

A Review on Interactions between Amino Acids and Surfactants as Well as Their Impact on Corrosion Inhibition

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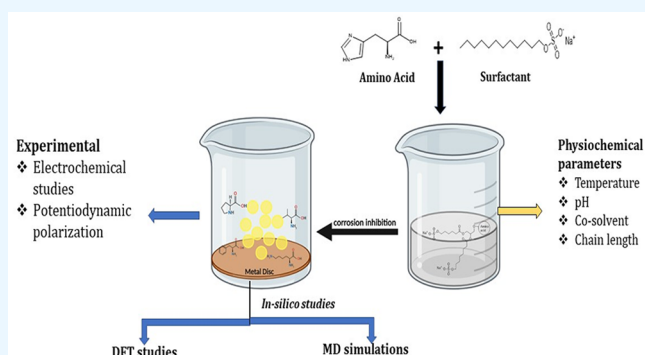
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ABSTRACT: Amino acid–surfactant interactions are central to numerous studies because of their increased effectiveness in chemical, biological, household and industrial use. This review will focus on the impact and effect of the physicochemical properties, temperature, pH, and surfactant chain length of the amino acid for detailed exploration of amino acids and surfactants in aqueous medium. The impact of cosolvent on self-aggregation, critical micelle concentration (CMC), and binding affinity with other biomolecules, as well as amino acid–surfactant interactions, are the epicenters. The results show that increasing the temperature causes negative enthalpy for ionic surfactants and micellization, implying that micellization and amino acids are thermodynamically spontaneous and exothermic, accompanied by positive entropy.

As these physicochemical studies are additive, the amino acid and ionic surfactant interactions provide clues on protein unfolding and denaturation under different media, which further changes with a change in physiological conditions like pH, cosolvent, chain length, and temperature. On varying the pH, the net charge of the amino acid also changes and, subsequently, the binding efficiency of the amino acids to the surfactants. The presence of cosolvent causes a lowering in the hydrophobic chain, which changes the surfactant's CMC. At a reduced CMC, the hydrophobic characteristic of amino acid–surfactant associations is amplified, leading to rapid denaturation of proteins that act as propulsion under the influence of extended chain surfactants. Amino acids are one of the most intriguing classes of chemicals that produce high inhibitory efficacy. Amino acids are also a component of proteins and therefore, found in a significant part of the human body, further making them a promising candidate as corrosion inhibitors. In this review article, authors have also focused on the collection and investigation for application of amino acid–surfactant interactions in corrosion inhibition. Various predictive studies/*in silico* studies are also reported by many research groups, such as density functional theory (DFT) calculations and molecular dynamics simulations to obtain tentative electronic, structural, and physicochemical characteristics like energies of the highest occupied molecular orbitals and lowest unoccupied molecular orbitals, binding energy, Gibb's free energy, electronegativity, polarizability, and entropy. *In silico* studies are helpful for the mechanism predictions of the process occurring on metal surfaces.



1. INTRODUCTION

Amino acids are naturally occurring building blocks that can act as polar head groups of amphiphilic molecules. Regarding the type of surfactant prepared, amino acids are more versatile than polyols. Many of the essential alpha-amino acids have been investigated as surfactant source materials. Although several amino-acid-based surfactants are on the market, producing such surfactants is still minimal. Amino acids also serve as flavor enhancers (monosodium glutamate, glycine, alanine) in the food industry; animal feed additives (lysine, methionine, threonine); antioxidants (tryptophan and cysteine) in the pharmaceutical industry; starting materials for the production of many chemical compounds (glycine is a precursor for the synthesis of glyphosate); and as intermediates

for the metabolism which is necessary for the synthesis of hormones and neurotransmitters. Biomembranes are well-organized structures of lipids and proteins. Investigating the interactions between amino acids and surfactants to reduce the interfacial tension is quite relevant and interesting. Their importance to humanity lies in various industrial applications ranging from food to pharmaceuticals, body-care-related

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products, and the cosmetics industry. In the current scenario, health and safety issues are the top priority worldwide. Thus, investigating amino acid–surfactant interactions has become essential and interesting research theme in various applications.

Surfactants are amphiphilic molecules, being both hydrophilic (head) and hydrophobic (tail). These surface-active molecules are used primarily as detergents, wetting agents, and softeners in soap manufacturing and pharmaceutical industries. Surfactants are classified as cationic (a positively charged head such as mono-alkyl quaternary systems), anionic (negatively charged hydrophilic head, for example, alkyl benzenesulfonates), and non-ionic (does not have an electrical charge),^{1–5} and investigations on amino acid–surfactant interactions have been present in the center of active research for the past few decades.⁶ Surfactants are wetting agents that lower surface tension and spread. Thus, they get adsorbed on the biomembrane and the outer protein coat of the virus as a charged film and try to stabilize it. Biosurfactants are a group of environmentally friendly surface-active agents produced or expelled extracellularly by microorganisms like bacteria, fungi, and yeast. Therefore, compounds that mimic the amphiphilic structures of naturally occurring substances like phospholipids, alkyl glucosides, and acyl substituted amino-acids may be designed and synthesized to serve as synthetic alternatives to biosurfactants. One form of surfactant that may be produced from agricultural or animal byproducts is amino acid surfactants (AASs). They are easily produced from renewable sources, biodegrade quickly, and make no harmful byproducts, AASs have attracted much attention from scientists over the past couple of decades as a unique class of surfactants.⁷ The amino acids are regularly used as parts of various food supplements to boost the natural immunity of the living system.⁸ L-Glutamine is a proven immunity enhancer and anti-inflammatory agent, and different surfactants such as sodium stearates and sodium dodecyl sulfate (SDS) interact with amino acids and form micelles in an aqueous medium.⁹ The alkyl chain of amino acids, except for Gln, Gly, Glu, Cys, Phe, Hyp, and Tyr do not significantly affect the interactions with the non-ionic surfactants as observed by chromatography.¹⁰ DFT calculations further suggest that long chains of these molecules also acquire some charge during surfactant interactions. This review article focussed to elaborate on the importance of amino acid–surfactant interactions under different temperatures, cosolvents, pH, and other physiological conditions, which will help to understand the wetting ability/interfacial phenomenon and can provide some vital information to the researcher for better designing of new molecules. We have also focused on the application part of the amino acid–surfactant interaction in corrosion inhibition. The binding mechanism predictions of the process occurring on the metal surfaces are done using density functional theory (DFT) calculations and molecular dynamics (MD) simulations that provide important information regarding physicochemical and structural properties.

