**FK Ekuma**
Department of Chemistry,
Michael Okpara University of
Agriculture Umudike, Abia
State, Nigeria

**UI Ekanem**
Department of Chemistry,
Michael Okpara University of
Agriculture Umudike, Abia
State, Nigeria

**HO Chukwuemeka-Okorie**
Department of Chemistry,
Michael Okpara University of
Agriculture Umudike, Abia
State, Nigeria

# Computational investigations on corrosion inhibition potentials of schiff bases synthesized from linoleic and benheric acids on mild steel in HCl medium

## FK Ekuma, UI Ekanem and HO Chukwuemeka-Okorie

**Abstract**
The inhibition efficiencies of two Schiff bases 2[2-diethylamino) ethyl methyl amino)-4-methy1-5-3 (3-methyl sulfanyl propy1 amino) methyliene cyclohedien-1-one (DEMS) and [1-(azepan-1-yl)2-2-[4-(2-tert-butyl sulfanylethyl piperazin-1-yl] ethanone (ATSP) synthesized from linoleic and benheric acids on mild steel coupons in 1M HCl were investigated at a temperature of 30 ℃ using weight loss and quantum chemical techniques. The schiff bases were characterized using Infrared (IR) Spectrophotometer. It was observed from the results that their inhibition efficiencies increased with increase in concentrations of the Schiff bases. From the calculated global reactivity parameter, it was seen that the inhibitor, DEMS has more potency to adsorb onto the surface of the mild steel than the inhibitor, ATSP due to its smaller energy gap ($\Delta E$), higher value of dipole moment ($\mu$), higher value of chemical softness ($\delta$), lower value of global hardness ($\eta$), higher electronegativity value (X) and higher value of maximum number of electrons transferred ($\Delta N$). All these make DEMS to exhibit high inhibition efficiency.

**Keywords:** Corrosion inhibition, inhibition efficiencies, quantum chemical parameters, mild steel, Schiff bases

## Introduction
Corrosion of metals and alloys constitute grave problems in the extraction, manufacturing, production and other allied industries and a great attention is channeled into ways of ameliorating the problem. Mild steel, which is one of the most widely used among the metals finds extensive applications in the chemical and petrochemical industries. Failures of petroleum pipelines have resulted in a number of oil wastages in the petroleum industries. The qualities and lifespan of metals can be improved upon by adopting strategies which could help to reduce or completely prevent anodic and or cathodic reactions in order to minimize corrosion. Inhibitors are used in these circumstances to control the metal dissolution. Green inhibitors, which are usually obtained from natural products of plant and animal are presently given considerable attention to replace some of the previously applied poisonous compounds that cause environmental pollution. The non-toxic inhibitors, of which Schiff bases are inclusive have been found to be eco-friendly, biodegradable and at the same time offer comparable performance [1]. Environmentally friendly corrosion inhibitors range from rare earth elements to organic compounds and are used as alternative corrosion inhibitors to reduce their harmful effects on humans, animals and environment. Organic compounds containing polar functional groups with oxygen, nitrogen, or sulfur as their constituent atoms have been widely studied as inhibitors for the acid corrosion of mild steel [2]. Some Schiff base compounds have recently been reported as effective corrosion inhibitors for mild steel [3, 4] and other metals [5, 6]. In consideration of the safety of metal corrosion inhibitors against the environment, their non-toxicity and effectiveness in terms of performance, eco-friendly inhibitors are considered more significant and desirable [7-11]. In studying the inhibition performance of corrosion inhibitors, quantum chemical computations have been extensively applied in studying reaction mechanisms and to offer clear interpretations to experimental results of corrosion inhibition [12]. The present work is therefore aimed at investigating the corrosion inhibition potentials of two Schiff bases synthesized from linoleic and benheric acids on mild steel in 1.0 M HCl using quantum chemical studies.

**Correspondence**
**FK Ekuma**
Department of Chemistry,
Michael Okpara University of
Agriculture Umudike, Abia
State, Nigeria

## Materials and Methods

The mild steel used for the present investigation was pressed-cut into different coupons of dimensions 3 cm by 3cm. Each coupon was sand-papered using different grades of sand papers (rough and then smooth) until a mirror polished surfaces were obtained. The surfaces of the coupons were washed with ethanol to remove any stains or grease, later washed with de-ionised water and then cleaned with acetone. They were finally air-dried for some hours before been kept in a desiccator. Different concentrations of the Schiff base inhibitors ($0.2$ g l$^{-1}$, $0.4$ g l$^{-1}$, $0.6$ g l$^{-1}$, $1.0$ g l$^{-1}$ and $2.0$ g l$^{-1}$) used in the study were prepared in 1 M concentration of HCl.

