Investigation of Sulfonium-Iodide-Based Ionic Liquids to Inhibit Corrosion of API 5L X52 Steel in Different Flow Regimes in Acid Medium

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ABSTRACT: The present work deals with the corrosion inhibition mechanism of API 5L X52 steel in 1 M H₂SO₄ employing the ionic liquid (IL) decyl(dimethyl)sulfonium iodide [DDMST⁺][I⁻]. Such a mechanism was elicited by the polarization resistance (R_p), potentiodynamic polarization (PDP), and electrochemical impedance spectroscopy (EIS) techniques, both in stationary and dynamic states. The electrochemical results indicated that the corrosion inhibition was controlled by a charge transfer process and that the IL behaved as a mixed-type corrosion inhibitor (CI) with anodic preference. The experimental results revealed maximal inhibition efficiency (IE) rates up to 93% at 150 ppm in the stationary state, whereas in turbulent flow, the IE fell to 65% due to the formation of microvortexes that promoted higher desorption of IL molecules from the surface. The Gibbs free energy of adsorption (ΔG°_ads) value of −34.89 kJ mol⁻¹, obtained through the Langmuir isotherm, indicated the formation of an IL monolayer on the metal surface by combining physisorption and chemisorption. The surface analysis techniques confirmed the presence of FeₓOᵧ, FeOOH, and IL on the surface and showed that corrosion damage diminished in the presence of IL. Furthermore, the quantum chemistry calculations (DFT) indicated that the iodide anion hosted most of the highest occupied molecular orbital (HOMO), which eased its adsorption on the anodic sites, preventing the deposition of sulfate ions on the electrode surface.

1. INTRODUCTION

In the oil industry, steel corrosion is regarded as one of the most serious problems to be dealt with due to the exposure of this metallic material to different conditions throughout a variety of industrial operations. In particular, during the extraction and transport of oil, the formation of acid media and flow conditions increase the corrosion rate, which provokes the degradation of metallic structures, and therefore, pipeline failures and damage of equipment and installations, which are part of different processes as a result of the shortening of the useful life of steel pieces.¹,² Diverse methods conceived to control corrosion at the industrial level have been put into practice; among these strategies, corrosion inhibitors (CIs) have been employed, which have been accepted willingly for their low cost and easy application with different alloys and corrosive media.³,⁴ CIs control the corrosion reactions that take place on the metal by an adsorption process that is affected by different factors such as the nature and surface charge of the metal, electronic structure, steric factors, aromaticity, functional groups with double and triple bonds, and high-density heteroatoms (N, O, S, and P) present in the inhibiting organic molecules.⁵,⁶

Inorganic compounds like chromates, nitrates, molybdates, phosphates, silicates, and arsenic have been used as CIs, which when combined with the oxide layer provide the metal surface with passivation protection.⁷ Notwithstanding, these compounds represent potential danger for the health, for they are highly toxic chemicals.⁸ Currently, environmental regulations concerning the use of chemical substances have limited the application of toxic compounds, which has led to the synthesis of low-toxicity CIs that are easy to handle and biodegradable, i.e., more environmentally friendly like the compounds known as ILs.⁹,¹⁰ These molecules are salts consisting of organic or inorganic anions and organic cations that display, in general, melting points below 100 °C, i.e., these are liquids at ambient temperature and possess unique features that stem from the
arrangement and chemical distribution of their ions; in addition, the ILs have negligible vapor pressure, thermal stability, nonflammability, high ionic conductivity, and wide electrochemical stability spectrum.\(^{11−13}\)

In the literature, the inhibiting properties in acid medium of ILs with imidazolium,\(^{14,15}\) pyridinium,\(^{16,17}\) ammonium,\(^{18−20}\) pyridazinium,\(^{21,22}\) and sulfonium\(^{23−25}\) cations have been reported. These last compounds have been studied in sulfamic,\(^{23}\) phosphoric,\(^{24}\) and hydrochloric and sulfuric\(^{25}\) acids, reporting IE values from 84 to 98%. Their inhibition behavior has been attributed to the nature of the substituent groups: the presence of π electrons that are capable of interacting with the negative charge of the metal, aliphatic chains that promote hydrophobic properties, but mainly due to the capacity of S to accept electrons.

The iodide anion effect has been the subject matter of several studies, and it has been reported that the IE values of ILs with iodide anion have been higher than those displayed by other

| Chemical structure | Medium/Metal | IE (%) | Ref |
|-------------------|--------------|--------|-----|
| Triethylsulphonium bis(trifluoromethylsulfonyl) imide | 304 stainless steel/5% sulfamic acid | 120 ppm: 97.8% | 23 |
| 4-nitrophenacyl-dimethyl-sulphonium bromide | Mild steel/0.67 M H\(_3\)PO\(_4\) | 5.0×10\(^{-3}\) M: 84% | 24 |
| Trimethylsulphonium iodide | Cr\(_3\) mild steel/0.5 M H\(_2\)SO\(_4\) | 300 ppm: 82% | 25 |
| 2-hydroxyethyl-trimethyl-ammonium iodide | Mild steel/1 M HCl | 17.91×10\(^{-4}\) M: 92.04% | 26 |
| 1-hexyl-3-methylimidazolium iodide | Mild steel/1 M HCl | 5×10\(^{-3}\) M: 93.1% | 27 |
| Cross-linked poly(N-methyl-4-vinylpyridinium) iodide | St-37 carbon steel/1 M H\(_2\)SO\(_4\) | 40 ppm: 94.5% | 17 |
| 1,1’[1,4 phenylenebis(methylene)]bis(3(carboxymethyl)imidazol-3-iium) chloride | Carbon steel/0.5 M HCl | 1 mM: 94.8% 1 mM+1 mM KI: 96.2% | 29 |
| L-tryptophane | Mild steel/1 M HCl | 0.2 mM: 72.8% 0.2 mM + 0.005 mM KI: 92.5% | 30 |
| (3-morpholinopropyl)-1-phenylmethanimine | API X65 steel/0.5 M H\(_2\)SO\(_4\) | 0.5 mM: 57.6% 0.5 mM + 50 mM KI: 98.6% | 31 |
anions, as shown in Table 1. In this context, in 2008, Verma et al. analyzed ILs with the cation 2-hydroxyethyl-trimethyl-ammonium and three different anions, finding that the IL with iodide anion had higher IE values than those with acetate and chloride anions. The anion influence on the inhibition process was studied by Mashuga et al. comparing ILs based on 1-heykyl-3-methylimidazolium with four different anions. It was reported that the IE obtained with the IL featuring the iodide anion (79%) or trifluoromethanesulfonate (81%) was slightly higher than those values given by fluoro-substituted anions such as tetrafluoroborate (78%) or hexafluorophosphate (73%).

In addition, iodide has also been employed in acid corrosion as synergic agent in inhibition processes of organic compounds. Cao et al. and Guo et al. showed that the IE of $\text{I}^-$[$1,4\text{-phenylenebis(methylene)}]$ bis[$3\text{(carboxymethyl)}$-imidazolium] chloride and $\text{I}$-tryptophane, respectively, increased significantly in the presence of KI as a synergic agent. Cao et al. indicated that the addition of KI could provide better IE by decreasing the IL concentration. Moreover, Guo et al. suggested that iodide adsorbed on a metal surface tended to form joining bridges between organic cations and the positively charged iron surface, thus stabilizing the CI adsorption process; the CI adsorption process; cations and the positively charged iron surface, thus stabilizing the metal surface tended to form joining bridges between organic molecules in the metal surface toward more negative values, facilitating the adsorption of positively charged species. According to the aforementioned, the inhibition properties that distinguish iodide from the halide group are its higher capacity to donate electrons, easy polarization, high hydrophobicity, greater atomic radius, and low electronegativity.

In addition to the effect exerted by the chemical structure on the corrosion inhibition mechanism, the medium conditions are essential factors that affect the performance of the CIs. Due to the multiple transfer phenomena of corrosive species and CI molecules in the metal–CI interphase, the proposal of a corrosion inhibition mechanism in the stationary state is complex. Moreover, in the presence of flow, the adsorption mechanism is affected by factors such as shear stress ($\tau_{\text{REE}}$) and formations of microvortexes that modify the adsorption and desorption of CI molecules and corrosive species. In contrast, the chemical structure of CIs is fundamental for the formation of stable films under flow conditions. For this reason, in the present work, a novel IL was synthesized, characterized, and evaluated in its inhibiting properties: decyl(dimethyl)sulfonium iodide [DDMS$^-$]. The IL was evaluated as CI of API 5L X52 steel under stationary and flow conditions [Reynolds numbers ($N_{\text{REE}}$) from 1000 to 5000] in 1 M H$_2$SO$_4$ solution. To analyze the inhibiting effect exerted by [DDMS$^-$], the $R_p$ potentiodynamic polarization (PDP), and electrochemical impedance spectroscopy (EIS) electrochemical techniques were used. Afterward, the obtained data were processed by different adsorption isotherm models. Scanning electron microscopy/energy-dispersive X-ray spectroscopy (SEM/EDS), diffuse reflectance infrared Fourier transform spectroscopy (DRIFTS), and X-ray photoelectron spectroscopy (XPS) surface analyses complemented the electrochemical results. Finally, to describe the behavior of the [DDMS$^-$] molecule, molecular simulation at DFT B3LYP/MIDIX theory level was carried out.

2. RESULTS AND DISCUSSION

2.1. Electrochemical Tests. 2.1.1. $E_{\text{OCP}}$ as a Function of Time. Figure 1 shows the open-circuit potential ($E_{\text{OCP}}$) values for API 5L X52 steel in 1 M H$_2$SO$_4$ with and without IL.