2. EFFECT OF PHYSICAL PARAMETERS ON AMINO ACID–SURFACTANT INTERACTIONS

2.1. Effect of Temperature. The physicochemical properties calculated from the amino acid–surfactant interactions are influenced by temperature. According to Ali and Ansari et al.,¹¹ SDS micellization values in taking amino acids (glycine, alanine, and glycylglycine) increase with temperature (Figure 1). The negative Gibbs free energy of micellization has been

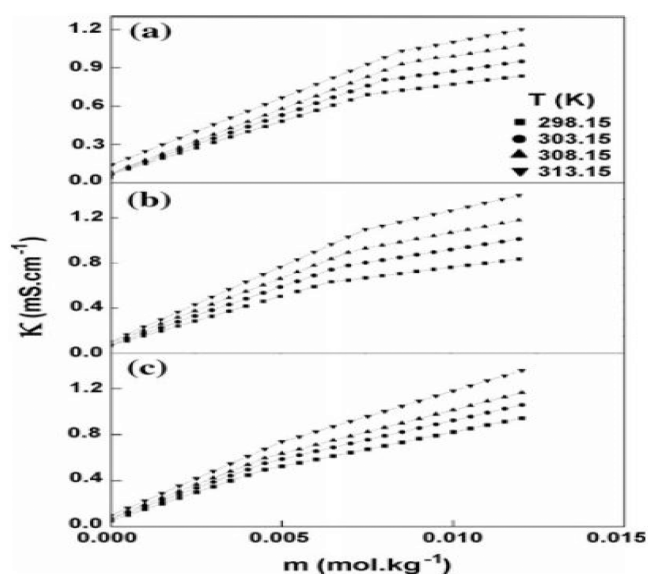


Figure 1. Variation of specific conductivity on SDS in 0–0.10 m aqueous (a) glycine, (b) alanine, and (c) glycylglycine at different temperatures. Reprinted with permission from ref 11. Copyright 2010 John Wiley and Sons, Ltd.

calculated for all amino acids (glycine, alanine, and glycylglycine), which may be due to the high positive values for entropy compared to those of enthalpy. This discussion concludes that the micellization process in this system is governed by entropy rather than enthalpy. The rise in entropy causes hampering in the structured water surrounded by the hydrophobic group at higher temperatures. At lower temperatures, the enthalpy of micellization is dominant over calculated entropy.

As the number of Na^+ counterions decreased, the Gibbs free energy decreased, revealing the impact on the micelles' surface polar headgroups regarding their electrostatic interactions. Furthermore, the entropic contribution increased in the presence of glycine and alanine, while the enthalpy decreased inversely with the temperature (Figure 2). The CMC was reported to be temperature-dependent: as the temperature increased, the CMC increased.¹¹

In general, when the CMC increased, the hydration of the hydrophobic group decreased, resulting in the aggregation of the headgroup. Further, an increase in temperature results in negative enthalpy and Gibbs free energy of micellization, while entropy is positive, indicating that the process is spontaneous. An increase in temperature disturbs the surrounding hydrophobic groups, thus decreasing the surfactant aggregation.¹² Noudeh et al. explained the micellization of some anionic surfactants (SDS) and cationic surfactants, benzalkonium chloride (BC), hexadecyl trimethylammonium bromide (HTAB), and tetradecyl trimethylammonium bromide (TTAB), using the du Nouy ring tensiometer. The CMC first decreased and then increased with an increase in temperature, giving a U-shaped graph depicting temperature dependence.¹³

The effect of glycine on cationic micellization was investigated using surface tension measurements. The surfactant hexadecylcetyltrimethylammonium bromide (CTAB) with other amino acids (L-serine and L-alanine) in Tris-HCl buffer solution is shown in Figure 3. The values of CMC increases with an increase in temperature without any

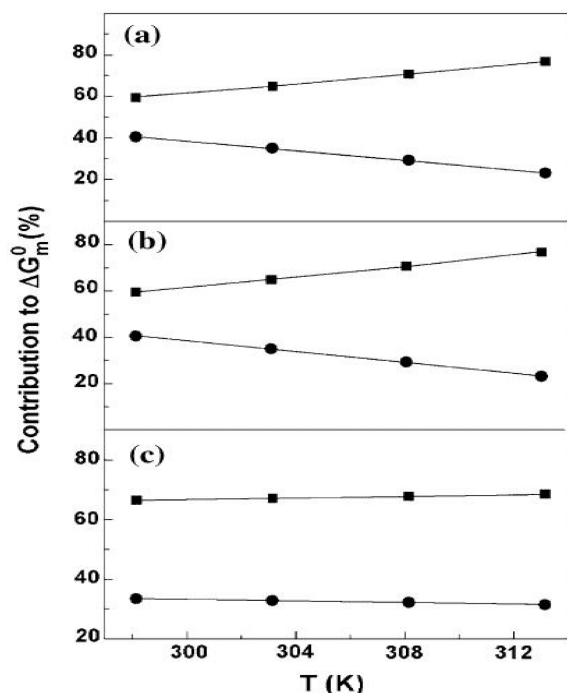


Figure 2. Enthalpic (●) and entropic (■) contributions to Gibb's free energy of micellization at different temperatures in 0.10 M aqueous (a) glycine, (b) alanine, and (c) glycylglycine. Reprinted with permission from ref 11. Copyright 2010 John Wiley and Sons, Ltd.