## Synthesis of the schiff bases
### Preparation of methyl esters from oils

Methyl esters were prepared from the linoleic and benheric oils by acid catalyzed esterification method according to Toliwal et al. [13]. Exactly 100 g of the oil was weighed into a 500 ml round bottomed flask then followed by the addition of 300 ml of methanol and 1ml of concentrated tetraoxosulphate (VI) acid into the flask. The content was refluxed for 4 h on a water bath. The unreacted methanol was distilled off, followed by the addition of 50 ml distilled water. The contents of the flask were poured into a separating funnel to collect the lower aqueous layer. The upper organic layer of the immissible mixture was extracted and washed three times with 1% solution of $Na_2CO_3$ to remove un-esterified fatty acids and were finally purified by distillation.

### Preparation of fatty acid hydrazide

Fatty acid hydrazide was prepared by measuring 0.1 M fatty acid ester into 150 ml ethanol in a refluxing flask, followed by addition of 0.2 M hydrazine hydrate (95%) into the mixture. The contents were refluxed for 4 h and cooled. The residue was washed and then separated from ethanol by recrystallization. Further, a solution of 0.02 M fatty acid hydrazide in 50 ml methanol was prepared using the method stated in Toliwal et al. [13]. A solution of 0.03 M potassium thiocynate and 3 ml of concentrated HCl were added with constant stirring into the round bottom flask. The mixture was evaporated to dryness immediately on a steam bath and then heated for an additional one hour with 150 ml ethanol. The resulting solid was mixed with 10 ml of distilled water and 20 ml ethanol and then separated from ethanol by recrystallization.

### Preparation of schiff bases

The preparation of the Schiff bases was done by adding to a solution of 0.02 M acetaldehyde in absolute alcohol a 0.02 M thiosemicarbazide according to Yaseen et al. [14] and the mixture refluxed for 7 h on a water bath. The contents were cooled and filtered and then separated from ethanol by recrystallization. The Schiff bases were characterized using FTIR spectrophotometer.

## Corrosion Studies
### Weight loss Technique

The pre-weighed coupons were suspended vertically in a 100 ml of 1.0 M HCl in the presence and absence of the Schiff bases under study for 3 h at a temperature of 30 °C. At the expiration of the 3 hours immersion time, the coupons were withdrawn from the test solutions with the aid of a fishing line hung through the holes bored at their upper edge and then transferred into the washing solution to quench the corrosion process. The metal coupons were scrubbed and washed in a distilled water. They were dried and re-weighed to determine the weight loss in grams. The measurements were done in triplicates and results obtained from the mean weight loss were used to calculate corrosion rate using the relation expressed in equation (1):

$$Corrosion\ rate = \frac{\Delta W}{At} \qquad (1)$$

Where $\Delta W$ is weight loss in grams, A is area of the metal coupon in cm$^2$ and t is the immersion time in hours.

The surface coverage and the inhibition efficiencies were calculated using the relations expressed in equations (2) and (3)

$$\theta = \left(\frac{CR_0 - CR_1}{CR_0}\right) \qquad (2)$$

$$(I\%) = \left(\frac{CR_0 - CR_1}{CR_0}\right) x100 \qquad (3)$$

Where, $CR_1$ and $CR_0$ are the corrosion rates in the presence and absence of the Schiff base inhibitors respectively

## Quantum Chemical Calculation

To study the effect of molecular structure on inhibition efficiency, quantum chemical calculations are usually carried out using Density Functional Theory (DFT) under the Generalized Gradient Approximation (GGA) with Pendix – Bunke –Fruzerhof (PBF) exchanging correlation function as implemented in D mol$^{-1}$ module using material studio software package version 6.0. A double numerical basis set augmented with polarization function is employed to describe the valence electrons. The geometries were fully optimised. Spin unpolarisation schemes were implored when carrying out the calculation.