![Figure 1. $E_{\text{OCP}}$ plot as a function of time of API 5L X52 steel in 1 M H$_2$SO$_4$ with and without IL.](https://doi.org/10.1021/acsomega.2c05192)

| Concentration (ppm) | $E_{\text{OCP}}$ (V vs Ag/AgCl) |
|---------------------|----------------------------------|
| 0                   | -420                             |
| 25                  | -430                             |
| 50                  | -435                             |
| 75                  | -440                             |
| 100                 | -445                             |
| 125                 | -450                             |
| 150                 | -455                             |

$E_{\text{OCP}}$ values were displaced toward more positive values with increasing IL concentration with respect to the blank. These $E_{\text{OCP}}$ displacements because of IL addition indicate both the adsorption of IL molecules on the metal surface and the formation of an inhibiting film. Furthermore, it was found that the $E_{\text{OCP}}$ stability started from 800 s.

2.1.2. Polarization Resistance. Figure 2 shows the $R_p$ behavior as a function of: (a) the [DDMS$^-$] concentrations and (b) different $N_{\text{REE}}$. In general, it is observed that the slope of the current density ($i$) vs overpotential ($\eta$) diminished with the CI concentration (C), indicating that the presence of IL increased the $R_p$ of the metal–electrolyte interphase due to the adsorption of inhibiting molecules from the formation of a layer on the steel surface in 1 M H$_2$SO$_4$. This inhibiting film produced resistance to the flow of electrons participating in the redox reactions, generating changes in the kinetics of the electrochemical reactions involved in the corrosion process. Furthermore, the slope increase at different $N_{\text{REE}}$ in the absence and presence of IL can be observed, which indicates that the diffusive processes under flow conditions modified the IL adsorption and interfacial properties of the metal–electrolyte system.

Table 2 displays the $R_p$ results and it can be seen that the maximal values were obtained at C above 100 ppm of CI and at the stationary state. The $I_{\text{IE}}$ was calculated from eq 1 [34–37]

$$I_{\text{IE}} = \left( \frac{R_p^{\text{in}} - R_p^{\text{max}}}{R_p^{\text{in}} \times 100} \right)$$

where the superindices $\text{in}$ and $\text{max}$ refer to the experiments in the presence and absence of CI, respectively.

2.1.3. Potentiodynamic Polarization. Figure 3 presents the PDP behavior as a function of C and different $N_{\text{REE}}$. It is observed that the increase in C caused the displacement of the potentiodynamic curves toward low current density values with
respect to the blank. Under flow conditions, the $N_{RE}$ increase intensified the corrosion process in the absence and presence of IL, displacing the potentiodynamic curves toward higher current density values, which indicates more serious surface damage in the presence of IL. At the stationary state (Table 2), lower current density values in the presence of CI are reported; this fact can be attributed to the growing blocking of active sites as a function of the [DDMS$^{+}$] concentration, which replaced water molecules and aggressive ions such as $H^+$, $H_3O^+$, $O_2^-$, and $SO_4^{2-}$ on the metallic substrate. The optimal adsorption process of the CI molecules on the metal surface occurred at a concentration of 100 ppm; in contrast, higher $i$ values were obtained under flow conditions due to the wall shear stress ($\tau_{RDE}$) increase. This behavior

Table 2. Electrochemical Parameters Obtained by the $R_p$ Technique of API SL X52 Steel in 1 M H$_2$SO$_4$ with Different Concentrations of [DDMS$^{+}$]$^-$

| system     | $N_{RE}$ | C (ppm mM$^{-1}$) | $E_{corr}$ (mV) | $R_p$ ($\Omega$ cm$^2$) | IE$_{R_p}$ (%) |
|------------|----------|-------------------|-----------------|--------------------------|----------------|
| blank      | 0        | 0/0               | 466 ± 0         | 50 ± 1                   |                |
| 1000       | 0        | 0/0               | 437 ± 0         | 44 ± 0                   |                |
| 2000       | 0        | 0/0               | 444 ± 0         | 38 ± 2                   |                |
| 3000       | 0        | 0/0               | 436 ± 0         | 23 ± 1                   |                |
| 4000       | 0        | 0/0               | 439 ± 0         | 16 ± 0                   |                |
| 5000       | 0        | 0/0               | 439 ± 0         | 16 ± 0                   |                |
| [DDMS$^{+}$]$^-$ | 0   | 25/0.076          | 444 ± 3         | 95 ± 2                   | 47.14 ± 1.78  |
|            | 0        | 50/0.151          | 426 ± 4         | 371 ± 7                  | 86.43 ± 0.45  |
|            | 0        | 75/0.227          | 429 ± 5         | 473 ± 24                 | 89.30 ± 0.34  |
|            | 0        | 100/0.303         | 418 ± 6         | 699 ± 35                 | 92.51 ± 0.22  |
|            | 0        | 125/0.378         | 420 ± 4         | 673 ± 18                 | 92.42 ± 0.23  |
|            | 0        | 150/0.454         | 419 ± 3         | 674 ± 17                 | 92.56 ± 0.22  |
| 1000       | 150/0.454| 394 ± 1           | 317 ± 0         | 85.98 ± 0.01             |                |
| 2000       | 150/0.454| 381 ± 1           | 278 ± 1         | 86.28 ± 0.06             |                |
| 3000       | 150/0.454| 376 ± 0           | 151 ± 1         | 84.49 ± 0.13             |                |
| 4000       | 150/0.454| 380 ± 4           | 87 ± 2          | 81.14 ± 0.48             |                |
| 5000       | 150/0.454| 388 ± 3           | 48 ± 1          | 67.36 ± 0.79             |                |

Figure 2. $R_p$ of API SL X52 steel in 1 M H$_2$SO$_4$ with (a) different [DDMS$^{+}$]$^-$ concentrations at the stationary state and (b) with 150 ppm of [DDMS$^{+}$]$^-$ under flow conditions at 298 K.

Figure 3. Potentiodynamic polarization of API SL X52 steel in 1 M H$_2$SO$_4$ with (a) different [DDMS$^{+}$]$^-$ concentrations at the stationary state and (b) with 150 ppm of [DDMS$^{+}$]$^-$ under flow conditions at 298 K.
pattern was originated by the flow regime change, which provoked higher desorption rate of the CI film as $N_{IE}$ was increased and then, the progressive diminution of IE. The $IE_{PDP}$ was calculated by eq 2\textsuperscript{34,35}

$$IE_{PDP} = \left( \frac{i_{corr}^{inh} - i_{corr}^{0}}{i_{corr}^{inh}} \right) \times 100$$

where the superindexes $inh$ and 0 refer to the experiments in the presence and absence of CI, respectively.

At the stationary state, the reported corrosion potential ($E_{corr}$) displacement values with respect to the blank fall within the interval ranging from 43 to 65 mV, i.e., within the ±85 mV interval, which indicates that [DDMS$^+$] matches the behavior pattern of a mixed-type CI, retarding both the cathodic and anodic reactions occurring during the corrosion process\textsuperscript{36,39} with anodic preference due to the displacement toward positive potentials ($E_{corr}^{inh} < E_{corr}^{0}$).\textsuperscript{40} This phenomenon is related to the preferential adsorption of [I$^-$/ and the contribution of the [DDMS$^+$] cations on the anodic and cathodic sites, respectively, which diminished the attack of water molecules and aggressive ions in the medium. Under flow conditions, the IL anodic preference was not affected sensibly. Notwithstanding, the $\beta$, values under flow conditions, reported in Table 3, are slightly higher than those obtained at the stationary state. This increase suggests that the IL modified the kinetics of the reduction reactions, thus retarding the hydrogen evolution by CI adsorption. Then, it can be concluded that the contribution by the IL anions and cations to the inhibition process is the same.

2.1.4. Electrochemical Impedance Spectroscopy. Figure 4 shows the Nyquist impedance curves at stationary and dynamic states and in the absence and presence of IL, where the formation of depreciated semicircles can be observed, which is attributed to the surface roughness and heterogeneity. In contrast, in the presence of [DDMS$^+$], an increase in the semicircle diameter as a function of C can be observed, which indicates that the corrosion process was controlled by the charge transfer resistance through the interface.\textsuperscript{41} This behavior pattern occurred at both stationary and dynamic states. In contrast, the diameter decrease in the semicircles as $N_{IE}$ increased indicates that the flow made the charge transfer and desorption rate of the species adsorbed on the metallic surface grow.\textsuperscript{42}

In the absence of IL and the stationary state, the formation of an inductive loop in the low-frequency region can be observed, which can be attributed to intermediate reactions related to the adsorption of water, aggressive ions ($H^+$, $H_2O^+$, $O^{2-}$, and $SO_4^{2-}$)
and/or insoluble solution corrosion products.\textsuperscript{43,44} This behavior pattern was also observed at the dynamic state in the absence and presence of IL, which was caused by diffusive processes of the electrolyte in the metal/IL interface. Nevertheless, in the presence of [DDMS\(\text{I}^-\)] at the stationary state, the inductive loop disappeared, which suggests the stabilization of the charge transfer processes because of the formation of a more homogeneous and stable inhibiting film than the one produced at the dynamic state.

Figure 5 shows the Bode plots at stationary and dynamic states. In the presence of IL, a higher displacement of the \(\mid Z\mid\) values and phase angle than those obtained with the blank can be observed, which suggests a reduction of the adsorption of aggressive ions, thus stabilizing the surface. Furthermore, the diagrams show a maximal point for the phase angle at intermediate frequencies, which indicates the existence of a relaxation time constant (\(\tau_{dl}\)) associated with the charge transfer resistance (\(R_{ct}\)) and capacitance of the electric double layer (\(C_{dl}\)).\textsuperscript{45} At the stationary state, the presence of another relaxation time constant is also observed, which is related to a capacitive process due to the accumulation of corrosion products/CI, despite the presence of the IL, the corrosive medium ions are adsorbed on the surface causing their damage.

The equivalent electrical circuits (EECs) employed to fit the experimental data from the impedance spectra are shown in Figure 6.\textsuperscript{45-48} What follows is the description of the physical interpretation of the EEC elements: \(R_s\) represents the solution resistance; \(R_{ct}\) is the resistance to the charge transfer on the surface, which depends on the charge transfer between the electronic conduction region (metal) and the ionic conduction region (solution); \(CPE_{dl}\) is a constant phase element (CPE) related to the \(C_{dl}\), which suggests the accumulation of charge in that interphase; \(R_f\) is an inductive resistance and \(L\) is an inductor and both elements represent the relaxation process of the intermediates involved in the oxidation reactions (H\(^+\), H\(_2\)O\(^+\), O\(^2^-\), and SO\(_4^{2-}\)); and \(CPE_f\) and \(R_f\) are the capacitance and resistance related to the formation of corrosion products and/or the IL film on the metal surface.