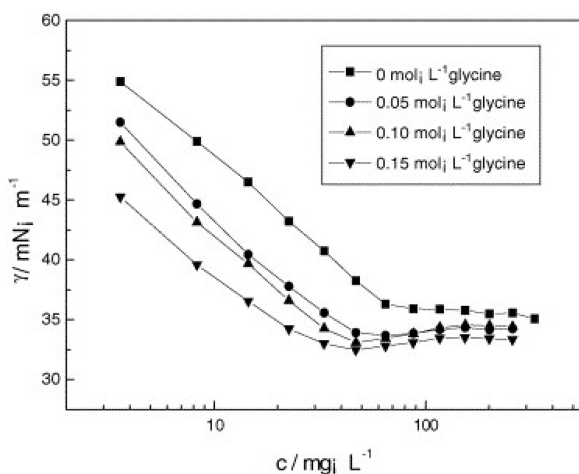


Figure 3. Surface tension of CTAB in the presence of different glycine concentrations in Tris-HCl buffer solution at 27 °C. Reprinted with permission from ref 14. Copyright 2005 Elsevier, Ltd.

effect of amino acid. When glycine was added to CTAB, it strengthens its hydrophobicity by enhancing its surface activity, resulting in easy micelle formation and surface tension, and CMC decreases. This may be with an increase in temperature, as the surface activity of CTAB also increases since the hydration ratio of the surfactant decreases.¹⁴ A negative Gibb's free energy of micellization is obtained with an increase in temperature, suggesting that dehydration of CTAB played a significant role in micelle formation at higher temperatures. The spontaneity of the process demonstrated by a positive entropy and enthalpy of micellization.

Yan et al. investigated the amino acid–BC surfactant interactions using UV absorption, density, conductivity, and

fluorescence spectra. The apparent molar volumes of the amino acids increase due to increase in the temperature and concentration of BC. This behavior is due to strong solute–solvent interactions that reduce the interaction of water molecules with the zwitterionic end of the surfactant. The CMC first decreases and then it increases with temperature, which may be because of the interplay of two opposing factors: initially, CMC decreases with an increase in temperature due to hydrophilic hydration, which got disrupted due to a further increase in temperature and hence leads to an increase in the CMC value. Both the CMC and aggregation number of BC decreases in the presence of the amino acids and dipeptides, which demonstrates that the micelles of BC are formed very easily and suggests that the interactions between the amino acids, dipeptide, and benzalkonium chloride are ionic–ionic and ionic–hydrophilic types.¹⁵

Naderi and Sadeghi studied the physicochemical properties of cationic surfactants, 1-decyl-3-methyl-imidazolium bromide, [C₁₀mim][Br], 1-dodecyl-3-methyl-imidazolium bromide, [C₁₂mim][Br], and anionic surfactant (SDS) in an aqueous solution of glycine, alanine, and proline at different temperatures. It has been observed that during the micellization process, the apparent molar volume decreases with temperature increase, which may be due to the break in the structure of solvent molecules around the alkyl chain. An increase in apparent molar isentropic compressibility of the surfactants with temperature has been observed. It has also been observed that the micellization had a linear relationship with apparent molar isentropic compressibility, which may be due to weak water–surfactant interactions during micelle formation. The CMC of surfactants decreases with amino acids in the following order: glycine > alanine > proline. The CMC of the surfactants in aqueous solution of proline is higher than that of other amino acids. This is due to the strong interactions that exist between proline and the hydrophobic part of the surfactants. The micelles formed due to hydrophobic–hydrophobic interactions between the amino acids and the aliphatic hydrocarbon chain of the surfactant seem to be less spontaneous compared to that of pure water, as observed from the values of Gibb's free energy of micellization.¹⁶

Mudawadkar and Patil (2016) explored the micellization of SDS along with non-polar additives like urea and acetamide at different temperatures. They found that the CMC of SDS increased as the temperature increases. However, the trend was reversed as the hydrophobic character increased from urea to acetamide. The thermodynamic parameters were calculated, and the negative Gibb's free energy indicated that the process of micellization is ruled by entropy, and it also increased with an increase in temperature.¹⁷

2.2. Effect of pH. As denaturation and unfolding of protein depend on the pH of the medium,^{18,19} the micelle formation of surfactants is also affected by the pH of the solution. It has been observed that at low pH and concentration, the interactions between amino acids and surfactants are mainly electrostatic, and the interactions become hydrophobic with an increase in the concentration of surfactants.^{20,21} Further, at low pH, amino acids become cationic, and at high pH, they behave as zwitterions/anionic.²² Numerous surfactants have been studied, and it has been shown that pH has no impact on aggregations.^{23,24} However, amino acids are neutral when the pH is near to the isoelectric point. Due to the lack of hydrophobic and electrostatic interactions, the amino-acid interacts poorly to the surfactant. The amino-acid has a