The self consistency field (SCF) and energy convergence threshold were set at $1.0$ x $10^{-5}$ Ha and $2.0$ x$10^{-5}$ Ha respectively. The quantum chemical parameters determined are energies of highest occupied and lowest unoccupied molecular orbital ($E_{Homo}$ and $E_{Lumo}$ respectively), energy gap ($\Delta E$) which was calculated using equation (4) [15],

$$\Delta E = E_{Homo} - E_{Lumo} \qquad (4)$$

Global hardness ($\eta$), which is a measure of the resistance of an atom to charge transfer was estimated using equation (5)

$$\eta = -1/2[\ E_{Homo} - E_{Luom}] \qquad (5)$$

Chemical softness ($\sigma$), another parameter which describes the capacity of an atom or group of atoms to receive electrons. It is the inverse of global hardness and was estimated using equation (6) [16].

$$\sigma = \frac{1}{\eta} \equiv -2/E_{Homo} - E_{Lumo} \qquad (6)$$

The maximum number of electrons transferred ($\Delta N_{max}$) in the chemical reaction was calculated using equation (7)

$$\Delta N_{max} = \frac{\chi}{2\eta} \qquad (7)$$

Where $\chi$ is the electronegativity and it is calculated as:

$$\chi = 1/2[E_{Homo} + E_{Lumo}] \qquad (8)$$

The electrophilicity index ($\omega$) as given by Yang and Parr [16] is expressed as equation (9)

$$\omega = \mu^2/4\eta \qquad (9)$$

The Mulliken charges (Q) for nucleophilic and electrophilic attacks were also determined.

## Results and Discussion
## Fourier Transform Infrared Spectroscopy
The Schiff base inhibitor molecules were characterized using infrared (IR) spectrophotometer. The (IR) spectra of the Schiff bases were recorded using a Perkin-elmer-1600 FT-IR spectrophotometer with resolving power of 4cm$^{-1}$.
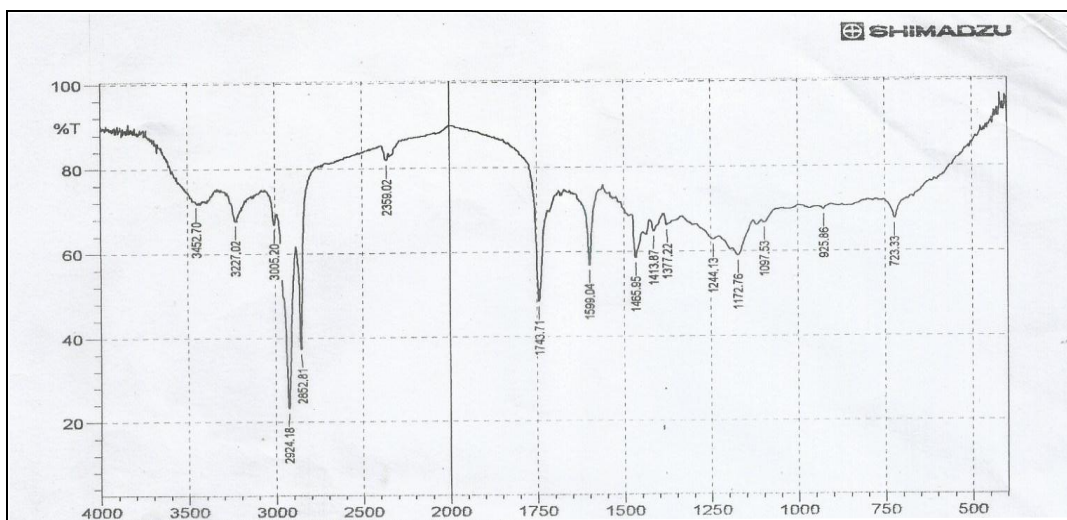