The constant phase elements (CPEs) in Figure 6 represent the nonideal capacitances of the EIS spectra, which were calculated with eq 3

\[
C = (Y_0 R^{1-n})^{1/n}
\]

where \(Y_0\) is the proportional factor and \(n\) is an empirical exponent between 0 and 1, which is related to the surface...
heterogeneity, where \( n \) values close to 1 are characteristic of homogeneous surfaces.39

Tables 4 and 5 show the EIS parameters at stationary and dynamic conditions, respectively. It is observed that the \( R_s \) values do not present variation (\( \Delta R_s \sim 1 \Omega \cdot \text{cm}^2 \)) at different \([\text{DDMS}^+^-]\) concentrations and flow conditions. Likewise, at the stationary state, the \( R_t \) and \( C_I \) values do not show significant changes in the inhibitor film—solution interphase with increasing \([\text{DDMS}^+^-]\) concentration.

In contrast, the \( R_s \) values diminished as the \( N_{\text{IE}} \) increased as shown by the diameter in the Nyquist spectra. However, in the presence of \([\text{DDMS}^+^-]\) and independent of the \( N_{\text{RE}} \) it is observed that the \( R_t \) values grew significantly with the IL concentration, suggesting that the corrosion process was controlled by the charge transfer resistance through the interface by the IL adsorption.41 The electrical double layer of the steel—electrolyte system behaves electrically as a capacitor, i.e., there is an electric charge and discharge process that leads to the corrosion process by electron transfer. This process is represented with the \( C_d \) electric element. At the stationary state, the \( C_d \) values diminished with respect to the blank, indicating the formation of an IL homogeneous film that blocked the reaction sites distributed uniformly in the interphase.46 Notwithstanding, with the \( N_{\text{IE}} \) increase, a gradual growth of the \( C_d \) values is observed, which suggests the modification of the metal—solution interphase due to the reduction of the double layer thickness and/or to the increase of the dielectric constant,40 i.e., to the formation of a thinner and more heterogeneous CI film than at the stationary state, which can be attributed to the electrolyte diffuse processes in the metal/IL interphase as a consequence of the surface damage caused by the partial hydromechanical removal of the film.51

The impedance parameter (\( \tau_{dl} \)) was calculated employing eq 4 and it is reported in Table 4

\[
\tau_{dl} = C_d R_{ct}
\]

It is observed that the \( \tau_{dl} \) values increased with the CI concentration. This parameter measures the time required by the metal—solution interphase to return to an equilibrium state. This fact indicates that a higher number of IL molecules adsorbed on the surface makes the electric charge and discharge process slower, which favors the reduction of the corrosion rate.52 In contrast, the process dynamic state provokes the diminution of \( \tau_{dl} \), i.e., the acceleration of electron transfer (Table 5).

Likewise, it is observed that the \( R_s \) and \( L \) values diminished with increasing \( N_{\text{RE}} \). This behavior pattern is observed at low frequencies in the Nyquist plots (Figure 3) and is associated with an increase in the desorption rate of the intermediate products of redox reactions (\( \text{H}^+, \text{H}_2\text{O}^+, \text{O}_2^{2-}, \text{and SO}_4^{2-} \)) and adsorbed \([\text{DDMS}^+^-]\) molecules.

At the stationary state (Table 4), the increase in CI concentration raised the \( n \) values, i.e., the surface homogeneity; this fact confirmed the diminution of the corrosion surface damage in the presence of an inhibitor. In contrast, under flow conditions, \( n \) values were diminished (Table 5), which indicated the increase in the corrosion rate by the desorption of inhibitor molecules from the surface as a consequence of the generated shear stress.

The \( R_s \) values were calculated by the sum of the resistive elements corresponding to each EEC. It can be observed that the \( R_s \) values were increased by the IL concentration, improving the IE \(_{\text{EIS}} \) calculated with eq 3. However, at the dynamic state, the reduction of the \( R_s \) values as a function of \( N_{\text{RE}} \) is revealed, which exerted a negative effect on the IE \(_{\text{EIS}} \) falling to 22% with the flow regime change.

2.1.5. Inhibition Efficiency. As it can be observed in Figure 7, \([\text{DDMS}^+^-]\) presented IEs within the interval ranging from 40 to 94% at the stationary state, which can be associated with the competition of chemical species to occupy available surface active sites and suggests that on the cathodic and anodic sites occurred the preferential adsorption of \([\text{DDMS}^+^-]\) and \([\Gamma^-]\) with respect to \( \text{H}^+, \text{H}_2\text{O}^+, \text{O}_2^{2-}, \text{and SO}_4^{2-} \). In addition, it is revealed that from the optimal CI concentration of 100 ppm, the maximal IE of 93% was reached.

According to the obtained results, the IL adsorption diminished slightly in laminar regime (\( N_{\text{RE}} = 1000–2000 \)), which can be attributed to the increase in the transport of CI molecules toward the metal surface that kept the IL adsorption and formation of complexes,53,54 which in turn reduced the \( \tau_{\text{EDE}} \) negative effect and IE in 8% with respect to the stationary state. The IE fell to 86% from the transitory regime (\( N_{\text{RE}} \geq 3000 \)) due to the formation of microvortexes that promoted higher desorption of IL molecules from the surface, making it difficult to form a continuous CI film.55 This negative effect exerted by the increasing electrode rotation speed was also reported by Ismail et al. and Bennhammed et al. who observed the
| Table 5. EIS Parameters Obtained for API 5L X52 Steel in 1 M H$_2$SO$_4$ with 150 ppm of [DDMS$^-$] in Flow Conditions |
|-------------------------------------------------------|
| **regimen** | **1000** | **1500** | **2000** | **2500** | **3000** |
|transient | 150/0.454 | 150/0.454 | 150/0.454 | 150/0.454 | 150/0.454 |
|laminar | 150/0.454 | 150/0.454 | 150/0.454 | 150/0.454 | 150/0.454 |
| turbulent | 150/0.454 | 150/0.454 | 150/0.454 | 150/0.454 | 150/0.454 |

| N$_a$ (ppm m$^{-1}$) | 0.148 ± 0.005 | 0.143 ± 0.006 | 0.149 ± 0.008 | 0.147 ± 0.010 | 0.149 ± 0.008 |
|C$_P$ (ppm m$^{-1}$) | 0.194 ± 0.028 | 0.194 ± 0.028 | 0.194 ± 0.028 | 0.194 ± 0.028 | 0.194 ± 0.028 |
|K$_c$ (Ω·cm$^{-2}$) | 2.8 ± 2.0 | 2.8 ± 2.0 | 2.8 ± 2.0 | 2.8 ± 2.0 | 2.8 ± 2.0 |
|R$_c$ (µG) | 0.149 ± 0.005 | 0.149 ± 0.005 | 0.149 ± 0.005 | 0.149 ± 0.005 | 0.149 ± 0.005 |
|C$_f$ (µG·m$^{-2}$) | 10.56 ± 1.30 | 10.56 ± 1.30 | 10.56 ± 1.30 | 10.56 ± 1.30 | 10.56 ± 1.30 |
|

The results confirm the influence of iodide on the inhibition process, which played a major role in the obtained IE of [DDMS$^-$]. Also, the presence of π orbitals in S with high capacity to donate electrons and the hydrophobic properties of the decyl chain contributed to the adsorption process as reported in the literature.

2.2. Adsorption Isotherms. To theoretically describe the nature of the interactions between the IL and the steel surface during the inhibition process, the experimental data were fitted employing adsorption isotherm models such as Langmuir, Freundlich, Temkin, and Frumkin, where θ is the surface fraction covered by the CI ($θ = 1/IE$), which was obtained by the average of the IE values by the $R_p$ and PDP techniques, C is the IL concentration in mM, and $K_{ad}$ is the adsorption equilibrium constant.

The Langmuir isotherm of the H$_2$SO$_4$–[DDMS$^-$] system is shown in Figure 8. The additional isotherm models are presented in Figure S1. The linear fitting of the experimental data produced a correlation coefficient ($R^2$) of 0.988, a slope of 0.99, and an intercept of 0.035. This empirical model suggests the formation of a [DDMS$^-$] monolayer, where the adsorption occurred only on a finite number of defined sites, energetically identical and equivalent with neither lateral interactions nor steric hindrance among the CI molecules, where just one of them can occupy an active site on the surface. The $K_{ad}$ value was equal to 2.82 × 10$^4$ m$^{-1}$ and was calculated by the reciprocal of the y-intercept ($K_{ad} = 1/b$) of the linear regression in Figure 8. This parameter allows the computation of the Gibbs free energy of adsorption ($ΔG_{ad}$) from eq 5.

$$ΔG_{ad}^{0} = -RT \ln(K_{ad})$$

where $R$ is the universal gas constant (8.314 kJ mol$^{-1}$K$^{-1}$), $T$ is the system absolute temperature ($K$), and 55.5 is the water concentration in the solution. The $ΔG_{ad}^{0}$ of [DDMS$^-$] was equal to $-35.36$ kJ mol$^{-1}$, which suggests that the IL adsorption mechanism involved the combination of physisorption (electrostatic forces) and chemisorption (coordinate bonds) which implied a higher interaction between the IL and the steel surface. The adsorption process can be mainly related to the chemical properties of [Γ] due to its high ionic radius and electronegativity lower than other halides, and the boosting inhibition effect by forming intermediate bridges between the metallic substrate and the [DDMS$^-$] cation, which promoted the production of a CI monolayer on the surface with a hydrophobic region (cation alkyl chains) toward the solution core. Furthermore, iron presents affinity to sulfur heteroatoms, which promoted the formation of [DDMS$^-$]–Fe complexes that were adsorbed directly on the metallic surface.

