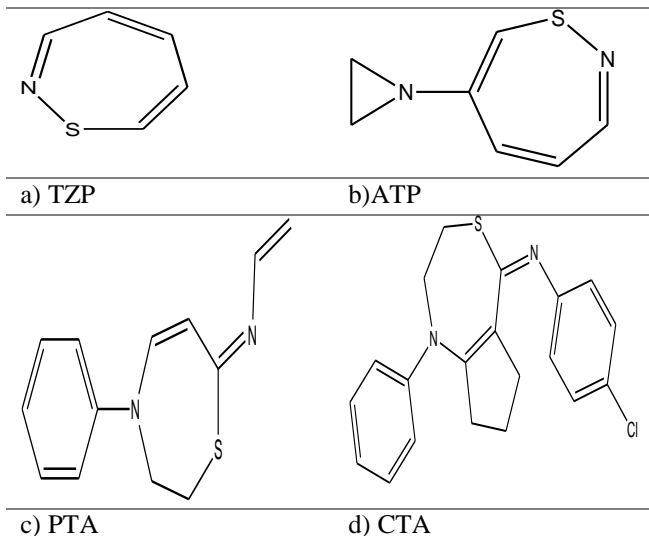


Fig 1. structures of Thiazepine derivatives

2. Materials and Methods

2.1. Quantum chemical Parameters Calculations

A DMol3 package in the BIOVIA/Material studio 8.0 (Accelrys, Inc.) was used for the quantum chemical calculation based on Density Functional Theory (DFT) principles. The molecules were sketch with the help of ChemDraw Ultra 7.0.3 CambridgeSoft. Calculations of parameters were conducted using B3LYP function with basis set as “double-numeric plus polarization” (DNP+) in liquid phase model. The electron density and distribution of frontier molecular orbitals, E_{HOMO} and E_{LUMO} , Fukui indices were assessed, with a view to establish the active sites that could be responsible for the effective transfer of electrons between the surfaces as well as local and global reactivity’s of the compound as instructed on the software. Ionization energy (IP), electron affinity (EA) and other functions which describe the reaction behaviors of molecules were calculated. Global reactivity parameters also were included. Such as electronegativity (χ), (ω) electrophilicity, global hardness (η), the chemical potential (μ), (ω^-) electron donating power, (ω^+) electron accepting power global softness (σ) global indices that describe the reactivity of a molecule in terms of the initial electron distribution in the molecule and local reactivity computing of Fukui function $f(r)$ from ab-initio quantum chemistry were evaluated based on Koopman’s extended theorem as described in the equations below.

$$\text{IE: Ionization energy (eV)} \quad IE = -E_{HOMO} \quad (1)$$

$$\text{AE: Electron affinity (eV)} \quad AE = -E_{LUMO} \quad (2)$$

$$\Delta\text{Eg: Energy gap (eV)} \quad E_g = E_{HOMO} - E_{LUMO} \quad (3)$$

$$\chi: \text{Absolute electronegativity (eV)}$$

$$\chi = \frac{I+A}{2} \approx \frac{-1}{2}(E_{HOMO} - E_{LUMO}) \quad (4)$$

$$\eta : \text{global hardness } \eta = \frac{I-A}{2} \approx -\frac{ELUMO-EHOMO}{2} \quad (5)$$

$$\sigma : \text{global softness} = -2/E_{HOMO}-E_{LUMO} \quad (6)$$

$$\omega \text{ electrophilicity } \frac{\mu^2}{2\eta} \approx \frac{(I+A)^2}{2(I-A)} \approx \frac{(ELUMO+EHOMO)^2}{2(ELUMO-EHOMO)} \quad (7)$$

$$\mu \text{ chemical potential (Debye)} \mu \approx -\frac{1}{2}(I+A) \approx \frac{1}{2} \quad (8)$$

$$\Delta N : \text{Fraction of electron transfer } \Delta N = \frac{\chi_{Al}-\chi_{Inh}}{2(\eta_{Al}+\eta_{Inh})} \quad (9)$$

The electron donating (ω^-) and electron accepting (ω^+) powers of the molecules has been defined as shown in the equations 10 and 11

$$\omega^- \text{ electron donating power} \approx \frac{(3I+A)^2}{16(I-A)} \quad (10)$$

$$\omega^+ \text{ electron accepting power} \approx \frac{(I+3A)^2}{16(I-A)} \quad (11)$$