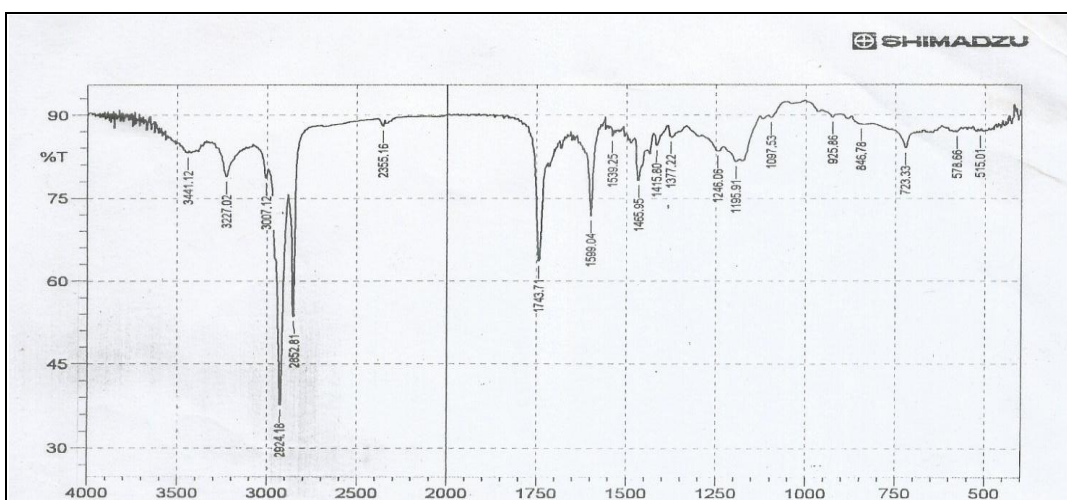**Fig 1:** The FTIR spectrum of the synthesized Schiff base (DEMS)



**Fig 2:** The FTIR spectrum of the synthesized Schiff base (ATSP)

The common features of the FTIR spectra of the studied Schiff base show bands at 1760- 1735 cm$^{-1}$ range which indicate the presence of C-C and C=O stretching bands of esters, and the carboxylic groups having the wave number ranges 3300- 2500 cm$^{-1}$. The absorption bands in the range of 2260 – 2220 cm$^{-1}$ show the presence of Nitrile (C= N). The strong bands around the wave number 1650- 1560 cm$^{-1}$ show the presence of NH$_2$ (amide) stretching vibration. The strong absorption broad sharp band around 3600- 3200 cm$^{-1}$ can be attributed to the presence of –OH (alcohol/phenol) stretching vibration. The wave number ranges 2950-2850 cm$^{-1}$ is associated with the stretching of alkyl -CH- vibration The wave number stretch with the range 1740- 1690 cm$^{-1}$ is associated with aldehyde (C=O) stretch. The band range 3500– 3300 cm$^{-1}$ shows the presence of primary and secondary amide. Of special interest in the study is the strong absorption bands at 1550- 1460 cm$^{-1}$, 1300 - 1100 cm$^{-1}$ which are associated with secondary amide and primary amide (NH$_2$) with wave number range 1200- 1050 cm$^{-1}$ and the absorption at 1600 – 1500 cm$^{-1}$, which is associated with (C-N= O) nitro amine and nitroso compounds (N-N-O). Also present is the spectra absorption at 860-680 cm$^{-1}$ associated with aromatic -CH stretching corresponding to aliphatic and aromatic C-H group.

The absorption spectra show that DEMS and ATSP inhibitor molecules contain S, O and N atoms in their functional groups (O-H, N-H, C=O, C=S, C-H and N=O) and are likely sites for coordination with the metal surfaces.

## Influence of inhibitor concentration on corrosion rate and inhibition efficiency
Despite the different concentrations of the inhibitors, DEMS and ATSP in the acidic solution, slight weight loses were still observed on the mild steel. The corrosion rate, surface coverage and inhibition efficiency (I%) of the inhibitors after 3 h exposure time and at temperature 303 K were evaluated using weight loss technique and are displayed in Table 1.

**Table 1:** Corrosion rate (CR), surface coverage (θ) and inhibition efficiency (I %) of the mild steel in 1.0 M HCl in different concentrations of the inhibitors (DEMS and ASTP) at 303 K