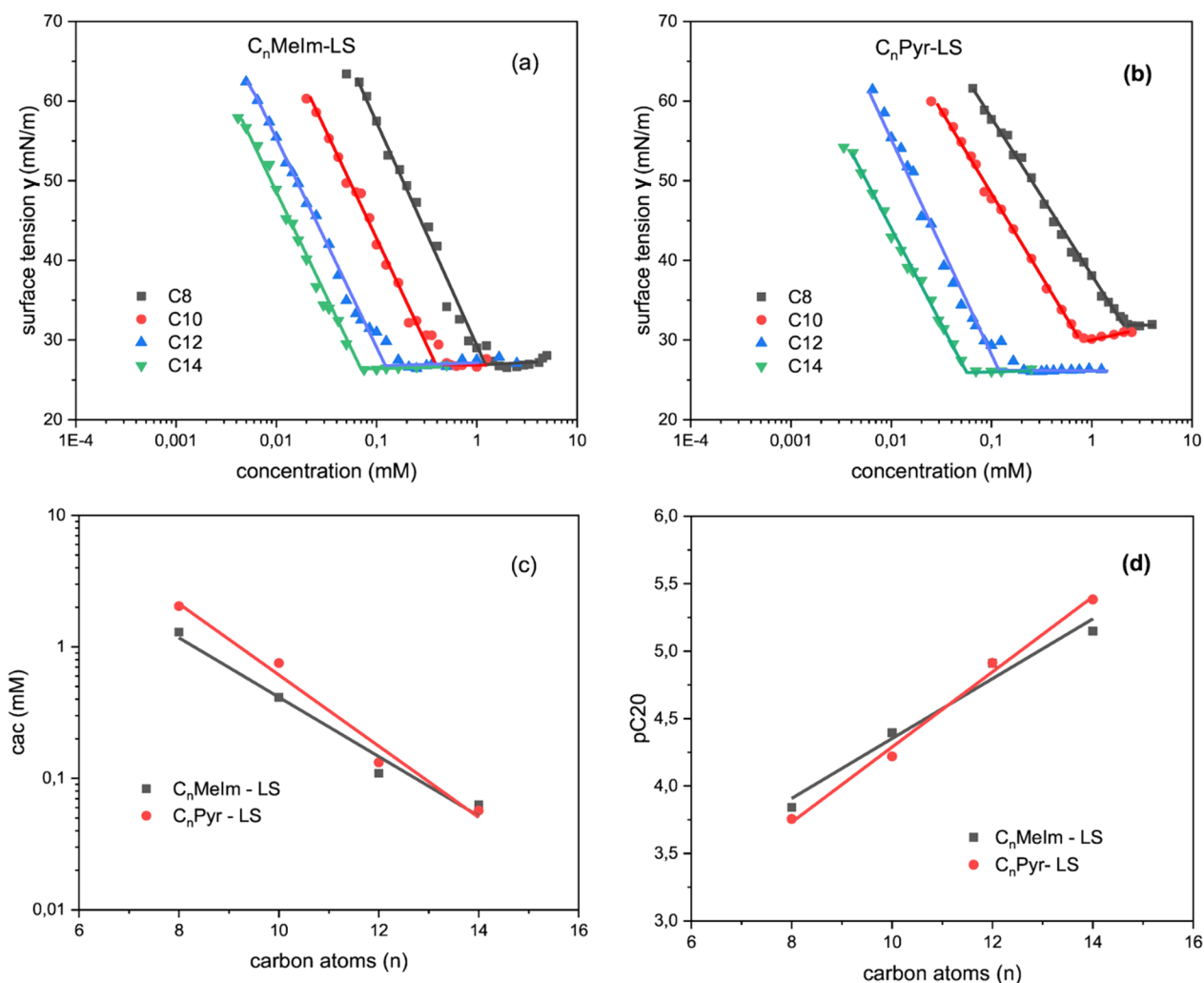


Figure 4. Plots of γ versus log C and log cac and pC_{20} versus the number of carbon atoms in the SAIL alkyl chain for C_n MeIm-LS (panels a, c, and d, respectively) and C_n Pyr-LS (panels b, c, and d, respectively) cationic mixtures. Reprinted with permission from ref 35. Copyright 2020 Elsevier, Ltd..

positive charge and forms a strong bond with the surfactant when the pH is below the isoelectric threshold. Likewise, hydrophobic interactions are formed between amino acids and surfactants when both are positively charged.²⁵

3. EFFECT OF COSOLVENT ON AMINO ACID–SURFACTANT INTERACTIONS

Das et al.²⁶ observed that micellization is affected by the nature of co-solvent used with the aqueous solution. The structural dynamics reveals that the intermolecular interactions between water and the cosolvent have a significant role to play. The CMC and the degree of dissociation are found to increase propositionally with the concentration of the cosolvent. However, Grace and Daniel et al.¹ showed that the CMC increased and the degree of counterion dissociation decreased with an increase in concentration of the cosolvent. Shirzad and Sadeghi²⁵ looked at the impact of short-chain alcohols as cosolvents on micellization. They reported that a 5% aqueous methanol solution increases the CMC of anionic SDS. Some cosolvents like ethane and propane are classified as penetrating since their presence decreases the CMC values. Other cosolvents like DMSO and DMF are classified as non-penetrating, as these result in the increase of CMC. Therefore,

addition of DMSO as a cosolvent to an aqueous medium shifts the CMC to a higher level by increasing the solubility of the hydrocarbon chain. The polarity of water is simultaneously lowered, which occurs due to different properties of the cosolvent.^{27,28}

Shah et al. explored the variation of surface tension and viscosity of SDS in the presence of aqueous methanol solutions and observed that methanol has an adverse effect on the surface tension and viscosity of solutions. It is observed that an increase in the viscosity coefficient occurs with an increase in methanol concentration, which may be due to the binding between SDS and the solvent. Moreover, it was shown that when the concentration of methanol decreased on the surface of the solution, the surface area increased. Also, with an increase in the fractional amount of methanol, the pressure at the surface decreased.²⁹

Sinha et al. studied the self-aggregation properties of some cationic monomeric and dimeric surfactants in polar organic solvents like ethylene glycol and diethylene glycol and observed that the aggregation phenomenon is affected positively with the addition of certain polar organic solvents. It was further revealed that the CMC of surfactants increased in water–organic solvents compared to pure water. When the

