Corrosion inhibition, surface adsorption and computational studies of *Momordica charantia* extract: a sustainable and green approach

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Abstract

The aerial parts extract of *Momordica charantia* plant were used for the corrosion resistance of carbon steel in the acidic medium (0.5 M H₂SO₄) utilizing weight loss method, Tafel and Electrochemical Impedance Spectroscopy. The state of mixed inhibitor adsorption on the carbon steel surface is shown by potentiodynamic polarization. *M. charantia* achieved the extraordinary inhibition efficiency of 93.51% at 500 mg/L of inhibitor concentration. Scanning electron microscopy and atomic force microscopy were used to know about the thin layer which was formed on the surface of carbon steel for its protection from corrosion and the adsorption of inhibitor was shown by UV–vis. spectroscopic technique. Fourier Transform Infrared Spectroscopy technique confirmed the existence of functional groups and the heteroatoms exhibit in the inhibitor. Adsorbance by the inhibitory molecules on the carbon steel surface followed the Langmuir adsorption isotherm. Hypothetical investigations (computational) showed a very valuable report. All acquired outcomes ensure that *M. charantia* extract can procedure an effectual preventing layer and restrict the corrosion procedure.

Keywords Carbon steel · EIS · Theoretical studies · Polarization · AFM · SEM

1 Introduction

Carbon steel is an alloy which can be easily found and have a lot of mechanical properties in its development, industrial process and its production [1]. We have used carbon steel here as carbon steel shows specific properties when it comes in contact of acidic medium [2, 3]. As we know that acidic medium is used by different modern processes like pickling, descaling and cleaning and in all these processes carbon steel get corroded. Green inhibitors adsorbed on the metal surface using π -electronic systems, and S, P, N, O [4]. They got adsorbed on the metal surface physically (physisorption) or/and chemically (chemisorption) and protect the metal from being corroded. This adsorption of inhibitory molecules can be chemical by creating a physical or covalent bond (chemisorption) or/and

through electrostatic interaction (physisorption) [5]. Corrosion inhibitors are accepted to act by engrossing and making a defensive film structure on the metal surface. As corrosion is an electrochemical procedure, the adsorbed layer can be considered as a twofold layer framed at the interface between the electrolyte and the outside of the metallic electrolyte [6]. The idea of the dealing of adsorbed particles on the carbon steel surface is evaluated utilizing adsorption and thermodynamic models. Sulfuric corrosive has been utilized in acidifying, formation fracture and improving oil recuperation was used to imitate the corroding media. Genuine alloys and metals respond chemically or electrochemically with the destructive media to make a steady compost where metal misfortune happens [7]. The manure in this manner made is known as a corrosion product, and the metal surface becomes rusts. Corrosion

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includes the exchange of metal particles into the solution at active zones (anode), expulsion of electrons from metal in less dynamic regions (cathode), ionic current in the solution, and electric flow in metal. The cathodic procedure is required to give an electron acceptor as oxygen or oxidizing operators or hydrogen particles [8]. Right now, because of its inexhaustible, biodegradable, cheap and non-harmful properties, biomaterials of plant can be utilized as a natural and sustainable corrosion inhibitors, like fruits, seeds, plant waste, and so on [9]. The phytochemicals in plant have incredible potential as economical, non-poisonous and inexhaustible sources of a wide scope of industrially significant natural chemical compounds. The yield of described green products as well as the corrosion reticence capabilities of the plant extracts differ extensively depending on the part of the plant and its location. Natural phytochemicals extracted from several portions of the plants are environmentally friendly, effective and economical [10]. A few investigations have been accounted for by different scientist utilizing such characteristic items as consumption inhibitor for various metals in various media [11–20]. But the vast majority of the natural corrosion inhibitors took higher inhibitor concentration to show their highest inhibition performance.