| DEMS | | | | | ASTP | | | | |
|---|---|---|---|---|---|---|---|---|---|
| Inhibitor conc (g l$^{-1}$) | Weight loss | (CR) | θ | I % | Inhibitor conc (g l$^{-1}$) | Weight loss | (CR) | θ | I % |
| Blank | 1.7476 | 0.0129 | - | - | Blank | 1.7476 | 0.0129 | - | - |
| 0.2 | 0.9437 | 0.007 | 0.4600 | 46.00 | 0.2 | 1.1495 | 0.0085 | 0.3422 | 34.22 |
| 0.4 | 0.9108 | 0.0067 | 0.4788 | 47.88 | 0.4 | 0.9701 | 0.0072 | 0.4449 | 44.49 |
| 0.6 | 0.7117 | 0.0053 | 0.5928 | 59.28 | 0.6 | 0.7849 | 0.0058 | 0.5509 | 55.09 |
| 1.0 | 0.5087 | 0.0038 | 0.7089 | 70.89 | 1.0 | 0.5866 | 0.0043 | 0.6643 | 66.43 |
| 2.0 | 0.3296 | 0.0024 | 0.8114 | 81.14 | 2.0 | 0.3983 | 0.003 | 0.7721 | 77.21 |

Results showed a decrease in weight loss with a corresponding increase in inhibition efficiency (% E) as concentrations of the inhibitors (DEMS and ATSP) increased. The obtained results suggest that the employed inhibitors suppressed the corrosion rate of the mild steel. This observation may be explained to result from the creation of a strong barrier between the mild steel and the HCl solution as the inhibitor molecules gradually adsorbed onto the mild steel surfaces leading to a retardation in the mild steel dissolution, and a similar interpretation had been made [17].
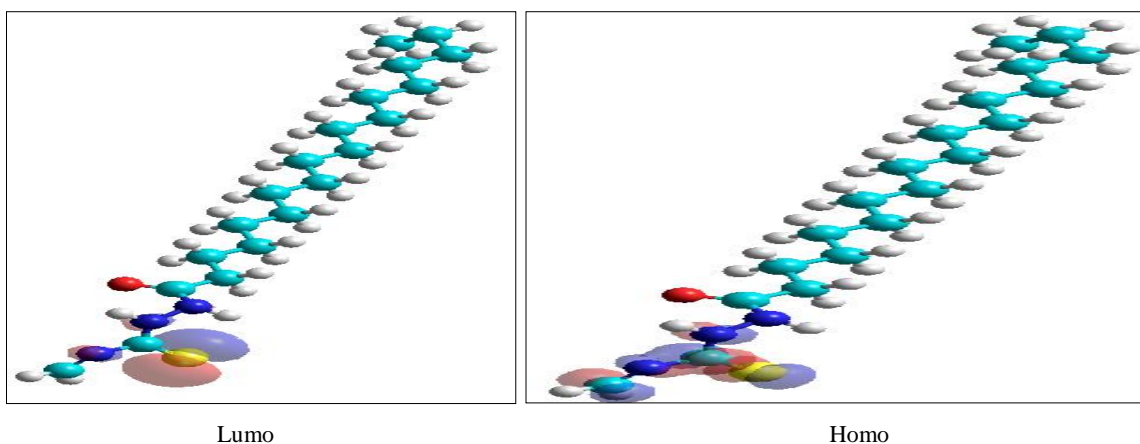
**Quantum Chemical Study**
The effects of molecular structure on inhibition efficiency of the Schiff bases were determined through quantum chemical parameters using semi-empirical (PM3) method. The geometries of the optimized lowest energy conformer together with the Homo and Lumo densities for each of the studied
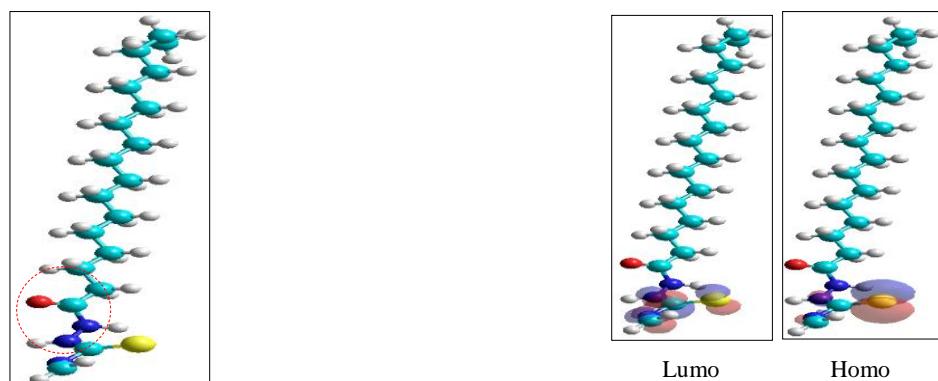
structures of DEMS and ATSP are shown in Figures 1-4.
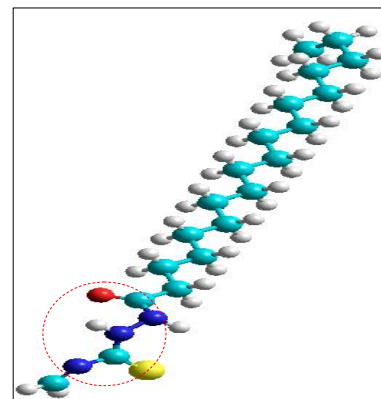