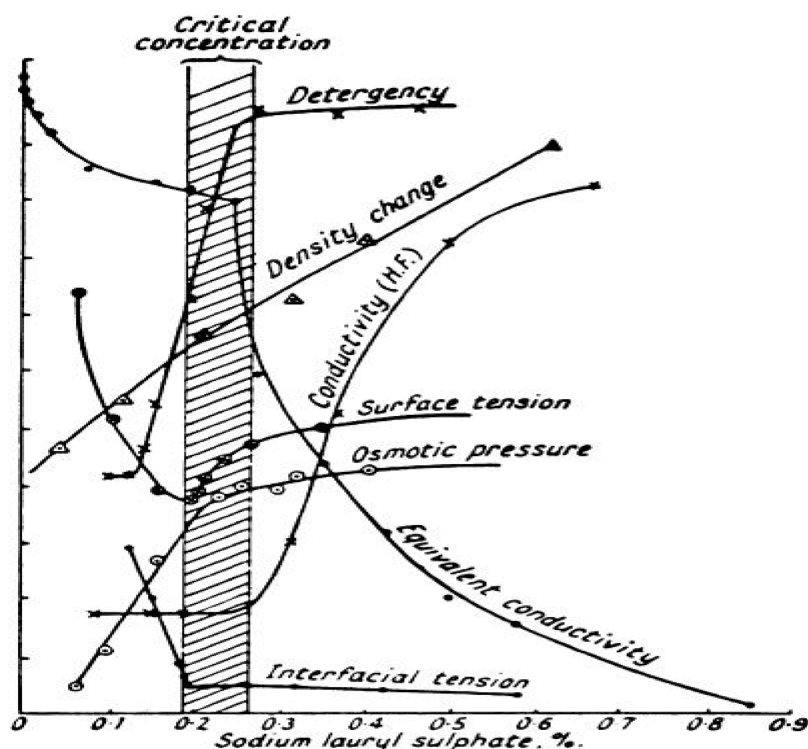


Figure 5. Variation in physical properties of surfactant solutions below and above the CMC value. Reprinted with permission from ref 41. Copyright 2003 Royal Society of Chemistry. Reproduced from ref 45. Copyright 1948 American Chemical Society.

volume of organic solvent increased, the aggregation decreased as a result of the change in Gibb's free energy. The negative value of ΔG of micellization and adsorption energy revealed that the process is spontaneous. Hence, various thermodynamic parameters showed that an increase in the volume percentage of glycols makes the micellization process less favorable.³⁰

Harutyunyan investigated the surface activity, micellar, viscometry, and aggregation properties of nonionic surfactant (HCA) in an aqueous solution and in the presence of neutral amino acids (alanine, phenylalanine, glycine, leucine, serine). The CMC of these surfactants was found to decrease in aqueous amino acid solutions, which may be due to the strong intermolecular interactions that exist in the component system. It was inferred that adsorption of hexadecyl alcohol ethoxylate, calculated using Gibb's adsorption equation at water/air interface, is favoured more than the micellization property. The negative viscosity B-coefficient values suggest that neutral amino acids behave as water structure breakers. With increased amino acid concentration, the aggregation number of the surfactant decreases, which may be due to interactions of the zwitterionic charged group of the amino acids.³¹ The effect of cosolvent on three different gemini surfactants [n -EO₁- n] ($n = 12, 14, 16$) was studied by Tiwari and Shah. They observed that the absence of a cosolvent significantly delayed the process of micellization in comparison to pure water which resulted in a positive Gibb's energy of transfer.³² The surfactants were shown to be functional even after being dissolved in the solvent, and the surface tension measurements showed that the surfactants' behavior was altered at various hydration concentrations.³³ The hydrophobic effect, which arises from the nonpolar hydrophobic chain of surfactants, also decreases upon the addition of a cosolvent and, thus, increased the critical micelle concentration.³⁴

4. EFFECT OF CHAIN LENGTH ON AMINO ACID–SURFACTANT INTERACTIONS

The hydrocarbon chain length is vital in amino acid–surfactant interactions because it provides information about the changes that occur below and above the CMC (Figure 4).³⁵ The influence of chain length of surfactant on the binding interactions of a biological photosensitizer with cationic micelles was investigated by Chakrabarty et al.³⁶ They found that varying the chain length of surfactant promoted a specific prototropic form of the probe molecule. An increase in the hydrophobic chain length resulted in shifting the prototropic equilibrium toward the cationic species. Thus, whenever the length of the surfactant chain increased, it led to an increase in the compactness of the micellar units. This, in turn, resulted in an increase in the population of the probe which resides in the interfacial region that is relative to the core region of the micellar environment.³⁶ Khan et al. explained the effect of the alkyl part of amine chain length on the CMC of the cationic gemini surfactant. Their findings showed that the CMC of the surfactant decreased with an increase in amine concentration. Also, they reported an increase in the synergism with an increase in alkyl amine concentration for the Gemini surfactant.³⁷ McGregor et al. and Rizvi et al. revealed that the hydrocarbon chain length plays a significant role in binding amino acids and surfactants. As the number of binding sites increases, so does the hydrocarbon chain length: more binding sites equates to more amino acid–surfactant interactions and vice versa.^{38,39}

5. APPLICATION OF AMINO ACID–SURFACTANT INTERACTIONS

Amino acid–surfactant interactions have a vast range of applications in many industries. In the food science, namely,

dairy, the formation of a milk during pasteurization is possible, due to the action of the surfactant on lactoglobulins, and surfactants are widely used as emulsifiers, where the action of surfactants on arginine creates an exceptionally good antimicrobial activity against the most common food borne pathogens *E. coli* and *Salmonella*, which show an increase in resistance to drugs. The presence of a guanidine side chain in arginine makes it a suitable and optimal raw material used in the preparation of cationic surfactants with significant biocidal and antiseptic properties. Surfactants lower the surface tension of water when the CMC is reached, thus promoting detergency (cleaning action of soap). Interactions of aspartic acid with surfactant have been reported to have an effective application in detergency due to its ampholytic and chelating characteristics. In drug delivery, surfactants and amino acids are used as excipients; for example, a synthetic acyl amino acid/peptide was reported to serve as a drug carrier and used in preparing functional liposomes with lipopeptide ligands. This is attributed to the existence of surface features such as hydrophobicity and surface charge, which have a significant impact on the particulate drug delivery system's cellular absorption. Hydrogels also serve as the foundation for fibrous proteins like fibroin, which are used for tissue regeneration and medication delivery. Gemini surfactants were reported to be good carriers for bioactive molecule transportation in gene therapy. These interactions of surfactants and amino acids also increase the efficacy of pesticides and insecticides when used as adjuvants along with agrochemical spray solutions because they have the ability to hydrolyze very easily into harmless components. Potassium *N*-cocoyl glycinate has the ability to cleanse and as a makeup remover and is mild to skin. *N*-acyl-*L*-glutamic acid has good water solubility due to the presence of two carboxylic groups in its molecule, making it useful in skin care products.⁴⁰ A change in CMC affects the protein interactions; when the value of CMC decreases, the proteins are more potent in forming micelles, and it also enhances hydrophobic–hydrophobic interactions (in the case of SDS) due to the increase in dielectric constant of the aqueous solutions of the protein. The strong electrostatic connection that binds the counterion with the ionic headgroup of the surfactant due to the reduced hydration radius results in a decrease in mutual repulsion among the ionic headgroup, resulting in a decrease in CMC. How various physical properties like density, conductivity, surface tension osmotic pressure change in the presence of surfactants is summarized in Figure 5.⁴¹ It is therefore necessary to further explore these interactions as they have tremendous benefits for humans.^{42–44}