Where χ_{Al} and χ_{inh} served as Eigen values for the absolute electronegativity of Al and the inhibitor molecule respectively, η_{Al} and η_{inh} are the absolute hardness of Al and the inhibitor molecule, respectively. A theoretical value for the electro-negativity of bulk Fe used was obtained as $\chi = 5.60$ eV and a global hardness of iron surface η_{Fe} as zero (0) and electro-negativity of inhibitor (χ_{inh}) = 0 eV by assuming that for a metallic bulk IP=EA because they are softer than the neutral metallic atoms. [1-6]

Fukui Second function (f^2) known as the dual descriptor $\Delta f(k)$, is another local descriptor defined as the difference between nucleophilic and electrophilic Fukui functions which also determine the electrophilicity or nucleophilicity of the molecules using the Fukui behavior of the atoms. [1] If $f^2(r) > 0$, then site k prefers nucleophilic attack, whereas if $f^2(r) < 0$; then site k prefers an electrophilic attack. This indicates that $f^2(r)$ serves as an index of selectivity towards nucleophilic or electrophilic attacks.

$$f(k)^+ = qk(N+1) - qk(N) \quad (\text{for nucleophilic attack}) \quad (12)$$

$$f(k)^- = qk(N) - qk(N-1) \quad (\text{for electrophilic attack}) \quad (13)$$

$$f(k)^0 = \frac{qk(N+1) - qk(N-1)}{2} \quad (\text{for radical attack}) \quad (14)$$

$$f(r) = f^+ - f^- = f^2 \quad (\text{Fukui function}) \quad (15)$$

Where qk is the gross charge of atom (k) in a molecule (the electron density at a point in space around the molecule N corresponds to the number of electrons in the molecule). N+1 corresponds to an anion, with an electron added to the LUMO of the neutral molecule: N-1 corresponds to the Cation with an electron removed from the HOMO of the Neutral molecules. All calculations were done at the ground state geometry. These functions were condensed to the nuclei by using an atomic charge partitioning scheme, such as Mulliken population analysis in equations

2.2. *Molecular dynamic simulations* All tables should Pyrimidine compound were simulated on the densely

packed Al (110) surface with a high stability. A Density Functional Theory (DFT) electronic using FORCITE tools package as incorporated in the BIOVIA Materials studio 8.0 (Accelrys, Inc.) software. for the simulation process of the surfaces. Calculations were carried out using condensed-phase optimized molecular potentials for atomistic simulation studies COMPASS in forcefield tool and Smart algorithm in a simulation box 17Å x 12 Å x 28 Å with a periodic boundary condition, to model a representative part of the surface. The Fe crystal was cleaved along the (110) Plane with a fractional depth of 3.0 Å. The geometry of the bottom layers was constrained before optimizing the surfaces which was subsequently enlarged into a 7 x 6 supercell to avoid edge effects due to the size of the molecules. Temperature fixed at 350 K which represents a trade-off between a system with too much kinetic energy where the molecule desorbs from the surface and a system with not enough kinetic energy for the molecule to move around the surface. Temperature was fixed with the NVE (microcanonical) ensemble with a time step of 1 fs and simulation time 5 ps. The quench process was design to quench every 250 steps to obtained the statistical values of the energies on the surfaces of the iron crystal (110). FORCITE optimized structures of the molecules and the surfaces were used to obtained different interactions of the molecule with the Fe surface. [1,2,13-20]. The Activation energy between the Al (110) surface and the pyrimidine derivatives were calculated using the equation 12 while the positive value of the activation energy was calculated as the binding energy using equation 13.

$$E_A = E_T - (E_I + E_S) \quad (12)$$

$$E_B = -E_A \quad (13)$$

Where E_A is the adsorption energy E_B is the binding Energy between the Al(110) and the moieties, E_T is the total energy of the molecule and E_S is the energy of the Al (1 1 0) surface when the molecule is removed, E_I is the energy of the inhibitor molecule when surface is removed.