M. charantia generally grows up to 5 m (16 ft). This herb bears simple, alternate leaves 4–12 cm across, with 3–7 deeply separated lobes. It belongs to the *Cucurbitaceae* family and known as Bitter gourd, Bitter melon, Bitter squash, and Karela. It is commonly found all throughout India, China, East Asia, South Asia and Southeast Asia. Aerial parts of *M. charantia* are very easily available in the market. This plant contains Kuguacin-F, Cucurbitane triterpenoid and Pentanorcucurbitacin as its key phytochemicals [21, 22]. Figure 1 shows the picture of *M. charantia*'s prime phytochemical constituents.

The current observation is expected for the *M. charantia* extraction and study the anti-corrosion assets in the acidic corrosive media which depends upon weight loss measurements followed by electrochemical estimations. In addition, the inhibitor adsorption on the carbon steel surface has been examined employing SEM and AFM. The UV–vis. and FT-IR spectroscopic measures have been implied to verify the adsorption phenomenon and the presence of various functional groups. Toward confirm the experimental results, quantum parameters were generated per the density functional theory (DFT) method.

Fig. 1 Major phytochemical constituents of *Momordica charantia* herb **a** Cucurbitane triterpenoid **b** Kuguacin-F and **c** Pentanorcucurbitacin

2 Experimental

2.1 Electrolytes preparation and applicable electrode, methodology for inhibitor

Dry *M. charantia* aerial parts were collected and they were verified by Dr. A. A. Bhat in Biotechnology department (Lovely Professional University) INDIA. The crude materials were washed well under the running tap water and then they were sterilize using distilled water. They were then dried under shade and crushed to powered. The powered material about 400 g were then extracted using 1000 mL of solvent in a round bottom flask. The filtrate was then collected and concentrated under controlled temperature and pressure in a rotatory evaporator. The extract was concentrated. Finally, around 15% of extract yield was acquired. 1.00 cm × 1.00 cm × 0.03 cm formed carbon steel specimen were applied in electrochemical and weight loss examinations. The elemental composition of used carbon steel coupon is recorded in Table 1. The carbon steel specimens were abraded by unique grades of emery papers then rinsed through distilled water and acetone. The sulfuric acid solution was mitigated to 0.5 M H₂SO₄ for use as an aggressive media.

2.2 Weight loss studies

Weight loss (gravimetric) assessments were carried out following the ASTM G 31–72 method for 24 h [23]. All the assessments of weight loss were made at 298 ± 0.5 K utilizing a water circulated thermostat (PPI Fini X48). The size of the corrosive solution was 500 mL for the weight loss experiments. The pre-weighted carbon steel coupons were dipped in the corrosive media. After the immersion time, the carbon steel coupons were left out, washed through acetone, dehydrated using nitrogen flow and finally weighted utilizing Shimadzu electronic balance (BL-220H/D455006313).

2.3 Electrochemical studies

The electrochemical techniques (Tafel and EIS) were conducted using the CHI760C electrochemical workstation. Examinations were get done at 298 ± 0.5 K in 0.5 M sulfuric corrosive, including a few inhibitor concentrations. The size of the corrosive media was 250 mL for the electrochemical tests. A regular three-electrode assembly was applied. The carbon steel with a working territory of 1 cm² was utilized as

the working electrode (WE). The platinum terminal utilized as an auxiliary electrode and the saturated calomel anode (SCE) fixed to a luggin capillary was utilized as the reference electrode. Prior to each investigation, the WE was drenched in the test solution for an hour to settle corrosion potential values (E_{corr}). The Tafel bends were acquired at ± 250 mV versus SCE with an scanning rate of 1 mV/s. The EIS spectra were examined with a frequency change between 100 kHz to 0.01 Hz through an amplitude perturbation of 0.005 V [24].