6. COMPUTATIONAL STUDY OF AMINO ACID–SURFACTANT INTERACTIONS

The various physiochemical study of the amino acid–surfactant complex from a thermodynamic standpoint is significant as it provides beneficial information about the various interaction and aid in the improvement of their applications in detergency, cosmetics, foods, biopharmaceutical processes, drug delivery, and so on. The study of micelle formation from the surfactant in amino acid is significant as they both are amphiphilic moieties and possess strong interactions due to ionic and nonpolar components.⁴⁶ The transferring data show that amino acids engaged in several ways with dodecyltrimethylammonium bromide (DTAB)/TTAB micelles having various interactions like hydrophobic–hydrophobic, ionic, and ionic–hydrophobic bonding. The

negative values of transfer volume show hydrophobic–hydrophobic and ionic–hydrophobic interactions between the surfactant and amino acid. This is confirmed further by the increasing endothermic conditions, and therefore it can be claimed that the formation of a peptide bond increases with cationic surfactant micelles.⁴⁷ The interactions are susceptible to environmental parameters such as pH, concentration, and temperature. As a result, the reported work investigated the interactions of cationic surfactant (CTAB) with various amounts of glycine in aqueous medium.⁴⁸

Hussain et al. studied the effect of amino acids on SDS at various temperatures. SDS self-aggregation characteristics are influenced by amino acids, as shown in Figure 6. The CMCs in MET, THR, and PHE solutions were decreased from 4.14 and 6.42×10^{-3} mol/dm³ to 4.59 and 3.70×10^{-3} mol/dm³, respectively.⁴⁹

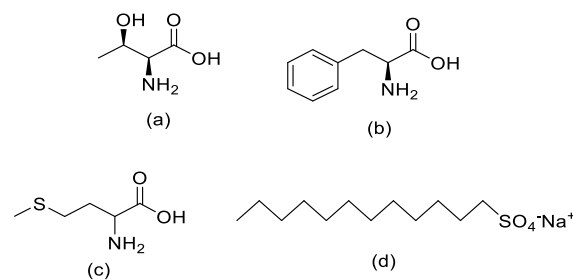


Figure 6. Chemical structure of (a) *L*-threonine, (b) phenylalanine, (c) DL-methionine, and (d) sodium dodecyl sulfate. Reprinted with permission from ref 49. Copyright 2022 Elsevier, Ltd.

Researchers have focused on the estimation of surface tension and fluorescence to investigate the interactions between anionic surfactant (SDBS) and cationic surfactant (DTAB) along with additives (histidine, glutamine, and methionine) on varying temperatures and composition. In SDBS, the value of CMC increases with the temperature, while in DTAB, it exhibits a U-type behavior, implying both hydrophobic and hydrophilic dehydration.⁵⁰ The physicochemical and toxicological characteristics of *N*-acyl surfactants generated from alanine and serine were examined and compared to SDS in this study. Although the carbon chain was demonstrated to have a significant influence on both surface characteristics and toxicological parameters, the impact of the polar head cannot be neglected.⁵¹ They synthesized a gemini surfactant (SDDC) from the amino acids cystine and decanoic acid in this study. The effect of various metallic salts on surfactant aggregation was investigated. This interaction resulted in an oxidation–reduction process in the SDDC/CuSO₄ combination examined in this work, with copper reduction happening concurrently with SDDC sulfur atom oxidation. Cu⁺ might interact with the surfactant in the final vesicular system.⁵² Wormlike micelles were tested in a surfactant combination that included an anionic surfactant (SLSar) and zwitterionic surfactant (CAHS). With the titration, the decrease in pH was from 7.5 to 4.5, as shown in Figure 7. Open symbols depict the turbidity in the solution, which was postulated to result from the precipitation of the acid form of SLSar. When the pH of four of the five examined systems was reduced, viscosity increased to a maximum and then dropped. The synergistic effect was found to be maximum in the the 6%/9% composition or an equivalent 1:1 molar ratio

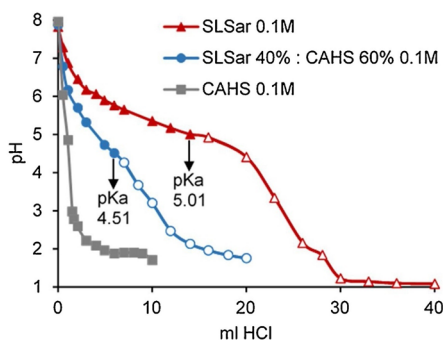


Figure 7. Titration curves of 0.1 M SLSar/CAHS systems with 0.1 M HCl. Reprinted with permission from ref 53. Copyright 2020 Elsevier, Ltd.

between two surfactants, with a maximum viscosity of 9.6 Pa·s at pH 4.0.⁵³

In further research, LaSrCoO₄ was synthesized using the amino-based surfactant (*N*-(2-hydroxylalkyl)-*L*-phenylalanine), and their electrocatalytic properties were studied. The resulting LaSrCoO₄ has a high surface area and strong electrocatalytic properties. The LaSrCoO₄ electrode displayed remarkable electrochemical performance and strong electrical conductivity. The designed LaSrCoO₄ exhibits promising cathodic properties in intermediate temperatures of solid oxide fuel cells.⁵⁴ The micellization in the aqueous solution of amino acid-based surfactant (SLS) and a zwitterionic surfactant cocamidopropyl betaine (CAPB) has been studied. The CAPB/SLS micelle

solution exhibits a maximum viscosity at 5500 mPa·s with a CAPB/SLS mass ratio of 8:4.⁵⁵ The volumetric properties of amino acid (glycine, serine, aspartic acid, lysine, alanine, leucine) with nonionic surfactant hexadecyl poly[oxyethylene] alcohol (C16A25) have been investigated. The changes in the transfer volumes (*t*₂) were explained in terms of interactions. They achieved low value for partial molar volume from aqueous to surfactant solutions for amino acids with varying hydrophobic compositions. These findings imply an equilibrium in the interactions of amino acid zwitterionic groups with the water-soluble moiety of C₁₆A₂₅, as well as amino acid hydrophobic/ionic/hydrophilic groups with the aquaphobic groups of C₁₆A₂₅.⁵⁶ The behavior of surfactants (RNC-*n*, *n* = 8, 12, 14) was studied both analytically and computationally, and its application was used as corrosion inhibitor in AA2024-T3 in NaCl solution. The corrosion inhibition performance enhanced with the carbon chain length.