2.3. Surface Analysis Techniques. 2.3.1. SEM. Figure 9a displays the micrographs of the steel surface after its immersion in the acid medium without IL. Surface damage and the palpable mass loss due to steel oxidation and the presence of corrosion products can be observed. In contrast, the metallic samples
protected with 150 ppm of [DDMS\(^-\)]. Figure 9b, present a homogeneous morphology, which confirms the adsorption of the IL molecule, thus blocking the active sites, diminishing the surface damage and mass loss of the metallic samples caused by the medium attack.

Figure 9c shows the EDS spectrum of API SL X52 steel in the absence of IL. Signals corresponding to S and O can be observed, which are characteristic elements of the corrosion products that are common in steel−H\(_2\)SO\(_4\) systems like Fe\(_{3}\)O\(_4\), FeOOH, and FeSO\(_4\). The low intensity of S and O peaks is related to the sample rinsing process after its retrieving from the corrosive medium, which favored the removal of excess corrosion products.

The EDS spectrum in the presence of IL, Figure 9d, displays the reduction of the O signal, which suggests the wind down of the production of corrosion products due to the formation of low-solubility complexes that limited the interaction between corrosive ions and the metallic surface. Likewise, a predominant Fe signal can be observed, which confirms the properties of [DDMS\(^-\)] as CI of steel in acid medium.

2.3.2. DRIFTS. Figure 10 shows the DRIFTS spectra of the steel surface attacked for 4 h in 1 M H\(_2\)SO\(_4\) in the presence of 150 ppm of inhibitor. The sample has a characteristic absorption band of the Fe−O bond of Fe\(_{3}\)O\(_4\) at 568 cm\(^{-1}\).\(^{69,70}\) The signal appeared at around 1130 cm\(^{-1}\), which corresponds to the alkysulfonium group. The bands at ~1643 cm\(^{-1}\) correspond to iron oxide and the alkysulfonium group too, while the band at 1736 cm\(^{-1}\) corresponds to the remaining H\(_2\)SO\(_4\).\(^{71,72}\) The O−H stretching bands from physisorbed molecular water can be observed at 3386 cm\(^{-1}\), while the signals at 2957 and 2854 cm\(^{-1}\) belong to the C−H stretching signal of the inhibitor aliphatic group and Fe\(_{3}\)O\(_4\).\(^{73,74}\) The C−H scissoring of the alkyl chain signals appears at 1459 cm\(^{-1}\).

2.3.3. XPS. XPS technique was used to analyze the oxidation state of the elements present on the API SL X52 steel surface attacked for 4 h in 1 M H\(_2\)SO\(_4\) in the presence of 150 ppm of inhibitor. The general XPS spectra indicate the presence of Fe\(_{2}\)p), O (1s), C (1s) S (2p), and I (3d). Fe is attributed to the metal substrate. Oxygen and sulfur signals are related mainly to corrosion products and salts deposited on the metal surface due to the corrosive medium type. The high carbon signal (60.4%) is ascribed not only to adventitious carbon but also to the presence of CI on the metal surface. There is also an iodine signal, which can be associated with the corrosion inhibitor structure.

Figure 11a shows the high-resolution C 1s peak, which deconvoluted to three peaks. The main peak at 284.8 eV corresponds to the remaining H\(_2\)SO\(_4\) while the signal at 286.4 \(\pm\) 0.8 eV is attributed to the corrosion inhibitor structure. The bands at 288.6 eV is attributed to the presence of C=S bonds present in the molecule; whereas the signal at 2957 and 2854 cm\(^{-1}\) correspond to sulfate species (SO\(_4^{2-}\)).

The O 1s region, Figure 11c, the main peak at 531.9 eV corresponds to oxygen in the hydroxide form, which is present in oxyhydroxides (FeOOH),\(^{76,77}\) whereas the signal at 530.1 eV is associated with oxygen in oxidized form as ferrosoferric oxide (Fe\(_{3}\)O\(_4\)),\(^{85,86}\) while the peak at 532.9 eV is ascribed to oxygen in the sulfate group (SO\(_4^{2-}\)).\(^{87}\)

The Fe 2p spectrum exhibits mainly three peaks (Figure 11d): (1) at 706.8 eV (Fe 2p\(_{3/2}\)) and 719.6 eV (Fe 2p\(_{1/2}\)), corresponding to metal Fe\(^{3+}\); (2) at 710.4 eV (Fe 2p\(_{3/2}\)) and

![Figure 7](https://example.com/image7.png)

**Figure 7.** IE for API SL X52 steel in 1 M H\(_2\)SO\(_4\) (a) at different [DDMS\(^-\)] concentrations under the stationary state and (b) with 150 ppm of [DDMS\(^-\)] under flow conditions.

![Figure 8](https://example.com/image8.png)

**Figure 8.** Langmuir isotherm for the API SL X52 steel electrode in 1 M H\(_2\)SO\(_4\) solution with [DDMS\(^-\)] at 298 K.

![Figure 10](https://example.com/image10.png)

**Figure 10.** DRIFTS spectra of the steel surface attacked for 4 h in 1 M H\(_2\)SO\(_4\) in the presence of 150 ppm of inhibitor.
The two main signals located at 619.3 and 630.8 eV (Figure 11e) can be ascribed to the photoemission peaks from I 3d$_1$ and I 3d$_3$, respectively, and correspond to the iodide ion.\textsuperscript{90,91}

2.4. Computer Simulation Analysis. 2.4.1. Geometry. Figure 12 shows the optimal [DDMS$^+$I$^-$] structure. The absence of imaginary frequencies confirms the system structural stability. To take the molecule to the ground state, neuter charge multiplicity 1 (singlet) was employed. In the optimal structure, the methyl and decyl groups were distributed outward to the plane with respect to sulfur (trigonal pyramidal shape). As for [I$^-$], it presented a preference to be located on the alkyl groups linked to sulfur, where the interaction with sulfur was minimized by the carbon and hydrogen atoms,\textsuperscript{92} being the most stable IL form. Regarding the decyl group, it displayed the characteristic linear conformation of a C$_{\geq 4}$ alkyl chain that has been reported in different ILs based on ammonium and imidazolium.\textsuperscript{93–95}

Table 6 reports the lengths and bond angles for each group of atoms. It is observed that the C–C, S–C, and C–H bonds did not present changes in vacuum and aqueous medium [employing COSMO (COnductor-like Screening MOdel) as the solvation model, which uses a dielectric constant of 78.4 to simulate the medium].\textsuperscript{96} In contrast, the space between sulfur and iodide shows slight distancing (∼0.33 Å), which increased the interaction capacity with other molecules. As for the bond angles of the different atom groups, they presented negligible variations when the medium was changed, suggesting that the distribution of the [DDMS$^+$I$^-$] atoms was not affected.
2.4.2. Energetic Analysis. As observed in Figure 13a, the highest occupied molecular orbital (HOMO) works as an electron donor and is located in the [I\(^-\)] ion, whereas (b) the lowest unoccupied molecular orbital (LUMO) functions as an electron acceptor, since it is the cation empty internal orbital and, in this case, it extended itself from [S\(^+\)] to the methyl groups and decyl (C\(_5\))

Regarding the molecular electrostatic potential (MEP) mapping, it is employed to determine reactive sites for electrophilic and nucleophilic attacks by visualizing the charge distribution, which is related to the molecule electron density.

Figure 14 shows the MEP of [DDMS\(\text{I}^-\)], where three different colors can be seen: the red color is associated with the IL most electronegative atom, the iodide anion, and electrophilic reactivity, i.e., with the most susceptible site to electrophilic attacks that cedes electrons to the steel surface to form coordinate bonds with the empty Fe orbital. The blue color located in the cation [S\(^+\)] is related to the nucleophilic reactivity, which is the most susceptible site to nucleophilic attacks, i.e., the site that accepts electrons from other species. Finally, the green color indicates that both the methyl and decyl groups present neutral charge, i.e., their electron configurations are full.

Figure 11. XPS deconvoluted profiles of (a) C 1s, (b) S 2p, (c) O 1s, (d) Fe 2p, and (e) I 3d on the iron sample surface exposed to 1 M H\(_2\)SO\(_4\) with 150 ppm of [DDMS\(\text{I}^-\)] for 4 h at 298 K.
behavior pattern has been observed in works on similar compounds like the one by Haque et al. on N-methyl-N,N,N-trioctylammonium chloride, where the blue region is located on the nitrogen atom of the cationic part, whereas the red region on the chloride ion.

The MEP and MO analyses confirmed that the $\Gamma^-$ anion worked as an electron donor and the $[\text{S}^+]$ cation as an electron acceptor, which represent sites associated with molecule adsorption processes.

2.4.3. Quantum Parameters. For the reactivity analysis of $[\text{DDMS}^+]$, the HOMO ($E_{\text{HOMO}}$) and LUMO ($E_{\text{LUMO}}$) energy values were calculated as shown in Table 7. According to the theory, high $E_{\text{HOMO}}$ values are associated with a higher tendency to donate electrons to appropriate receiving molecules with low-energy empty molecular orbitals. In contrast, low $E_{\text{LUMO}}$ values suggest higher probability of accepting electrons on the metallic surface. The latter indicates that if a CI exhibits high $E_{\text{HOMO}}$ and low $E_{\text{LUMO}}$ it will have better interaction with the metallic surface. As observed in Table 7, $E_{\text{HOMO}}$ is relatively higher and $E_{\text{LUMO}}$ is relatively lower in both media, which suggests that $[\text{DDMS}^+]$ presents a strong tendency to donate and accept electrons.

As for the formation of a transition state, it is due to the interaction between the MOs, i.e., to the energy gap between $E_{\text{HOMO}}$ and $E_{\text{LUMO}}$ ($\Delta E_{\text{LUMO-HOMO}} = E_{\text{LUMO}} - E_{\text{HOMO}}$). This parameter is considered as a descriptor of the molecular activity, where low $\Delta E_{\text{LUMO-HOMO}}$ values indicate higher polarization and an increase in the metal surface reactivity, which is associated with better CI behavior. Table 7 shows that $[\text{DDMS}^+]$ presented a significant difference regarding $\Delta E_{\text{LUMO-HOMO}}$ in both media, which facilitated the adsorption. The $\mu$ values for $[\text{DDMS}^+]$ were equal to 10.77 and 15.92 Debye in vacuum and water, respectively, which resulted to be higher than those reported for water (1.85 Debye), suggesting the preference to replace the adsorbed water molecules on the metallic surface by the IL.