2.4 Surface examinations

To know about the morphology carbon steel surface, AFM-Model: NT-MDT-INTEGRA followed by SEM-Model: LEO-435 VP techniques were used. The micrographs of pre-treated carbon steel coupons in 0.5 M sulfuric acid were examined, without and with the inhibitor extract [25]. After immersing the pre-treated carbon steel specimens from 0.5 M H₂SO₄ solution without and with 500 mg/L extract for 24 h, the surfaces of carbon steel specimens were rinsed with ultrapure water and acetone, and dried.

2.5 Spectroscopic studies

The carbon steel specimen before and after the immersion in the test solution has been investigated by Shimadzu UV-1800 UV–visible absorption spectrophotometer. The obtained spectrums was used to explain the inhibition mechanism. The information of the presence of various functional groups was also obtained using FT-IR technique. The plant extract blended with KBr pallet for FT-IR investigation in the Shimadzu FTIR 8400S spectrophotometer with wavenumber 400–4000 cm^{−1} [26].

2.6 Theoretical investigation

Theoretical findings were conducted to a meaningful understanding of the adsorption mechanism. Quantum chemical calculations were operated as theoretical investigations. It is well known that plant extracts contain several phytochemicals. For theoretical studies, we monitored the presence of the main phytochemical component in the *M. charantia* extract. Theoretical studies were performed using DFT (Density Functional Theory) in combination with the Hyperchem software package. Key factors are extracted from molecules whose structure is optimized [27]. The MD simulation was performed employing the Forcite module of Materials Studio 8.0 software developed by BIOVIA Inc. They

Table 1 Nominal composition (wt%) of the used carbon steel

Element Symbol	Fe	Ni	Cu	P	Mn	Cr	Si	C
% Composition	97.83	0.27	0.43	0.12	0.43	0.45	0.39	0.08

were run in a simulation box (1.98 nm × 1.98 nm × 4.01 nm) with periodic boundary conditions. The lower Fe sheet box consisted of an upper solvent layer (containing the particle of interest containing 500 water molecules per liter). Fe (110) was selected as the iron substrate as the test surface because it has a densely packed structure, the most stable, cast on a six-layer Fe plate. In this model, each layer had 64 Fe atoms representing a unit cell (8 × 8). Andersen's thermostat applied the entire system at 298 K, controlled by Canon NVT set under simulation of 1.0 ffs μ 1500 cm, utilizing the COM-PASSIA force field. The electrostatic interactions were calculated using the Ewald sum technique sum of the collection method based on atoms for the Van der Waals interactions.

3 Outcomes and analysis

3.1 Spectroscopic analysis

FT-IR technique has been conducted to verify the several functional groups existing in the plant extract. FT-IR spectra of pure inhibitor extract has been shown in Fig. 2. Peaks obtained for different functional groups have been shown in Table 2. In pure inhibitor, peaks for different functional groups like; -OH, C-O and CH₂ confirmed the presence of heteroatoms in the plant extract.

The adsorption fact was also checked with UV-visible spectroscopy procedure. The analysis was done twice that is before and after the corrosion examination. The UV-vis. spectra of inhibitor in both the modes shown in Fig. 3. Prior to the corrosion measurement, the inhibitor solution shows an adsorption peak at 276.00 nm which shows the n-π* transition. It is clear from Fig. 3 that this peak reallocated afterwards the corrosion assessment. When looking

Fig. 2 FT-IR spectra of pure *Momordica charantia* extract

at both spectra, a huge change in the adsorption band was discovered, which is associated with the inhibiting molecules adsorption on the outside of carbon steel [28].

3.2 Weight loss (gravimetric) and electrochemical measurements

The weight loss technique is the easiest procedure for obtaining a basic idea of the relation between the inhibitor concentration and corrosion resistance efficiency of the inhibitor. These experiments have been carried out at 298 ± 0.5 K for 24 h with various inhibitor concentrations. The following comparison was employed to obtain the corrosion rate [29]:

$$C_R = \frac{K \times W}{A \times t \times \rho} \quad (1)$$

Here

- C_R = corrosion rate (mmy⁻¹)
- W = weight loss of carbon steel (g)