3. Results and Discussion

3.1 Quantum Chemical Calculations

3.1.1 Frontier molecular orbitals

Organic Molecules show greater reactivity when the bonds connecting atoms are weak and easier to break [2,3,4]. The reactivity of the inhibitors also has said to depend on the partial charges of the molecules. The effectiveness of this inhibition cannot be limited to molecular structure but the distribution of the electronic orbitals. Hence density functional theory has proven to be one of the powerful tools for the ground state molecular properties calculation

and it's powerful in pointing out the changes in electronic structure responsible for inhibitive nature of the molecules. [3,21,22]. These electronic properties are also important in Quantum chemical calculations which enable theoretical study of molecules on the surfaces of metals [1-5]. Frontier molecular orbitals of the inhibitor's molecules provide important information on the selectivity in relation to the

molecules used for solving corrosion issues [1,17]. From the structures presented in figure 2, the optimized structure is presented with a blue Nitrogen, yellow Sulphur, grey carbon and a white hydrogen with a light blue chlorine. The optimized structure, total electron density and HOMO/LUMO orbitals of the studied molecules are presented in Figure 2.

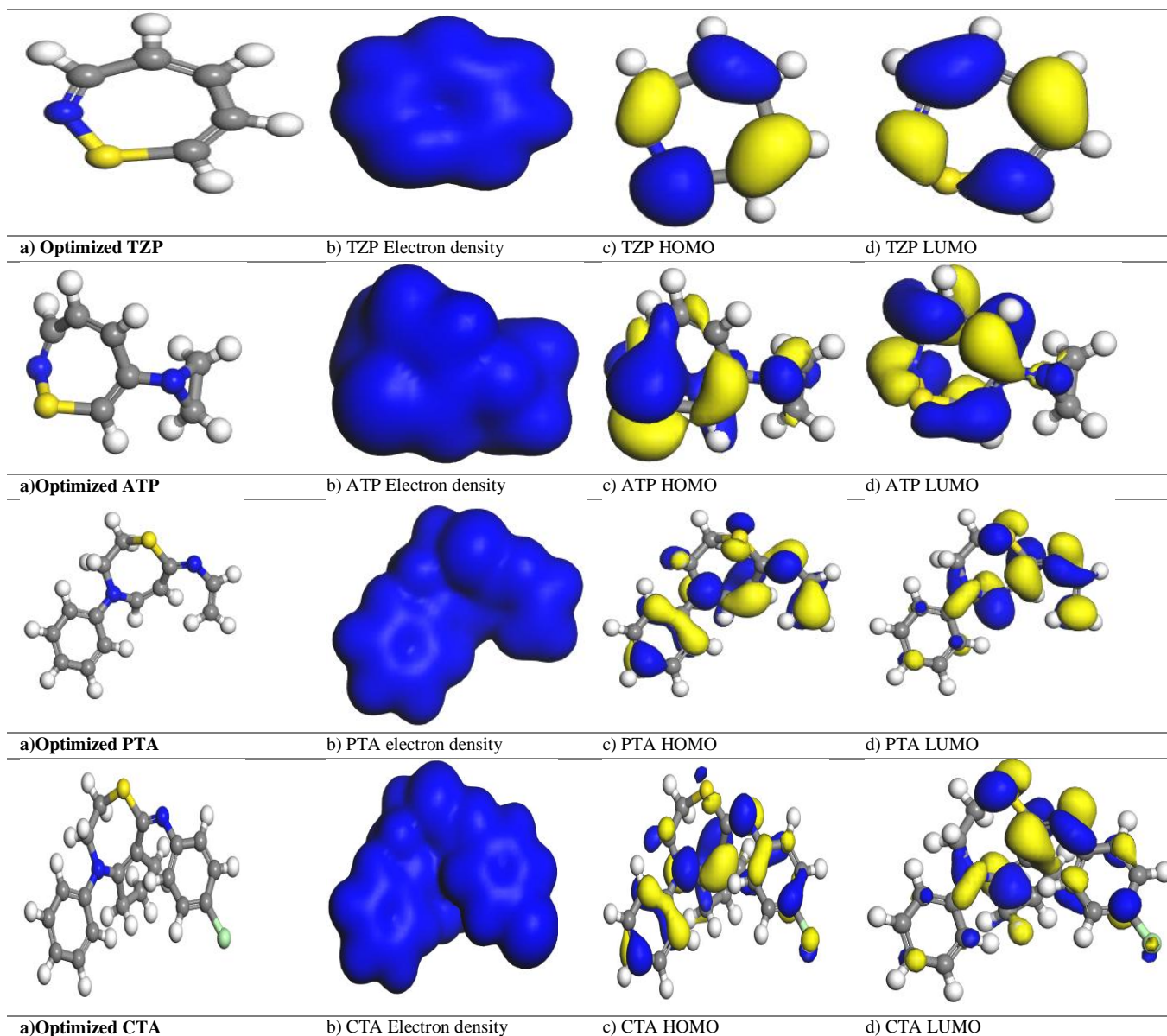


Fig 2. A 3D Snap shots of structural and electronic properties of Thiazepine derivatives

The density occupies the entire molecule. This notified that, the molecules can use the entire surface during inhibition on the surface of metal [10-20]. The HOMO and LUMO orbitals occur around the functional groups like Chlorine (Cl), Sulphur (S), Nitrogen (N) and the methylene (-CH₂-) the pi-bonds (double bond) in the molecules [1,2,5,10]. This shows a clear possibility of atom with Pi-

bond or different functional groups as a good corrosion inhibitor on the surface of metals [21-23].

3.1.2 Frontier orbital energies