2.5. Corrosion Inhibition Mechanism. As it is known, iodides exert an inhibitory effect on corrosion, which occurs mainly in the anodic sites of the metal surface, slowing down the dissolution of iron in the form of iron cations ($\text{Fe}^{2+}$). Based on theoretical calculations, the iodide anion hosts the most part of HOMO, which attracts it to the anode sites. $\text{Fe}^{2+}(\text{OH})_{\alpha{\text{aq}}}^-$ or $\text{Fe}^{3+}(\text{OH})_{\alpha{\text{aq}}}^-$ are formed at the anodic sites after adsorption of water and hydroxide anions ($\text{OH}^-$), which in turn form corrosion products like magnetite ($\text{Fe}_3\text{O}_4$) or through the path of “green rust” to form iron oxyhydroxides ($\text{FeOOH}$), usually lepidocrocite; the presence of these corrosion products was confirmed by XPS analysis. In the presence of corrosion inhibitor, very few corrosion products typical for the sulfuric acid medium such as rozenite and melanterite were detected, which means that $\Gamma^-$ ions prevented the deposition of sulfate ions on the electrode surface, and hindered sulfate passivation, slowing down the formation on a larger scale of corrosion products that contain the sulfate anion in their structure.

However, since the CI is a mixed-type inhibitor, it acted not only on anodic sites, but also on cathodic sites (Figure 15). As the CI cation is a trialkyl sulfonium derivative, where LUMO is located, it accepted electrons. The sulfonium ion approached the cathode sites on the metal surface by competing with $\text{H}_3\text{O}^+$ and displacing water. Since the CI cation is much larger than $\text{H}_3\text{O}^+$, it removed the protons from the metal surface in the cathode zone and thus slowed down the hydrogen formation reaction. Based on the electrochemical analysis, the CI concentration of 50 ppm caused notable inhibition of the corrosive process (greater than 80%), while from the concentration of 75 ppm, there was no big change in the anticrocorrosive effect (>90%) in laminar and (>80%) transitory flows.

3. CONCLUSIONS
From the present work, the following conclusions were drawn.

- Electrochemical measurements showed that the charge transfer rate in the presence of CI was lower than the blank, which evidenced the formation of a protecting film.
- It was observed that the IE values increased with the IL concentration. Furthermore, under hydrodynamic con-
ditions, the IE values diminished by the desorption of IL molecules due to sheer stress.

- $\Delta G^\circ_{\text{ads}}$ values suggested that the IL adsorption process was a combination of physisorption and chemisorption.
- The surface analyses supported the [DDMS]$^+$ inhibition process, exhibiting less damage of the metallic surface by IL adsorption.

Table 7. Dipole Moment, HOMO and LUMO Energies, and Energy Gap ($\Delta E_{L-H}$) of [DDMS]$^-$

| system   | $-E_{\text{HOMO}}$ (eV) | $-E_{\text{LUMO}}$ (eV) | $\Delta E_{L-H}$ (eV) | $\mu$ (Debye) |
|----------|--------------------------|--------------------------|------------------------|---------------|
| vacuum   | 5.98                     | 1.77                     | 4.21                   | 10.77         |
| water    | 5.91                     | 1.63                     | 4.29                   | 15.92         |

Figure 13. (a) Highest occupied molecular orbital (HOMO) and (b) lowest unoccupied molecular orbital (LUMO) of [DDMS]$^-$]. All are obtained at the optimized geometry in vacuum.

Figure 14. MEP isosurface of [DDMS]$^-$ obtained at the B3LYP/MIDIX level.
The HOMO of [DDMS\(^+\)I\(^-\)] suggested that the iodide anion had the capacity to donate electrons, which eased its adsorption on the anodic sites, thus preventing the depositing of sulfate ions on the electrode surface.

### 4. METHODS

#### 4.1. Synthesis and Characterization of Decyl-(dimethyl)sulfonium Iodide.

The molecular structure of the synthesized IL is depicted in Table 8. Iodomethane (≥99%, Sigma-Aldrich), n-decyl methyl sulfide (97%, Alfa Aesar), and trifluoroacetic acid (99%, Sigma-Aldrich) were employed in the synthesis. The compound was characterized by NMR. The \(^1\)H (300 MHz) spectrum was recorded on a JEOL Eclipse-300 equipment in DMSO-\(d_6\), and chemical shifts were expressed in ppm relative to tetramethylsilane as the internal standard.

Decyl(dimethyl)sulfonium iodide was synthesized according to a similar previously described procedure.\(^{104}\)

4.1.1. Decyl(dimethyl)sulfonium Iodide [DDMS\(^+\)I\(^-\)]. In total, 3.17 g (22.3 mmol) of methyl iodide, 1.60 g (8.47 mmol) of n-decyl methyl sulfide, and 3.12 g (27 mmol) of trifluoroacetic acid were mixed in a 25 mL round-bottom flask, which was closed with a stopper. The reaction was performed at room temperature without stirring. After 30 min, diethyl ether (100 mL) was added to precipitate the product as a white solid. Yield: 2.50 g (89%). \(^1\)H NMR (300 MHz, DMSO-\(d_6\)): 3.34 (s, 6H), 3.88 (m, 2H), 1.91 (s, 2H), 1.60 (m, 2H), 1.33−1.20 (m, 14H), 0.85 (t, \(J = 6\) Hz, 3H).

#### 4.2. Materials and Test Solutions.

API 5L X52 steel coupons with the exposed surface area of 0.289 cm\(^2\) were employed with the following chemical composition (wt %): C ≤ 0.28%, Mn ≤ 1.4%, P ≤ 0.030%, S ≤ 0.030%, V ≤ 0.15%, Nb 0.15%, Ti ≤ 0.15%, Cu 0.25%, Ni 0.25%, Cr 0.25%, Mo 0.15%, and Fe as the main element. Before each test, the metal samples were polished with SiC emery paper (from 400 to 1200). Afterward, they were degreased with acetone−ethanol and exposed to an ultrasonic bath to eliminate particles adhered to the surface. Finally, the polished samples were dried under nitrogen flow.\(^{105}\) 1 M H\(_2\)SO\(_4\) was the corrosive solution and it was prepared with analytic-grade acid and deionized water. [DDMS\(^+-\)] was evaluated at concentrations ranging from 25 to 150 ppm.

#### 4.3. Electrochemical Tests.

Electrochemical tests were performed employing a Potentiostat/Galvanostat AutoLab apparatus model PGSTAT302N. The software NOVA 2.1.4 was used to obtain and analyze the experimental data. A glass electrochemical cell equipped with three electrodes was used:

![Figure 15. Corrosion inhibition mechanism of API 5L X52 steel in 1 M H\(_2\)SO\(_4\) containing [DDMS\(^+-\)].](http://pubs.acs.org/journal/acsodf)

### Table 8. Chemical Structure of the IL Evaluated as CI

| Entry | Name                                      | Chemical Structure | Molecular weight (g/mol) |
|-------|-------------------------------------------|--------------------|--------------------------|
| [DDMS\(^+\)I\(^-\)] | Decyl-(dimethyl)sulfonium Iodide | S\(^+\)C\(_{10}H_{21}\)I | 330.32                   |
counter electrode (platinum 99%), working electrode (API 5L X52 steel), and reference electrode (Ag/AgCl). All of the tests were carried out at 25 ± 1°C in aerated medium. In addition, the tests were run in triplicate and the reported results represent the average.

The working electrode was immersed in the electrolytic solution for 20 min until reaching the \( E_{\text{OCP}} \). The \( R_p \) measurements were carried out within a potential interval of ±25 mV vs \( E_{\text{OCP}} \) whereas that of PDP was of ±250 mV vs \( E_{\text{OCP}} \). Both tests took place at a scanning rate of 0.1666 mV s\(^{-1}\). EIS tests were developed within a frequency interval ranging from 100 kHz to 10 mHz using a sinusoidal wave with 5 mV of amplitude after stabilizing the \( E_{\text{OCP}} \).

The flow tests were performed with a rotating disc Metrohom RDE II 309. The \( N_{\text{RE}} \) was calculated from eq 6\(^{110,111}\),

\[
N_{\text{RE}} = \frac{U \cdot d}{v}
\]

where \( U \) is the cylinder peripheral speed (m s\(^{-1}\)), \( d \) is the electrode diameter (m), and \( v \) is the electrolyte kinematic viscosity (m\(^2\) s\(^{-1}\)). The \( \tau_{\text{RDE}} \) generated on the surface was calculated with eq 7\(^{112,113}\),

\[
\tau_{\text{RDE}} = 0.079 N_{\text{RE}}^{-0.3} \rho r^{-1} \omega^2
\]

where \( \rho \) is the density (kg m\(^{-3}\)), \( r \) is the cylinder radius (m), and \( \omega \) is the electrode angular velocity (rad s\(^{-1}\)). In Table 9, \( \omega, N_{\text{RE}} \), and \( \tau_{\text{RDE}} \) values under laminar, transitory, and turbulent hydrodynamic regime conditions, respectively, can be observed.