Based on Figure 8, the diameter capacitive loop might result from the adsorption of the inhibitor on the metal surface. With increasing concentrations, the diameter of the loop of RNC-14 increases. The impedance factor increases initially and is subsequently reduced as the concentration increased in the lower frequency range. The Nyquist plot corresponds to a single time constant, which agrees with the Bode and phase angle charts.⁵⁷

A research group investigated the conductometric interaction of the cationic surfactant (CTAB) with amino acids (lysine and serine) in water. The solution creation approach was used to investigate the influence of numerous factors on

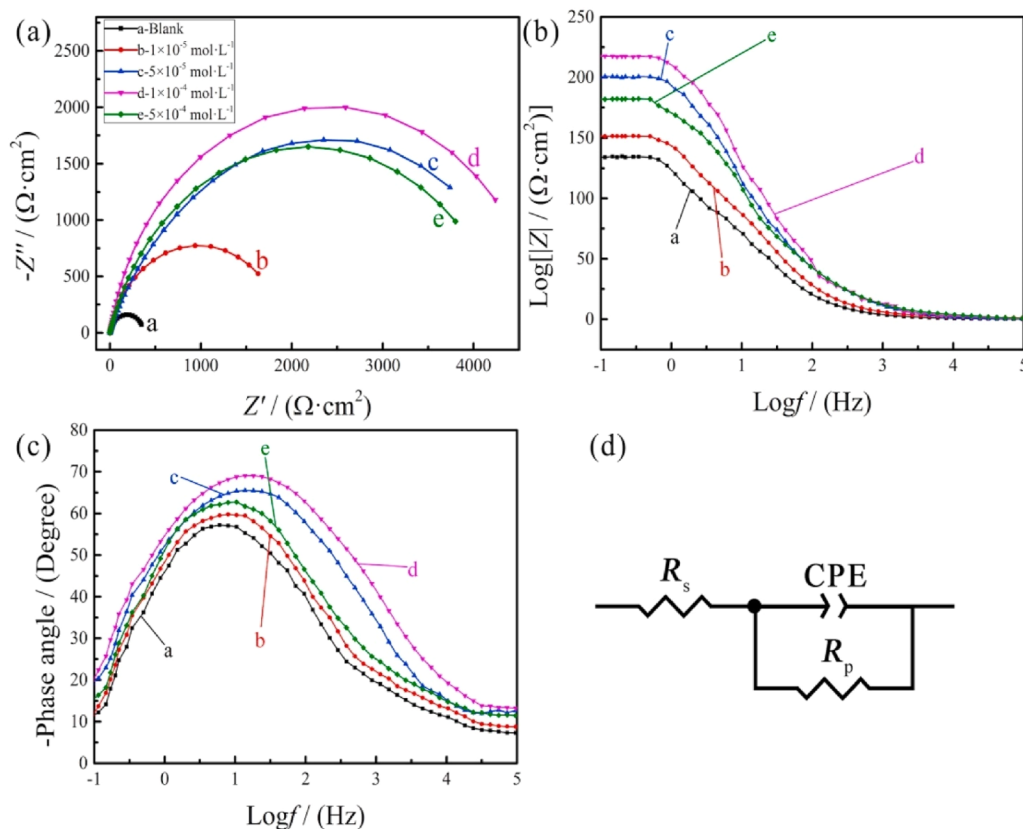


Figure 8. Series of Nyquist plot, Bode plot, and phase angle plot for AA2024-T3 in the absence or the presence of RNC-14 at various concentrations for AA2024-T3 without and with surfactants at different concentrations in 3.5% sodium chloride solution: (a) RNC-8, (b) RNC-12, and (c) RNC-14. (d) Equivalent circuit. Reprinted with permission from ref 57. Copyright 2022 Elsevier, Ltd.

interactions. Thermodynamic parameters for micellization including ΔH_m , ΔS_m , and ΔG_m have also been calculated with amino acids (serine and lysine). The results show that increasing the concentration of additional amino acids produces an increase in CTAB CMC; however, CMC decreases with rise in temperature, leading to a decrease in CMC.⁵⁸ Feng worked on the adsorption of 20 amino-acids with surfactant on the gold metal using molecular dynamics in dilute solution with the intermolecular CHARM-METAL potential. All amino acids appeared between -3 and -26 kcal mol⁻¹, and the degree of adsorption is related to the strength of coordination of polarizable atoms (O, N, C) to multiple sites. Large molecules possessing sp² hybridization (Gln, Arg, Asn, Trp, Tyr, and PPh₃) adsorb strongly followed by sp³ hybridization.⁵⁹ The potential of specific amino acid derivatives to bind to the metal surface has been investigated theoretically. Molecular features were identified and compared using DFT calculations, while binding behavior was investigated using molecular dynamics simulations on different metal surfaces and in different conditions. According to the results, each chemical tested showed a striking affinity for reacting with metallic substrates. However, the research on various metal surfaces reveals that the binding energy of the molecule varies greatly depending on the surface type following the order Fe₂O₃ < FeS₂ < Fe (110) < FeCO₃.⁶⁰ Researchers have used SCA along with four amino acid surfactants due its solubility in a solvent at ambient temperature. The micelle formation becomes highly endothermic and entropy-driven and also shows the greater capacity to reduce oil–water interfacial tension than SDS. SCA was also shown to be more effective than SDS and CTAB in changing the wettability of quartz and carbonate rocks in Figure 9.⁶¹