The Frontier orbital energies of the molecules are presented in Table 1. The energy studied includes, E_{HOMO} , E_{LUMO} , energy gap (ΔE), dipole moment (μ), electronegativity (χ), global hardness, global softness and fraction of electron

transfer (ΔN). The E_{HOMO} Eigen value shows the capability of a molecule to donate electrons to the empty orbitals of the p-orbitals of the Aluminum surface while the E_{LUMO} Eigen value show potential of electrons to be accepted by the molecule from the p-orbital of the Aluminum surface [2,3, 10,22-27]. The Eigen energy values of the molecules is presented in Table 1.

Table 1. Frontier Eigen Energies values of the Molecules

Parameters	TZP	ATP	PTA	CTA
E_{HOMO} (eV)	-4.786	-4.879	-4.930	-4.819
E_{LUMO} (eV)	-3.622	-2.780	-2.517	-2.399
ΔE (eV)	1.164	2.099	2.413	2.420
I	4.786	4.879	4.930	4.819
A	3.622	2.780	2.517	2.399
χ	4.204	3.829	3.724	3.609
η	0.5820	1.0495	1.2065	1.2100
ω^+	17.36	9.03	7.76	7.34
ω^-	13.15	5.20	4.03	3.73
σ	1.718	0.953	0.829	0.826
ΔN	1.199	0.844	0.777	0.823

From the Eigen energy values of the molecules studied, the E_{HOMO} , E_{LUMO} were calculated and the molecules with the highest E_{HOMO} is likely to be the molecule with the highest nucleophilic attacks and the molecule with the lowest value of E_{LUMO} is also expected to have the highest electrophilic attack [10,22,25]. The Energy gap between the E_{HOMO} and E_{LUMO} has expectation that the molecule with the lowest energy gap is a compound likely to have a least possible distance for easy transfer of electron between the molecules or metal surface and the molecule [20-26]. From the derivatives of the Thiazepine studied, TZP has the lowest energy gap and therefore an indication of the higher frequency of transfer of electrons between the molecule and the surface, which are in order of: TZP < ATP < PTA < CTA. This is might be as the result of presence of the functional groups of the molecules as well of the size. From the result presented the bigger the molecule and more functional group the less the energy gap experience by the moles [11,21-25].