**Fig 1:** Optimised geometry of DEMS Schiff base inhibitor



Lumo                                    Homo

**Fig 2:** Molecular orbital of DEMS Schiff base showing Lumo and Homo



**Fig 3:** Optimised geometry of ATSP Schiff base (inhibitor)



Lumo          Homo

**Fig 4:** Molecular orbital of ATSP Schiff base showing

**Table 2:** Derived quantum chemical parameters from semi - empirical (PM3) method for the Schiff bases, DEMS and ATSP

| Quantum chemical parameters | DEMS | ATSP |
|---|---|---|
| $E_{Homo}(eV)$ | -9.175 | -9.175 |
| $E_{Lumo}(eV)$ | -1.382 | -1.380 |
| Total energy($kJmol^{-1}$) | -90835.100 | -87386.500 |
| $\Delta E(eV)$ | 7.793 | 7.795 |
| $\eta(eV)$ | 3.8965 | 3.8975 |
| $\delta(eV^{-1})$ | 0.25664 | 0.25658 |
| $\mu(D)$ | 1.664 | 1.654 |
| X | 5.2785 | 5.2775 |
| $\Omega$ | 3.5753 | 3.5731 |
| $\Delta N_{max}$ | 0.6773 | 0.6771 |

## Global Molecular Reactivity

The chemical parameters that are related to the reactivity of the two inhibitor molecules (DEMS and ATSP) are shown in Table 2. These parameters help in predicting the reactivity of a molecular species. According to the Frontier molecular Orbital theory [15], the energy of the molecular orbital ($E_{Homo}$ and $E_{Lumo}$) are significant parameters for the prediction of a chemical species. Molecular reactivity is mainly located at the $E_{Homo}$ and $E_{Lumo}$ and it plays vital roles in the prediction of molecular reactivity of a molecule (the inhibitor).

## Homo Energy ($E_{Homo}$)

This indicates the tendency of the molecule to donate electrons. Inhibition efficiency of an inhibitor increases with increasing $E_{Homo}$. A high $E_{Homo}$ values indicate that a molecule has the tendency to donate electrons to appropriate acceptor molecule with low empty molecular orbital. The inhibitor molecules, DEMS and ATSP have tendency to donate electron(s) as shown in Table 2. The negative sign of the $E_{Homo}$ indicates that the adsorption of the inhibitors on the metal surface follow the mechanism of physisorption and a similar interpretation had been given [18].

## Lumo Energy ($E_{Lumo}$)

The $E_{Lumo}$ indicates the tendency of the molecule to accept electrons. Inhibition efficiency increases with decrease in the value of $E_{Lumo}$ of a molecule, thus an $E_{Lumo}$ indicates the tendency of a molecule to accept electron from an appropriate donor molecule [19, 20]. The inhibitor molecules, DEMS and ATSP have low tendency to accept electron from any donor as seen from the estimated values shown in Table 2.

## Energy gap ($\Delta E$)

The energy gap ($\Delta E$) has to do with excitation of an electron from $E_{Homo}$ to $E_{Lumo}$. It determines the reaction activity between the inhibitor molecules and the metal surface [21]. Low $\Delta E$ indicates strong interaction and results in high inhibition efficiency [22]. From Table 2, the energy gap with respect to inhibition efficiency follows the trend DEMS > ATSP, indicating that DEMS is a better inhibitor compared to ATSP.

## Dipole Moment ($\mu$)

It was reported by Tang *et al.* [23] and Zhang *et al.* [24] that high values of dipole moment enhance inhibition efficiency. From the results shown in Table 2, inhibitor molecule DEMS has higher inhibition efficiency when compared to the ATSP inhibitor molecule.