Table 2 FT-IR peaks for pure *Momordica charantia* extract

FT-IR (Wavenumber; cm ⁻¹)		
1	3304.17	O-H stretching of alcohol
2	2926.11	C-H stretching
3	1043.52	C-O stretching

Fig. 3 Ultraviolet-visible spectra of *Momordica charantia* extract before and after immersion of carbon steel specimen for 24 h at 298 K

- $K=8.76 \times 10^4$ (constant)
- $\rho=7.86 \text{ g cm}^{-3}$ (density of Fe)
- t =immersion time (h)
- A =area of the carbon steel coupon

The following equations were used to calculate the efficiency of the inhibitor and the coverage values of the surface [2]:

$$IE(\%) = \frac{C_R^0 - C_R^i}{C_R^0} \times 100 \quad (2)$$

$$\theta = \frac{C_R^0 - C_R^i}{C_R^0} \quad (3)$$

Here

- θ shows surface coverage values
- C_R^i shows the corrosion rate in the presence of inhibitor
- C_R^0 shows the corrosion rate of the carbon steel in the absence of the inhibitor

The outcomes acquired with the weight loss measurements are introduced in Table 3, which show an expansion in the inhibitor concentration, an abatement in the consumption rate and an expansion in the restraint effectiveness. The most noteworthy corrosion resistance value of 90.80% was accomplished at 500 mg/L. The outcomes were utilized to follow the Langmuir adsorption isotherm. Langmuir adsorption isotherm shows a chart between C/θ and C , appeared in Fig. 4(a), which shows a straight line with a regression coefficient (R^2) near 1. It verifies the development of a monolayer on the outside of the carbon steel. This can be depicted as [30]:

$$\frac{C}{\theta} = \frac{1}{K_{ads}} + C \quad (4)$$

Here

- θ denotes the surface coverage
- C denotes inhibition concentration
- K_{ads} denotes the equilibrium adsorption constant

The polarization curves were obtained for the carbon steel in 0.5 M H_2SO_4 at $298 \pm 0.5 \text{ K}$ nonappearance and existence of different concentrations of *M. charantia*. Figure 4b demonstrates the Tafel curves, starting with zero to different concentrations of *M. charantia* inhibitor in 0.5 M H_2SO_4 . Obtained Tafel plots give the values for Corrosion current density (i_{corr}), Corrosion potential (E_{corr}), Cathodic and Anodic Tafel slopes (β_c and β_a), and corrosion inhibition efficiency (IE) applying the following equation [31]:

$$IE(\%) = \frac{i_{corr}^0 - i_{corr}^i}{i_{corr}^0} \times 100 \quad (5)$$

Here

- i_{corr}^0 represents the corrosion current density without inhibitor
- i_{corr}^i represents the corrosion current density with inhibitor

Table 3 represents the polarization results for the carbon steel in the nonappearance and appearance of several inhibitor concentrations. The corrosion potential (E_{corr}) is within 85 mV in relation to the blank, suggesting its behaviour as a type of mixed inhibitor. The Tafel bends show abatement in the incline of the anode and cathode bends with the expansion of the inhibitor. This is because of the way that the particles of the active inhibitor molecules are get adsorbed on the outside of the carbon steel and the reduction of the steel. With every expansion of the inhibitor concentration, the thickness of the corrosion current density (i_{corr}) decreases constantly. β_a and β_c changed essentially with inhibitor concentration. This

Table 3 Corrosion parameters for carbon steel in 0.5 M H_2SO_4 without and with various concentrations of *M. charantia* extract obtained by weight loss, and electrochemical experiments (EIS and Tafel) at $298 \pm 0.5 \text{ K}$