### Table 9. Angular Velocity, \( N_{\text{RE}} \) and Shear Stress as Functions of the RDE Rotation Rate

| Regimen      | Rotation Rate (rpm) | \( \omega \) (rad s\(^{-1}\)) | \( N_{\text{RE}} \) | \( \tau_{\text{RDE}} \) (Pa) |
|--------------|---------------------|-----------------|-----------------|-----------------|
| Laminar      | 343                 | 35.9            | 1000            | 0.320           |
| Transitory   | 686                 | 71.84           | 2000            | 1.040           |
| Turbulent    | 1029                | 107.76          | 3000            | 2.073           |
|              | 1372                | 143.68          | 4000            | 3.381           |
|              | 1715                | 179.6           | 5000            | 4.940           |

### 4.4. Surface Analysis.

The samples employed for the surface analyses were prepared by following the methodology for electrochemical tests and polished with 1 μm alumina. The metal coupons were immersed in the corrosive medium in the absence and presence of 150 ppm of Cl for 4 h at 25°C. Afterward, the metal samples were retrieved from the medium and rinsed with deionized water and dried with nitrogen.\(^{103}\) The surface of API 5L X52 steel was analyzed by SEM/EDS on a JEOL-JSM-6300 microscope. The study of the treated metal surfaces was carried out using DRIFTS; these measurements were performed in situ using a Thermo Scientific Nicolet 560 Spectrometer in a series of spectra recorded with identical resolution (4 cm\(^{-1}\)). The XPS analysis was performed with a K-Alpha Thermo Fisher Scientific spectrometer with monochromatic Al Kα (1486.6 eV) and vacuum pressure of 1 × 10\(^{-9}\) Torr. The pass energy values for the study and high-resolution spectra were set at 160 and 20 eV, respectively. The obtained spectra were referred to adventitious carbon (284.8 eV) and the peak fitting was performed using the software Thermo Avantage v.5.9915.

### 4.5. Computational Details.

The IL corrosion inhibition performance was supported with first-principles energy calculations. The \([\text{DDMST}^-]\) cation was optimized structurally considering different positions of the \([I^-]\) anion without symmetry restriction and singlet state (Multiplicity 1). The computations were developed with the density functional theory (DFT) by the Gaussian 09W software\(^{114}\) with B3LYP/MIDIx theory level.\(^{115,116}\) The entries were generated with the software Gauss View v6.0. The properties were obtained employing the lowest total energy configuration, whereas the Cl theoretical performance was established through the analysis of the molecular orbitals and dipolar moment (\(\mu\)),\(^{117}\) which were calculated from the optimized structure under standard temperature and pressure conditions.\(^{117}\)

### ASSOCIATED CONTENT

**Supporting Information**

The Supporting Information is available free of charge at https://pubs.acs.org/doi/10.1021/acsomega.2c05192.

Other analyzed models of adsorption isotherms for API 5L X52 steel in 1 M H\(_2\)SO\(_4\) solution with [DDMST\(^-\)] (PDF)

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**Notes**

The authors declare no competing financial interest.

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REFERENCES

(1) Bhardwaj, N.; Sharma, P.; Singh, K.; Rana, D.; Kumar, V. Phyllanthus emblica seed extract as corrosion inhibitor for stainless steel used in petroleum industry (SS-410) in acidic medium. Chem. Phys. Impact 2021, 3, No. 100038.

(2) Bhardwaj, N.; Sharma, P.; Kumar, V. Corrosion Inhibition Property and Adsorption Behavior of P. tremula Leaf Extract in Acidic Media for Steel used in Petroleum Industry (SS-410). Prot. Met. Phys. Chem. Surf. 2021, 57, 1076–1084.

(3) Wan, S.; Wei, H.; Quan, R.; Luo, Z.; Wang, H.; Liao, B.; Guo, X. Soybean extract firstly used as a green corrosion inhibitor with high efficacy and yield for carbon steel in acid medium. Ind. Crops Prod. 2022, 187, No. 113354.

(4) Zhang, W.; Zhang, D.; Li, X.; Li, C.; Gao, L. Excellent performance of dodecyl dimethyl betaine and calcium gluconate as hybrid corrosion inhibitors for Al alloy in alkaline solution. Corros. Sci. 2022, 207, No. 110556.

(5) Yang, L.; Fan, H.; Yan, R.; Zhang, J.; Liu, S.; Huang, X.; Zhang, D. N-substituted methyl ethylenediamine derivatives as corrosion inhibitors for carbon steel in 1 M hydrochloric acid. J. Mol. Struct. 2022, 1270, No. 133975.

(6) Gholivand, K.; Sarmadi-babae, L.; Faraghi, M.; Badalkhani-khameh, F.;Fallah, N. Heteroatom-containing phosphoramide as carbon steel corrosion inhibitors: Density functional theory and molecular dynamics simulations. Chem. Phys. Impact 2022, 5, No. 100099.

(7) Verma, D. K.; Aslam, R.; Aslam, J.; Quraishi, M. A.; Ebenso, E. E.; Verma, C. Computational Modeling: Theoretical Predictive Tools for Designing of Potential Organic Corrosion Inhibitors. J. Mol. Struct. 2021, J236, No. 130294.

(8) Zhang, Q.; Zhang, R.; Wu, R.; Luo, Y.; Guo, L.; He, Z. Green and high-efficiency corrosion inhibitors for metals: A review. J. Adhes. Sci. Technol. 2022, 1–24.

(9) Al-Rashed, O.; Nazeer, A. A. Effectiveness of Some Novel Ionic Liquids on Mild Steel Corrosion Protection in Acidic Environment: Experimental and Theoretical Inspections. Materials 2022, 15, No. 2326.

(10) Verma, C.; Alrefae, S. H.; Quraishi, M. A.; Ebenso, E. E.; Hussain, C. M. Recent developments in sustainable corrosion inhibition using ionic liquids: A review. J. Mol. Liq. 2021, 321, No. 114484.

(11) Salim, R.; Hajjaji, F. E. L.; Ech-chihbi, E.; Titi, A.; Messali, M.; Nahle, A.; Kaya, S.; El Ibrahim, B.; Taleb, M. Experimental and theoretical approach for novel imidazolium ionic liquids as Smart Corrosion inhibitors for mild steel in 1.0 M hydrochloric acid. Arab. J. Chem. 2015, 15, No. 103967.

(12) Tian, G.; Yuan, K. Adsorption and inhibition behavior of imidazolium tetrafluorooborate derivatives as green corrosion inhibitors for carbon steel. J. Mol. Model. 2021, 27, 195.

(13) Zuniga, M.; Kevin, Y. J. Results in Engineering Ionic liquids as corrosion inhibitor: From research and development to commercialization. Results Eng. 2022, 15, No. 100562.

(14) Bhaskan, Pancharatna, P.; D.; Lata, S.; Singh, G. Imidazolium based ionic liquid as an efficient and green corrosion constraint for mild steel at acidic pH levels. J. Mol. Liq. 2019, 278, 467–476.

(15) Gurjar, S.; Sharma, K.; Sharma, A.; Ratnani, S. Performance of imidazolium based ionic liquids as corrosion inhibitors in acid medium: A review. Appl. Surf. Sci. Adv. 2021, 6, No. 100170.

(16) El-Hajjaji, F.; Salim, R.; Taleb, M.; Benhiba, F.; Rezk, N.; Singh-Chauhan, D.; Quraishi, M. A. Pyridinium-based ionic liquids as novel eco-friendly corrosion inhibitors for mild steel in molar hydrochloric acid: Experimental & computational approach. Surf. Interfaces 2021, 22, No. 100881.

(17) Hamidi, Z.; Mosavian, S. Y.; Sabbaghi, N.; Karimi-Zarchi, M. A.; Noroozifar, M. Cross-linked poly(N-alkyl-4-vinylpyridinium) iodides as new eco-friendly inhibitors for corrosion study of St-37 steel in 1 M H2SO4, Iran. Polym. J. 2020, 29, 225–239.

(18) Wang, S.; Sun, J.; Shan, B.; Fan, W.; Ding, R.; Yang, J.; Zhao, X. Performance of dodecyl dimethyl benzyl ammonium chloride as bactericide and corrosion inhibitor for 7B04 aluminum alloy in an aircraft fuel system. Arab. J. Chem. 2022, 15, No. 103926.

(19) Zheng, T.; Liu, J.; Wang, M.; Liu, Q.; Wang, J.; Chong, Y.; Jia, G. Synergistic corrosion inhibition effects of quaternary ammonium salt cationic surfactants and thiourea on Q235 steel in sulfuric acid: Experimental and theoretical research. Corros. Sci. 2022, 199, No. 110199.

(20) Kannan, P.; Varghese, A.; Palanisamy, K.; Abousalem, A. S. Evaluating prolonged corrosion inhibition performance of benzyl-tributylammonium tetrachlorolaurum ion liquid using electrochemical analysis and Monte Carlo simulation. J. Mol. Liq. 2020, 297, No. 111855.

(21) El-Hajjaji, F.; Salim, R.; Messali, M.; Hammouti, B.; Chauhan, D. S.; Almutairi, S. M.; Quraishi, M. A. Electrochemical Studies on New Pyridazinium Derivatives as Corrosion Inhibitors of Carbon Steel in Acidic Medium. J. Bio-Trio-Corros. 2019, S, 1–13.

(22) Gurjar, S.; Ratnani, S.; Kandwal, P.; Tiwari, K. J.; Sharma, A.; Sharma, S. K. Experimental and theoretical studies of 1-Benzyl pyridazinium bromide as green inhibitor for mild steel corrosion. Adv. Electr. Eng. Electron. Energy 2022, 2, No. 100054.

(23) Deyab, M. A. Sulfonium-based ionic liquid as an anticorrosive agent for thermal desalination units. J. Mol. Liq. 2019, 296, No. 111742.

(24) Arab, S. T.; Al-Turkustani, A. M. Corrosion Inhibition of Steel in Phosphoric acid by Phenacyldimethyl Sulfonium Bromide and some of its p-Substituted Derivatives. Prog. Electrochem. Acta 2006, 24, 53–69.

(25) Shein, A. B.; Nedugov, A. N. Examination of Trialkyl-Substituted Sulfonium, Selenonium, and Telluronium Salts as Inhibitors of Acid Corrosion of Iron and Steel. Prog. Met. 2000, 36, 240–243.

(26) Verma, C.; Oboi, I. B.; Bahadur, I.; Sherif, E.-S. M.; Ebenso, E. E. Choline based ionic liquids as sustainable corrosion inhibitors on mild steel surface in acidic medium: Gravimetric, electrochemical, surface morphology, DFT and Monte Carlo simulation studies. Appl. Surf. Sci. 2018, 457, 134–149.