## Softness ($\delta$)

Softness ($\delta$) is one of the properties which help in determining molecular stability and reactivity. The results in Table 2 show that the inhibitor molecule DEMS, which has a higher $\delta$ and lower $\Delta E$ value has a higher reaction activity compared to the inhibitor molecule ATSP with lower $\delta$ and higher $\Delta E$ value. Inhibitor molecule, DEMS with high $\delta$ and low $\Delta E$ has higher reaction activity and thus induces higher efficiency and this is in accordance with interpretations given in previous work [25].

## Hardness ($\eta$)

Hardness ($\eta$) is the measure of the resistance of an atom to charge transfer. Hard molecules have large energy gap. Table 2 shows that the inhibitor molecule, DEMS has $\Delta E$ value as 7.793 and $\eta$ value as (3.8965) while the inhibitor molecule ATSP has $\Delta E$ value as 7.795 and $\eta$ value as 3.8975. Hardness for these inhibitors follows the trend ATSP > DEMS, indicating that DEMS is a better inhibitor for the mild steel surfaces due to the lower energy gap.

## Electronegativity (X)

This is used to describe the intrinsic capability of an atom in a molecule to attract electron and could be estimated using equation (8). From Table 2, it could be seen that the inhibition efficiencies for the inhibitors follow the order DEMS >ATSP, for the higher the value of X, the stronger it attract electrons [26].

## Electrophilicity Index ($\omega$)

Electrophilicity as defined by equation (9) [27]. The inhibitor with higher ($\omega$) tends to have stronger interaction with the metal surface and as such induces higher inhibition efficiency. Table 2 shows the value of $\omega$ for the inhibitor molecules, DEMS (3.5753) and ATSP (3.5731). The inhibition efficiencies (I %) of the inhibitor molecules follow the trend, DEMS > ATSP.

## Number of transferred electrons ($\Delta N$)

This is an indication of the ability of a molecule to donate electrons and bind onto the surface of a metal. It does not represent the actual number of electrons transferred during an electrochemical reaction but rather gives a rough estimate of the possible trend in electron transfer among selected molecules. The compound that has the highest ability to transfer electron is considered to have the highest tendency to interact with metal surface. From the results shown in Table 2, the $\Delta N$ for the inhibitor molecules, DEMS and ATSP follows the trend DEMS > ATSP. According to Lukovits *et al.* [28], if the value of $\Delta N$ is less than 3.6, the efficiency of inhibition increases with increasing electron donating ability of the inhibitor at the metal surface.

From the calculated global reactivity parameter, it can be concluded that the inhibitor, DEMS has more potency to adsorb onto the surfaces of the mild steel than the inhibitor, ATSP for it has smaller value of $\Delta E$, higher value of $\mu$, high value of $\delta$, lower value of $\eta$, higher value of X, and higher value of $\Delta N$. All these make DEMS to have high inhibition efficiency.

## Conclusion

The quantum chemical studies showed that there exit a relationship between inhibition efficiencies of the inhibitors (ATSP and DEMS) and $E_{Lumo}$, $E_{Homo}$, $\Delta E$, dipole moment ($\mu$), hardness ($\eta$), softness ($\sigma$) and $\Delta N$. The negative value obtained for $E_{Homo}$ indicates that the mechanism of adsorption was physisorption.

Weight loss measurement established that inhibition

efficiency increased with increase in concentration of inhibitor from 0.2 g/l to 2.0 g/l at a temperature of 303 K. The two inhibitors, DEMS and ASTP had inhibition efficiencies of 81.14 % and 77.212 % respectively at a concentration of 2.0 g/l in 1M HCl for the immersion period of 3 h. From quantum analysis, DEMS had highest inhibition efficiency because it possessed highest $E_{HOMO}$ energy in comparison with ASTP and it was more capable of releasing electrons to the mild steel active sites. Mulliken population analysis on DEMS and ASTP revealed sites for nucleophilic and electrophilic attacks that aid anchorage onto mild steel surface as obtained from quantum chemical calculations.

The inhibition of the mild steel could be generally attributed to the adsorption of the Schiff base molecules on the surfaces of the metals which leads to blocking of the active sites of the mild steel and consequently suppressed the mild steel dissolution.

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