Chemical hardness the resistance against electron cloud polarization is the resistance against inhibition efficiency. meaning higher value of chemical hardness decrease inhibition efficiency of the molecules during corrosion inhibition. Though, soft molecules allow electron transfer and therefore behave as good corrosion inhibitors, the higher the softness value of the molecule the greater inhibition efficiency of the molecule. From the points above, the global hardness and softness are good parameters that determine the corrosion efficiency of the

molecule on the surface of the metal. [15]. In light of the result presented in Table 1 with regard to hardness and softness, the trend in inhibition efficiency of Thiazepine derivatives follows: TZP > ATP > PTA > CTA. But the higher value of global hardness resists the inhibition. As the molecules increase and the functional group in the molecules increase the global softness ability increase. Thus, global hardness and softness are inversely proportional. The increase of global hardness decreases the value and efficient of global softness [1,25]. The dipole moment is related to the polarity of the molecule [26-27]. This depends on the electronegativity of the molecules as the dipole moment in the studied molecules increase in similar trend to the increase values of electronegativity. The molecules with the least electronegativity value turn out to be more stable and in turn tells how reactive a bond or the molecule is hence reactivity is ability to loss/gain of electron(s) [20,28]. Fraction of electron transfer (ΔN) was investigated to understand the transfer of electrons from one surface to another. This is another parameter useful in the mechanism of corrosion inhibition during corrosion of metals. The result of ΔN presented on Table 1 for all the four molecules TZP, ATP, PTA, CTA, are positive and less than 3.6. This is an indication that electron transfer can occur between the molecules and the metal surface and thus inhibition efficiency of the molecules is directly proportional to the electron donating ability of the molecules [1,2,10,14,21,23,25,28,29]. The ω^- electron donating power and ω^+ electron accepting power of the molecules were calculated. It follows that a larger (ω^+) electron accepting power value corresponds to a better capability of accepting charge, whereas a smaller value of (ω^-) electron donating power value of a system makes it a better electron donor [30].

3.1.3 Fukui Function

Reactivity of molecules during electron transfer also depends on the local reactivity of molecules as a contribution to selecting the region where reaction is likely to occur through donation or accepting electrons. This to understand the specific atoms responsible for the highest frequency of the reactivity [2,10].

Nucleophilic Fukui function (f^+), electrophilic Fukui function (f^-) were important in electron transfer of molecules during corrosion inhibition. The condensed Fukui function as presented in Table 2 showed the actual region where the transfer of electron is possible which also reduce corrosion by exchanging electron with the surface of the metal [20-26]. From the result, TZP has the highest values of (f^+) and (f^-) at S (1), ATP at C (1), PTA at S (11) and CTA at N (3).

Table 2. Showing Fukui Function of the molecules

Compound	Atom	Nucleophilic Attack (+)		Electrophilic Attack (-)	
		Milliken	Hirshfield	Milliken	Hirshfield
CTA	N(3)	0.100	0.096	0.273	0.191
PTA	S(11)	0.149	0.106	0.365	0.403
ATP	C(1)	0.104	0.086	0.102	0.099
TZP	S(1)	0.164	0.133	0.314	0.293

The electrophilic Fukui function correspond to the HOMO and the Nucleophilic Fukui function correspond to the LUMO [29]. The mechanism of the reaction expected electrons to move during adsorption from HOMO to LUMO orbitals for possible bond formation [7-9]. Table 2 indicate the orbital reaction with the highest Eigen values of nucleophile or electrophile which indicate the atom with the highest reactivity in the molecule [8-10]. Both molecules have their Eigen values on a single functional group per molecule. CTA molecule has its Eigen values at N (3) Amine functional group for both Nucleophilic and electrophilic attack. PTA highest Eigen values occurs at S (11) thionic functional group for both nucleophilic and electrophilic attack. The ATP highest Eigen values

occurred at the C (1) aryl-halide functional group on the molecule for both nucleophilic and electrophilic attack for the molecule. TZP has its highest Eigen value at S (1) for both nucleophilic and electrophilic attack. Therefore, it could be seen that the heteroatoms namely: Nitrogen, Sulphur and chlorine could be responsible for the nucleophilic and electrophilic attacks on the surface of Al in the corrosion inhibition process of the metal [11,20,22,25]. The screenshot in figure below shows the Fukui function at different atomic position among the molecules. The highest values of the Fukui functions occurred as prescribed in table 2.