Weight loss			Tafel					EIS		
Conc. (mg/L)	C_R (mm y^{-1})	IE (%)	$-E_{corr}$ (mV vs. SCE)	i_{corr} ($\mu\text{A cm}^{-2}$)	β_a (mV/dec)	$-\beta_c$ (mV/dec)	IE (%)	R_{ct} ($\Omega \text{ cm}^2$)	C_{dl} ($\mu\text{F cm}^{-2}$)	IE (%)
Blank	11.33	–	465	890.90	141.66	164.25	–	15.71	269.00	–
100	2.48	78.09	446	160.90	44.52	110.87	81.93	86.41	155.00	81.82
200	1.85	83.61	458	108.30	46.81	118.56	87.84	115.78	154.00	86.43
300	1.53	86.45	467	99.40	44.48	115.86	88.83	156.11	153.00	89.93
400	1.28	88.62	474	79.60	46.16	116.86	91.05	174.62	137.00	91.00
500	1.04	90.80	468	63.10	49.43	117.59	92.91	242.22	120.00	93.51

Fig. 4 **a** Langmuir adsorption isotherm, **b** polarization curves, **c** Nyquist, **d** bode plots for carbon steel in 0.5 M H₂SO₄ with 0–500 mg/L concentrations of *M. charantia* extract at 298 K, **e** used equivalent circuit and **f** OCP plots

demonstrates the adsorption of the dynamic segments of *M. charantia* was impacted both by the components of iron disintegration and by the systems of the oxygen

decrease response. This is because of the solid coordination bond between the free iron orbital and the free electrons, which are available in the active parts of the

concentrate of *M. charantia*. *M. charantia* inhibitor shows the lowest value of i_{corr} ($63.10 \mu\text{A cm}^{-2}$) specifies its best corrosion resistance with 92.91% IE at 500 mg/L.

To examination the impact of *M. charantia* extract concentration for the carbon steel in 0.5 M H_2SO_4 at 298 ± 0.5 K, the electrochemical impedance spectroscopy technique was performed to obtain a stable state. E_{OCP} (open circuit potential) was showing a stable steady state following an hour of immersion as shown in Fig. 4f. A charge transfer resistance (R_{ct}), a double layer capacitance (C_{dl}) and a solution resistance (R_s) are portions of the circuit. The outcomes are appeared in Table 3. Figure 4c shows Nyquist outlines for carbon steel without and with specific concentration of *M. charantia*. Figure 4d shows the Bode outlines for carbon steel and Fig. 4e shows the used equivalent circuit. The impedance values were acquired utilizing the accompanying equation [32]:

$$IE(\%) = \frac{R_{ct} - R_{ct}^0}{R_{ct}} \times 100 \quad (6)$$

Here

- (R_{ct}) shows the charge transfer resistance with inhibitor
- (R_{ct}^0) shows the charge transfer resistance without inhibitor

As the inhibitor concentration expands, C_{dl} reduces and R_{ct} increments, as appeared in Table 3. These outcomes affirm the high adsorption level of *M. charantia* on the outside of carbon steel. *M. charantia* indicated 93.51% hindrance effectiveness at 500 mg/L with R_{ct} ($242.22 \Omega \text{ cm}^2$) and confirms its better performance against the corrosive medium.

3.3 Theoretical analysis

3.3.1 Quantum chemical calculations

As it was discussed earlier that the plant extract contains various phytochemicals. Here, in the present study, three main phytochemicals of the *M. charantia* were selected for the computational studies. Figure 5 shows the optimized, HOMO and LUMO orbitals of the Kuguacin-F, Cucurbitane triterpenoid and Pentanorcucurbitacin. Followings equations have been used to calculate different quantum chemical parameters [33]:

$$\Delta E = E_{LUMO} - E_{HOMO} \quad (7)$$

$$\eta = \frac{1}{2} (E_{LUMO} - E_{HOMO}) \quad (8)$$

$$\chi = -\frac{1}{2} (E_{LUMO} + E_{HOMO}) \quad (9)$$

$$\Delta N = \frac{\chi_{Fe} - \chi_{inh}}{2(\eta_{Fe} - \eta_{inh})} \quad (10)$$

$$\sigma = \frac{1}{\eta} \quad (11)$$

$$\Delta E_{BackDonation} = -\frac{\eta}{4} \quad (12)$$

$$\pi = -\chi \quad (13)$$

Here;