(27) Mashuga, M.; Olausankanni, L.; Adekunle, A.; Yesudass, S.; Kabanda, M.; Ebenso, E. Adsorption, Thermodynamic and Quantum Chemical Studies of 1-hexyl-3-methylimidazolium Based Ionic Liquids as Corrosion Inhibitors for Mild Steel in HCl. Materials 2015, 8, 3607–3632.

(28) Azeez, F. A.; Al-Rashed, O. A.; Nazeer, A. A. Controlling of mild-steel corrosion in acidic solution using environmentally friendly ionic liquid inhibitors: Effect of alkyl chain. J. Mol. Liq. 2018, 265, 654–663.

(29) Cao, S.; Liu, D.; Ding, H.; Wang, J.; Lu, H.; Gui, J. Corrosion inhibition effects of a novel ionic liquid with and without potassium iodide for carbon steel in 0.5 M HCl solution: An experimental study and theoretical calculation. J. Mol. Liq. 2019, 275, 729–740.

(30) Guo, L. Synergistic Effect of Potassium Iodide with L-Tryptophane on the Corrosion Inhibition of Mild Steel: A Combined Electrochemical and Theoretical Study. Int. J. Electrochem. Sci. 2017, 166–177.

(31) Farag, A. A.; Hegazy, M. A. Synergistic inhibition effect of potassium iodide and novel Schiff bases on X65 steel corrosion in 0.5M H2SO4. Corros. Sci. 2013, 74, 168–177.

(32) Feng, L.; Zhang, S.; Qiang, Y.; Xu, S.; Tan, B.; Chen, S. The synergistic corrosion inhibition study of different chain lengths ionic liquids as green inhibitors for X70 steel in acidic medium. Mater. Chem. Phys. 2018, 215, 229–241.

(33) Qi, Y.; Tu, X.; Lu, X.; Yang, J. A novel insight into synergistic corrosion inhibition of fluoride and DL-malate as a green hybrid inhibitor for magnesium alloy. Corros. Sci. 2022, 199, No. 110177.

(34) Satri, V. S.; Ghali, E.; Elboujdaini, M. Corrosion Prevention and Protection Practical Solutions; John Wiley & Sons Ltd, 2007.

(35) Papavinasam, S.; Doiron, A.; Shen, G.; Revie, R. W. Prediction of Inhibitor Behaviour in the Field From Data in the Laboratory; NACE Corrosion 2004: New Orleans, Louisiana, 2004.
Cisneros, M. G.; Chacon-Nava, J. G. Evaluation of composite coatings with regular textures. Int. J. Corros. 2011, 2011, No. 718626.

Zhang, K.; Yang, W.; Xu, B.; Liu, Y.; Yin, X.; Chen, Y. Corrosion inhibition of mild steel by bromide-substituted imidazoline in hydrochloric acid. J. Taiwan Inst. Chem. Eng. 2015, 57, 167–174.

Kamali-Ardakani, E.; Kowsari, E.; Ehsani, A. Imidazolium-derived polymeric liquid as a green inhibitor for corrosion inhibition of mild steel in 1.0 M HCl: Experimental and computational study. Colloids Surf., A 2020, 586, No. 124195.

Wang, X.; Yang, H.; Wang, F. An investigation of benzimidazole derivative as corrosion inhibitor for mild steel in different concentration HCI solutions. Corros. Sci. 2011, 53, 113–121.

Aldana-González, J.; Espinoza-Vázquez, A.; Romero-Romo, M.; Uruchurtu-Chavarin, J.; Palomar-Pardavé, M. Electrochemical evaluation of cephalothin as corrosion inhibitor for API 5L X52 steel immersed in an acid medium. Arab. J. Chem. 2015, 12, 3244–3253.

Ismail, A.; Irshad, H. M.; Zeino, A.; Toor, I. H. Electrochemical Corrosion Performance of Aromatic Functionalized Imidazole Inhibitor Under Hydrodynamic Conditions on API X65 Carbon Steel in 1 M HCl Solution. Arab. J. Sci. Eng. 2019, 44, 5877–5888.

Burdusos-Nergis, D.-P.; Vizureanu, P.; Sandu, A. V.; Bejinariu, C. Evaluation of the Corrosion Resistance of Phosphate Coatings Deposited on the Surface of the Carbon Steel Used for Carabiners Manufacturing. Appl. Sci. 2020, 10, 2753.

Xu, L.-N.; Zhu, J.-y.; Lu, M.-x.; Zhang, L.; Chang, W. Electrochemical impedance spectroscopy study on the corrosion of the weld zone of 3Cr steel welded joints in CO2 environments. Int. J. Miner., Metall. Mater. 2015, 22, 500–509.

Tan, Z.; Yang, L.; Zhang, D.; Wang, Z.; Cheng, F.; Zhang, M.; Jin, Y. Development mechanism of internal local corrosion of X80 pipeline steel. J. Mater. Sci. Technol. 2020, 49, 186–201.

Mo, M.; Zhao, W.; Chen, Z.; Liu, E.; Xuea, Q. Corrosion inhibition of functional graphene reinforced polyurethane nanocomposite coatings with regular textures. RSC Adv. 2016, 6, 7780–7790.

Bojangi, A. A.; Wu, H. S. Characterization of Electrode Performance in Enzymatic Biofuel Cells Using Cyclic Voltammetry and Electrochemical Impedance Spectroscopy. Catalysts 2020, 10, No. 782.

Delgado, M. C.; García- Galvan, F. R.; Barranco, V.; Feliu-Batlle, S. A. Measuring Approach to Assess the Corrosion Rate of Magnesium Alloys Using Electrochemical Impedance Spectroscopy. In Magnesium Alloys, Allolkhazraei, M., Ed.; IntechOpen: London, 2017; pp 129–160.

Hsiissou, R.; Benhiba, F.; Dagdag, O.; El Bouchti, M.; Nouneh, K.; Assouag, M.; Briche, S.; Zarrouk, A.; Elharfi, A. Development and potential performance of prepolymer in corrosion inhibition for carbon steel in 1.0 M HCl: Outcomes from experimental and computational investigations. J. Colloid Interface Sci. 2020, 574, 43–60.

Chafqa, M.; Chaouki, A.; Al-Hadeethi, M. R.; Ali, I. H.; Mohamed, S. K.; Touni, K.; Salghi, R. Naproxen-Based Hydrazones as Effective Corrosion Inhibitors for Mild Steel in 1.0 M HCl. Coatings 2020, 10, 1–17.

Barmatov, E.; Hughes, T. L. Effect of corrosion products and turbulent flow on inhibition efficiency of propargyl alcohol on AISI 1018 mild steel in 4 M hydrochloric acid. Corros. Sci. 2017, 123, 170–181.

Singh, A.; Ansari, K. R.; Chauhan, D. S.; Quraishi, M. A.; Lgaz, H.; Chung, I.-M. Comprehensive investigation of steel corrosion inhibition at macro/micro level by ecofriendly green corrosion inhibitor in 15% HCl medium. J. Colloid Interface Sci. 2020, 560, 225–236.

Rodríguez-Clemente, E.; Gonzalez-Rodríguez, J. G.; Valladares-Cisneros, M. G.; Chacon-Nava, J. G. Evaluation of Allium sativum as corrosion inhibitor for carbon steel in sulphuric acid under hydrodynamic conditions. Green Chem. Lett. Rev. 2015, 8, 49–58.

Vakili-Azghandi, M.; Davoodi, A.; Farzi, G. A.; Kosari, A. Water-base acrylic terpolymer as a corrosion inhibitor for SAE1018 in simulated sour petroleum solution in stagnant and hydrodynamic conditions. Corros. Sci. 2012, 64, 44–54.

Zhao, J.; Liu, Y.; Yang, X.; He, X.; Wang, L.; Xiong, D.; Gu, Y. Corrosion Behavior of Pipeline Steel in Oilfield Produced Water Under Dynamic Corrosion System. J. Wuhan Univ. Technol. 2022, 37, 677–691.

Benmahammed, I.; Douadi, T.; Issaadi, S.; Al-Noaimi, M.; Chaafa, S. Heterocyclic Schiff bases as corrosion inhibitors for carbon steel in 1 M HCl solution: hydrodynamic and synergetic effect. J. Dispersion Technol. 2020, 41, 1002–1021.

Obot, I.-B.; Onyeachu, I.-B.; Umosen, S. A. Alternative corrosion inhibitor formulation for carbon steel in CO2-saturated brine solution under high turbulent flow condition for use in oil and gas transportation pipelines. Corros. Sci. 2019, 159, No. 108140.

Guo, L.; Obot, I. B.; Zheng, X.; Shen, X.; Qiang, Y.; Kaya, S.; Kaya, C. Theoretical insight into an empirical rule about organic corrosion inhibitors containing nitrogen, oxygen, and sulfur atoms. Appl. Surf. Sci. 2017, 406, 301–306.

Hsiissou, R.; Abbout, S.; Safi, Z.; Benhiba, F.; Wazzan, N.; Guo, L.; Nouneh, K.; Briche, S.; Erramli, H.; Ebn Touhami, M.; et al. Synthesis and anticorrosive properties of epoxy polymer for CS in [1 M] HCl solution: Electrochemical, AFM, DFT and MD simulations. Constr. Build. Mater. 2021, 270, No. 121454.

Hsiissou, R.; Abbout, S.; Seghiri, R.; Rehioui, M.; Berisha, A.; Erramli, H.; Assouag, M.; Elharfi, A. Evaluation of corrosion inhibition performance of phosphorus polymer for carbon steel in [1 M] HCl: Computational studies (DFT, MC and MD simulations). J. Mater. Res. Technol. 2020, 9, 2691–2703.

Fernandes, C. M.; Alvarez, L. X.; Escarpini-dos Santos, N.; Maldonado-Barrios, A. C.; Ponzio, E. A. Green synthesis of 1-benzyl-4-phenyl-1H-1,2,3-triazole, its application as corrosion inhibitor for mild steel in acidic medium and new approach of classical electrochemical analyses. Corros. Sci. 2019, 149, 185–194.