Table 3. Calculated molecular dynamic simulation parameters for the studied

Properties (Kcal/mol)	TZP	ATP	PTA	CTA
Total Kinetic Energy	8.680±3.3	12.210±5.7	19.070±16	39.620±4.9
Total potential Energy	-38.790±0.0	89.860±0.0	-123.35±2.1	-75.460±1.2
Energy of the molecule	-10.650±4.2	126.95±0.0	-69.210±0.0	-34.770±0.4
Energy of the surface	0.000±0.0	0.000±0.0	0.000±0.0	0.000±0.0
Adsorption Energy	-28.130±0.0	-37.09±0.0	-54.140±0.0	-40.680±1.6
Binding Energy	28.130±0.0	37.09±0.0	54.140±0.0	40.680±1.6

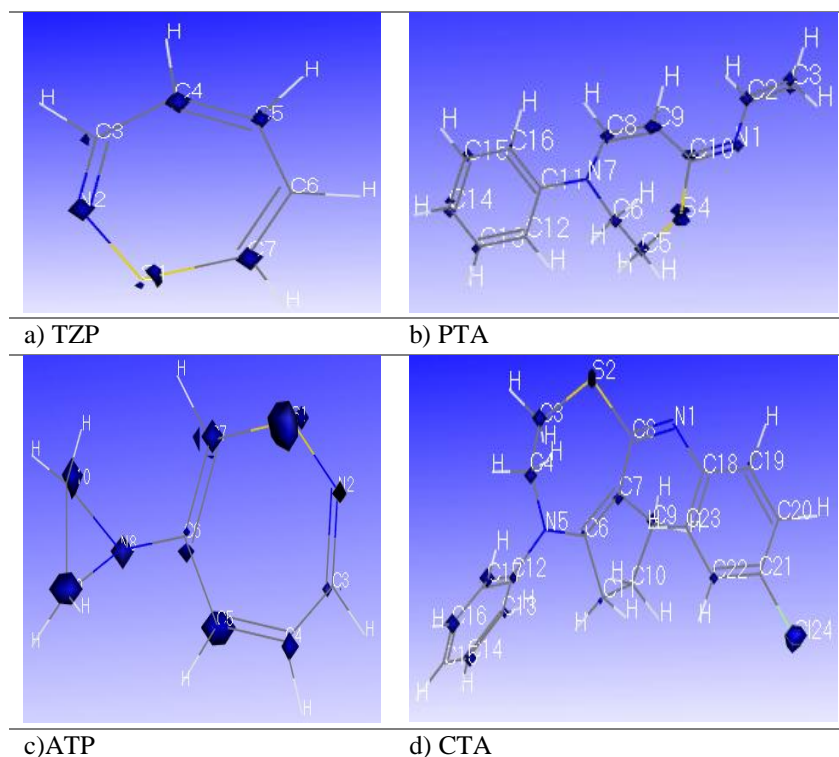


Fig 3. Showing the Fukui points of the molecules

3.2. Molecular Dynamic Simulation

Thiazepine derivatives as simulated on the Al (110) surface present the insight at which molecules interact with the surface of metals to reduce the extent of corrosion on the surface when exposed in a harmful environment [18-20]. The densely occupied surface of the Aluminum Al (110) was used hence the surface of the Aluminum been covered by many atoms among others [17,31,32]. The snapshot of

the thiazepine derivatives on the Aluminum surface during simulation is presented in Figure 3. The parameters of the calculated molecular dynamic explain the potential of the inhibition of the molecule on the surface of the simulated metal [15]. The properties determine were: total energy (kinetic and potential), others include, Surface energy, energy of the molecule, adsorption and binding energy [12].