- χ_{inh} and η_{inh} represents the electronegativity and hardness of inhibitor molecule
- χ_{inh} and η_{Fe} means the electronegativity and hardness of iron

Table 4 covers the fundamental assets of Kuguacin-F, Cucurbitane triterpenoid and Pentanorcucurbitacin, which are of enormous significance due to their impact on the collaboration of electrons among the inhibitor molecule and the carbon steel surface.

- Cucurbitane triperpenoid (-3.15 eV) indicates a high value of E_{HOMO} representing its extraordinary ability to deliver the electrons to the carbon steel.
- Pentanorcucurbitacin has the lowermost values of E_{LUMO} (-2.17 eV) shows the highest capacity to donate electrons to Fe.
- Again, Cucurbitane triperpenoid (1.36 eV) demonstrates the at a low level value of ΔE representing its strong power of the [Fe-Cucurbitane triperpenoid] complex.

As a conclusion, as the various molecule shows different values for different parameters, suggesting a mixture of different interactions may take place and the inhibitor as a mixture of various phytochemical performances as a mixed kind of inhibitor and support the experimental outcomes.

3.3.2 MD simulations

The dynamic process was performed and the whole system was balanced until the temperature and energy of the system were balanced [34]. The low energy adsorption configurations of the three inhibitors adsorbed on the Fe

Fig. 5 Optimized structures and HOMO & LUMO obtained by DFT/B3LYP/6-31G+ (d,p) method of major phytochemical constituents (Cucurbitane triterpenoid, Kuguacin-F and Pentanorcucurbitacin) of *Momordica charantia*

Table 4 Calculated quantum chemical parameters of major phytochemical compounds of *Momordica charantia* obtained from the DFT/B3LYP/6-31G+ (d,p) method

Molecule	E_{HOMO} (eV)	E_{LUMO} (eV)	ΔE (eV)	ΔN (e)	$\Delta E_{\text{Back-Donation}}$ (eV)	η (eV)	σ (eV^{-1})	χ (eV)	π (eV)
Cucurbitane triperpenoid	−3.15	−1.79	1.36	3.31	−0.17	0.68	1.46	2.47	−2.47
Kuguacin-F	−4.12	−0.81	3.31	1.36	−0.41	1.65	0.60	2.47	−2.47
Pentanorcucurbitacin	−9.30	−2.17	7.13	0.17	−0.89	3.56	0.28	5.73	−5.73

(110) surface are shown in Fig. 6. As can be seen in Fig. 6, the adsorption centres of the examined inhibitors on the surface of Fe (110) are the electrons of the benzene rings, the oxygen, sulphur and nitrogen atoms. Inhibitor molecules are adsorbed in a nearly flat orientation on the iron surface to maximize coating and surface contact, providing a strong interaction for the adsorbate/substrate system

[35, 36]. The strength of corrosion inhibitors absorbed on iron surface can be expressed by the adsorption energy (E_{ads}), so it will be very interesting to study the adsorption energies of inhibitors absorbed on iron surface when considered the inhibition performance. The adsorption energy in solution can be calculated by the following equations [37]:

Fig. 6 Side and top views of most stable adsorption configurations for three inhibitors on Fe(110) surface

$$E_{\text{interaction}} = E_{\text{total}} - (E_{\text{surface+solution}} + E_{\text{inhibitor}}) \quad (14)$$

$$E_{\text{binding}} = -E_{\text{interaction}} \quad (15)$$

where E_{total} is the total potential energy of the system, which include iron crystal, the adsorbed inhibitor molecule and solution; $E_{\text{surf+water}}$ and $E_{\text{inh+water}}$ are the potential energies of the system without the inhibitor and the system without the iron crystal, respectively; E_{water} is the potential energy of the water molecules [38].