Kowsari, E.; Payami, M.; Amini, R.; Ramezanazdeh, B.; Javanbakht, M. Task-specific ionic liquid as a new green inhibitor of mild steel corrosion. Appl. Surf. Sci. 2014, 289, 478–486.

Tang, Y.; Zhang, F.; Hu, S.; Cao, Z.; Wu, Z.; Jing, W. Novel benzimidazole derivatives as corrosion inhibitors of mild steel in the acidic media. Part I. Gravimetric, electrochemical, SEM and XPS studies. Corros. Sci. 2013, 74, 271–282.

Okafor, P. C.; Zheng, Y. Synergistic inhibition behaviour of methylbenzyl quaternary imidazoline derivative and iodide ions on mild steel in H2SO4 solutions. Corros. Sci. 2009, 51, 850–859.

Umoren, S. A.; Ebenso, E. E.; Okafor, P. C.; Ekpe, U. J.; Ogbohe, O. Effect of halide ions on the corrosion inhibition of aluminium in alkaline medium using polyvinyl alcohol. J. Appl. Polym. Sci. 2007, 103, 2810–2816.

Bentiss, F.; Lebrini, M.; Traisnel, M.; Lagrenée, M. Synergistic effect of iodide ions on inhibitive performance of 2,5-bis(4-methoxyphenyl)-1,3,4-thiadiazole during corrosion of mild steel in 0.5 M sulfuric acid solution. J. Appl. Electrochem. 2009, 39, 1399–1407.

Sastri, V. S.Green Corrosion Inhibitors: Theory and Practice; John Wiley & Sons, Inc., 2011.

Godinez, L. A.; Meas, Y.; Ortega-Borges, R.; Corona, A. Corrosion inhibitors. Res. Metals 2003, 39, 140–158.

Cha, Y.-J.; Kim, M.-J.; Choa, Y.-H.; Kim, J.; Nam, B.; Lee, J.; Kim, D. H.; Kim, K. H. Synthesis and Characterizations of Surface-Coated Superparamagnetic Magnetite Nanoparticles. IEEE Trans. Mag. 2010, 46, 443–446.

Raghuv, M. S.; Kumar, K. Y.; Prashanth, M. K.; Prasanna, B. P.; Vinuth, R.; Pradeep-Kumar, C. B. Adsorption and antimicrobial studies of chemically bonded magnetic graphene oxide-Fe3O4 nanocomposite for water purification. J. Water Process. Eng. 2017, 17, 22–31.

Lachkar-Zamouri, O.; Brahim, K.; Bennoun-Mrad, F.; Khatte, I. Attack of Tunisian Phosphate Ore by a Mixture of Sulfuric and...
Phosphoric Acid: Thermochemical Study by Means of Differential Reaction Calorimetry. Adv. Mater. Phys. Chem. 2018, 8, 411–427.

(72) Kurniawan, C.; Eko, A. S.; Ayu, Y. S.; Sihite, P. T. A.; Ginting, M.; Simamora, P.; Sebayang, P. Synthesis and Characterization of Magnetic Elastomer based PEG-Coated FeO3 from Natural Iron Sand. In IOP Conference Series. Materials Science and Engineering; IOP Publishing, 2017.

(73) Chirita, M.; Banica, R.; Ieta, A.; Grozescu, I. Superparamagnetic Unusual Behavior of Micrometric Magnetite Monodisperse Monocrystals Synthesized by Fe-EDTA Thermal Decomposition. Part. Sci. Technol. 2012, 30, 354–363.

(74) Nguyen, Q.; Quyen, D.; Hoang, T. A new route of emulsifier-free emulsion polymerization for the preparation of polymer coated magnetite nanoparticles. Mater. Sci. Pol. 2014, 32, 264–271.

(75) Hou, Y.; Li, J.; Gao, X.; Wen, Z.; Yuan, C.; Chen, J. 3D Dual-Confining Sugar Encapsulated in Porous Carbon Nanosheets and Wrapped with Graphene Aerogels as Cathode for Advanced Lithium Sulfur Batteries. Nanoscale 2016, 8, 8228–8235.

(76) Liu, H.; Xu, C.-Y.; Ou, Y.; Ma, F.-X.; Li, Y.; Yu, J.; Zhen, L. Ultrathin Cds nanosheets vertically aligned on Ns/gO for low voltage electrolytic water in alkaline media. Sci. Rep. 2019, 9, No. 1951.

(77) Hummel, H.-U.; Forner, W. Investigation of the Charge Distribution of Free and Bound 1,1-Dicyanoethylene-2,2-dithiolate. An ab initio HF-MO and XPS Study. J. Inorg. Gen. Chem. 1986, 540, 300–306.

(78) Ning, L.; Wang, D.; Wang, L.; Wu, L.; Yang, J.; Wang, X.; Ma, H.; Feng, S.; Lu, H. Interesting Corrosion Inhibition Performance and Mechanism of Two Silanes Containing Multiple Phosphorus Group. Silicon 2020, 12, 1455–1468.

(79) Orfanoudaki, T.; Skodras, G.; Dolios, I.; Sakellaropoulos, G. P. Production of carbon molecular sieves by plasma treated activated carbon fibers. Fuel 2003, 82, 2045–2049.

(80) Moura, C. A. d. S.; Belmonte, G. K.; Reddy, P. G.; Gonsalves, K. E.; Weibelf, D. E. UV photofragmentation study of hybrid nonchemically amplified resists containing anthimine as an absorption enhancer. RSC Adv. 2018, 8, 10930.

(81) Belmonte, G. K.; Moura, C. A. d. S.; Reddy, P. G.; Gonsalves, K. E.; Weibelf, D. E. UV photofragmentation and oxidation of a polyaniline—Sulphonium resist: XPS and NEXAFS study. J. Photochem. Photobiol., A 2018, 364, 373–381.

(82) Gassman, P. G.; Callstrom, M. R.; et al. XPS Data for Linear Three-Center, Four-Electron Bonding in Sulfur Species. J. Am. Chem. Soc. 2011, 133, 8716–8725.

(83) Kolomen, S. B.; George, G. N.; Gorbaty, M. L. Direct determination and quantification of organic sulfur forms by X-ray photoelectron spectroscopy (XPS) and sulfur k-edge absorption spectroscopy. Fuel Proc. Technol. 1990, 24, 425–429.

(84) Zhang, Q. H.; Hou, B. S.; Xu, N.; Xiong, W.; Liu, H. F.; Zhang, G. A. Effective inhibition on the corrosion of X65 carbon steel in the oilfield produced water by two Schiff bases. J. Mol. Liq. 2019, 285, 223–236.

(85) Allen, G. C.; Curtis, M. T.; Hooper, A. J.; Tucker, P. M. X-Ray Photoelectron Spectroscopy of Iron-Oxygen Systems. J. Chem. Soc., Dalton Trans. 1974, 52, 1445–1451.

(86) Wagner, C. D.; Zatko, D. A.; Raymond, R. H. Use of the oxygen KLL Auger lines in identification of surface chemical states by electron spectroscopy for chemical analysis. Anal. Chem. 1980, 52, 1445.

(87) Siriwardane, R. V.; Cook, J. M. Interactions of SO2 with Sodium Deposited on CaO. J. Colloid Interface Sci. 1986, 114, 525.

(88) Hallam, P. M.; Gómez-Mingot, M.; Kumpouris, D. K.; Banks, C. E. Facile synthetic fabrication of iron oxide particles and novel hydrogen superoxide supercapacitors. RSC Adv. 2012, 2, 6672.

(89) Puech, L.; Dubarry, C.; Ravel, G.; de-Vito, E. Modeling of iron oxide deposition by reactive ion beam sputtering. J. Appl. Phys. 2010, 107, No. 054908.

(90) Luo, J.; Du, X.; Gao, F.; Yang, Y.; Hao, X.; Li, S.; Hao, X.; Tang, K.; Guan, G. Iodide ion trapping polyprolyrle film: Selective capture of iodide ions by electrochemically switched ion extraction (ESIE) process. Chem. Eng. J. 2019, 380, No. 122529.
(109) ASTM G185-06-(2016). Evaluating and Qualifying Oil Field and Refinery Corrosion Inhibitors Using the Rotating Cylinder Electrode; West Conshohocken: PA, 2016. DOI: 10.1520/g0185-06r16.

(110) Childs, P. R. N. Rotating Flow; Elsevier Ltd, 2011. DOI: 10.1016/C2009-0-30534-6.

(111) Ibrahim, I. M.; Jai, J.; Daud, M.; Hashim, M. A. Inhibition effect of fatty amides with secondary compound on carbon steel corrosion in hydrodynamic condition. IOP Conf. Ser.: Mater. Sci. Eng. 2018, 334, No. 012048.

(112) ASTM G170-06-(2012). Evaluating and Qualifying Oilfield and Refinery Corrosion Inhibitors in the Laboratory; West Conshohocken: PA, 2012. DOI: 10.1520/g0170-06r12.

(113) Barmatov, E.; Hughes, T.; Nagl, M. Efficiency of film-forming corrosion inhibitors in strong hydrochloric acid under laminar and turbulent flow conditions. Corros. Sci. 2015, 92, 85–94.

(114) Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; et al. Gaussian 09, revision D.01; Gaussian, Inc.: Wallingford, CT, 2013.

(115) Easton, R. E.; Giesen, D. J.; Welch, A.; Cramer, C. J.; Truhlar, D. G. The MIDI! basis set for quantum mechanical calculations of molecular geometries and partial charges. Theor. Chim. Acta 1996, 93, 281–301.

(116) Thompson, J. D.; Winget, P.; Truhlar, D. G. MIDIX basis set for the lithium atom: Accurate geometries and atomic partial charges for lithium compounds with minimal computational cost. PhysChemComm 2001, 4, 72–77.

(117) Singh, A.; Ansari, K. R.; Quraishi, M. A.; Lin, Y. Investigation of Corrosion Inhibitors Adsorption on Metals Using Density Functional Theory and Molecular Dynamics Simulation. In Corrosion Inhibitors, Singh, A., Ed.; IntechOpen, 2019.