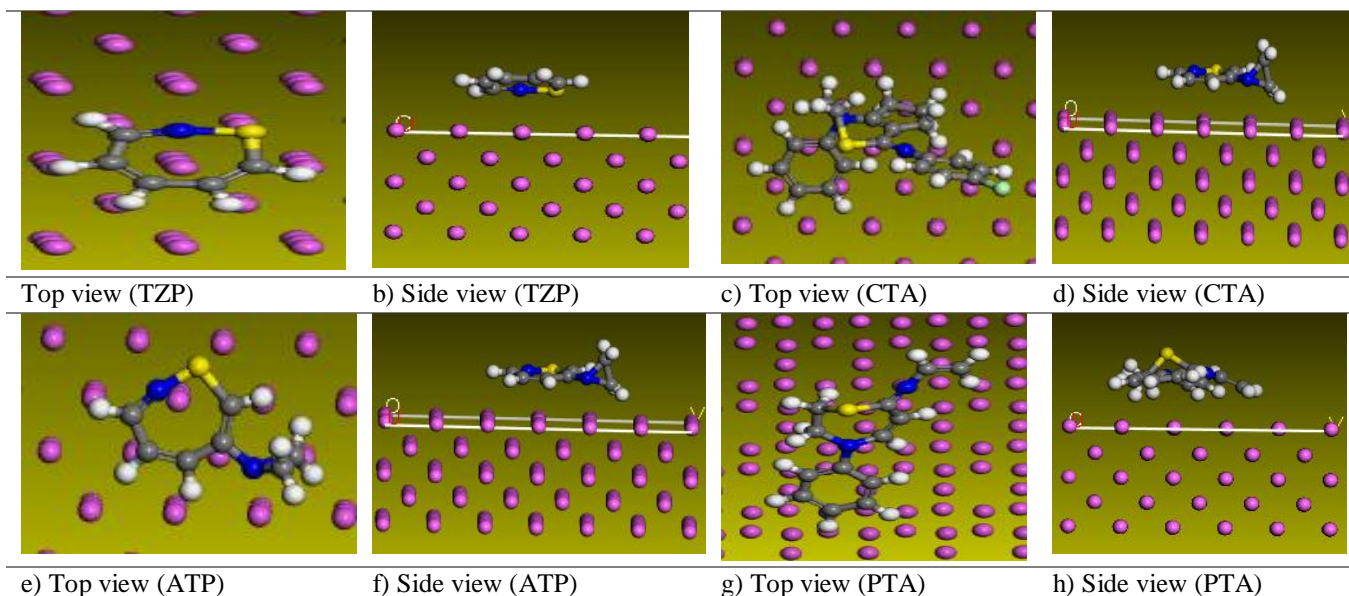


Fig 4. The snap short of thiazepine derivatives on the Al (110) surface showing the top and side view

3.2.1: Mechanism of inhibition

The *ab initio* of mechanism in any corrosion inhibitor is at which extend the adsorption of such inhibitor is with the surface [15-20]. From the result of the molecules on Aluminum surface studied, the negative adsorption energy on the surfaces indicates that, the molecule is feasible and spontaneous on the surfaces [10,21,29] The binding energy and adsorption energy of the simulation was less than -100Kcal/mol on Al surface suggesting physical adsorption mechanism [2,5,10-11]. This shows that, the derivatives are charged molecule with strong inductive and strong resonance effect because of the different functional groups present in the molecules. [20]. With such value, Ayuba and Nyijime, Nyime and Iorhuna, Lawal and Bashir concluded in their separate experiment that, for a mechanism to be physisorption, the value of binding energy would be less than 100Kcal/mol [11,15, 29]. As such, mechanism of Thiazepine derivatives show a binding energy value of less than 100Kcal/mol in the order $PTA > CTA > ATP > TZP$ Hence the reference molecule TZP has the lowest binding and adsorption value with a clear indication that, its derivatives are more promising for the corrosion inhibition of the metal. This further prove that the bigger the molecule is the larger the value of binding energy hence binding energy is the negative of the adsorption energy,

this leaves with an explanation, that the larger the molecule the larger the adsorption of molecule on the surface and more effective would the molecule protect or reduce the corrosion of such metal.

4. Conclusion

The result of this research work indicated that, established adsorption or binding energy of the thiazepine derivatives on the Al surface is relatively low which signifies a physical adsorption mechanism. The frontier energy values and Fukui function show the effectiveness of the molecule as the potential molecules capable of corrosion inhibition. The reference molecule (TZP) Hence has the lowest binding and adsorption value which is an indication that its derivatives are more promising for the corrosion inhibition of the Aluminum metal and functional group of thiazepine alone are insufficient in the corrosion inhibition of Aluminium surface. Both E_{HOMO} and E_{LUMO} were evaluated and were observed to produce an energy gap responsible for the efficient transfer of electrons. In the study, atoms such as Nitrogen, Sulphur, Oxygen Chlorine and methylene group (-CH₂-) were responsible for the transfer of electrons between the molecule and the empty p-orbital of the Aluminium surface.

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Conflict of Interest

The authors declare that they have no conflict of interest

Reference

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