The adsorption energies in this work were calculated from the average adsorption energy of the obtained equilibrium configurations. The E_{ads} obtained are -336.9 , -380.3 and -413.4 kJ/mol for THA-H, THA-Br and THA-OCH₃, respectively [39]. It is seen that the adsorption energies are negative and therefore spontaneous adsorption can be expected [40]. In general, the higher the absolute value of E_{ads} , the stronger the interaction between the inhibitor and the metal surface [41]. It is obvious that THA-OCH₃ has higher absolute

values of E_{ads} than THA-H and THA-Br, and, therefore, exhibits better inhibitory properties for carbon steel, which is in agreement with experimental results [42].

3.4 SEM and AFM analysis

Figure 7 shows micrographs (SEM & AFM) of carbon steel surfaces before and after corrosion tests with and without inhibitors.

- Figure 7a shows polished carbon steel SEM and AFM micrographs. The minimum surface roughness reached (2.99 nm) and the maximum height (60 nm).
- Figure 7b shows the corroded surface of carbon steel after a corrosion test without inhibitors. Rough micrographs can be seen because metals are very sensitive to corrosion and shows the highest surface roughness at (138.81 nm) and maximum height (2100 nm).
- Figure 7c shows the carbon steel surface after a corrosion test with the inhibitor. This shows that the pres-

Abraded
CS

(a)

Without
inhibitor

(b)

With
inhibitor

(c)

Fig. 7 SEM micrographs and AFM images of the carbon steel surface after 24 h of immersion at 298 K in 0.5 M H_2SO_4 : **a** abraded carbon steel, **b** without inhibitor and **c** with the inhibitor (500 mg/L)

ence of inhibitors covers the surface and prevents corrosion processes with much lower surface roughness (16.22 nm) and maximum height of 0.25 μm (250 nm).

This is much less than the results obtained without inhibitors. This shows that *M. charantia* absorbs on the metal surface, creating a protective layer to prevent corrosion on carbon surfaces [43].

Fig. 8 Proposed mechanism of the adsorption behaviour of Cucurbitane triperpenoid on carbon steel surface

3.5 The proposed mechanism

To decide the impact of resistance of *M. charantia* on the carbon steel surface with the presence of 0.5 M sulfuric acid, it is essential to compute the consequences of this test and associate them with the chemical, electronic and structural properties of the inhibitor particles [44]. The *M. charantia* contains numerous phytochemical substances that contain heteroatoms. These molecules behave as Lewis bases and structure coordination bonds with free d-orbital of iron and adsorb on the carbon steel surface, framing a defensive covering on the outside of the carbon steel to secure against corrosive media. Thus, it tends to be said that the connection between inhibitor particles and iron can be interceded by chemisorption and physisorption. Retro-donation can likewise be made utilizing electronic pair-electrons [45]. This phenomenon likewise been demonstrated by hypothetical examinations and the after effects of polarization [46–49]. Figure 8 shows the proposed system for carbon steel surface adsorption strategy by Cucurbitane triperpenoid.

4 Conclusion

The result of the anti-corrosion properties of *M. charantia* in the 0.5 M H_2SO_4 corrosive medium for carbon steel was investigated by electrochemical analysis followed by weight loss tests, SEM & AFM. Electrochemical examination evaluations verified that *M. charantia* signifies inhibition efficiency of more than > 93% at 500 mg/L to prevent corrosion of the carbon steel. Authentication of numerous

functional groups including heteroatoms and unsaturation in the plant extract constituents was done with the help of FT-IR technique. Verification of the formation of coordination bonds between inhibitor molecules and Fe^{2+} was done with the help of UV-vis. technique. The surface adsorption of *M. charantia* inhibitor was investigated by SEM supported by AFM technique. Computational investigation has been done using DFT and MD simulations for the main constituents.

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Compliance with ethical standards

Conflict of interest All the authors declare that they do not have any conflict of interest.

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