The behavior of micellization and molecular interaction of amino-acid-based amphoteric surfactant sodium *N*-acyl diaminosulfonate based on castor oil (AAS-CO) and cationic

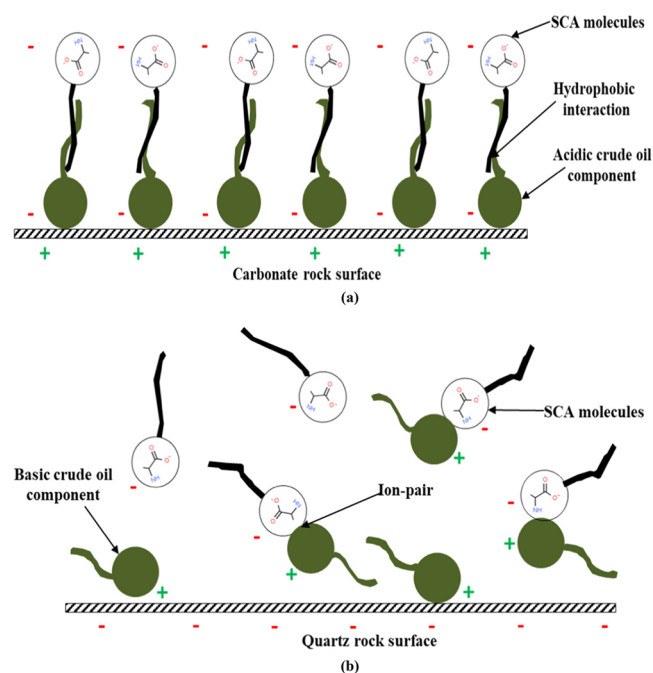


Figure 9. Interaction of SCA molecules on (a) carbonate and (b) quartz rock surface. Reprinted with permission from ref 61. Copyright 2020 Elsevier, Ltd.

surfactant (STAB) in aqueous solution were evaluated by both conductometry and tensiometry. Thermodynamic characteristics demonstrate that the proposed method of micellization is enthalpically spontaneous. When amounts of AAS-CO were added to an aqueous solution, the free energy increased, favoring the formation of mixed micelle represented in Figure 10.⁶²

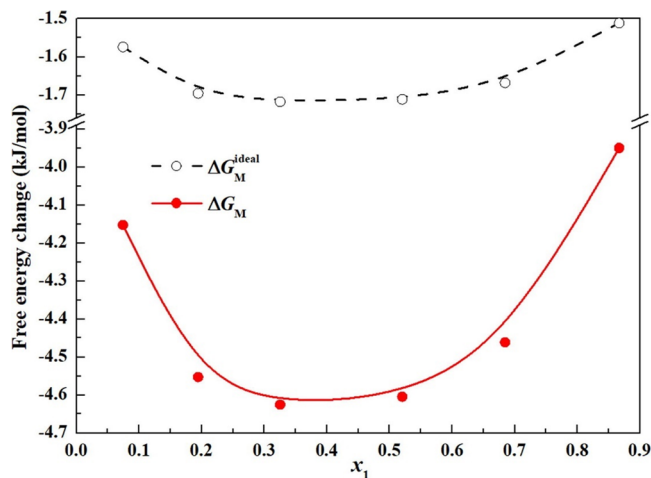


Figure 10. Variation of free energy change of micellization with the composition in bulk solution at $T = 298.15$ K. Reprinted with permission from ref 62. Copyright 2021 Elsevier, Ltd.

This work described the formation of a viscoelastic wormlike micellar system in a mixed non-ionic surfactant system. The anionic surfactant (LAD) was neutralized by 2,2',2''-nitrilotriethanol (TEA) at various degrees of neutralization (1:1 via 1:1.5 to 1:2), and the influence of concentration and temperature was studied. At low shear rates, the samples display Newtonian behavior shown in Figure 11, whereas shear thinning occurs above critical shear rates.⁶³

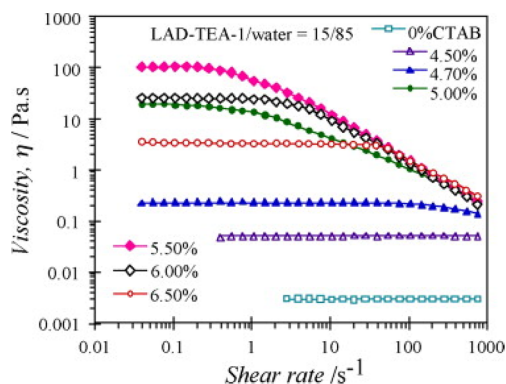


Figure 11. Viscosity versus shear rate curves for the LAD-TEA-1/water/CTAB system as a function of CTAB at fixed LAD-TEA-1/water = 15/85 at 25 °C. Reprinted with permission from ref 63. Copyright 2007 Elsevier, Ltd.

A research group has synthesized the cationic surfactant, namely, 4,4'-(((1*Z*,5*Z*)-pentane-1,5-diylidene)-bis-(azaneylylidene))-bis(1-dodecyl-1,5-dimethyl-3-oxo-2-phenyl-2,3-dihydro-1*H*-pyrazol-1-ium bromide (QABCS)), and surface tension measurements were taken to investigate the surface-active factors. Numerous methodologies were used to assess QABCS's performance as an inhibitor for carbon steel

(CS) in 1.0 M HCl. The interpretation of DFT and Monte Carlo (MC) studies demonstrates that the Q_{ABCS} seems to have a high adsorption capacity on the surface of CS due to active sites present in Q_{ABCS}' structure.⁶⁴

Based on the research of the effects of amino acids on the micelle characteristics of C₁₄-C₆ AOS in aqueous environments, it is possible to conclude that the reported characteristics are due to the influential intermolecular forces. The micellization of C₁₄-C₁₆AOS in AA aqueous solutions is greatly influenced by hydrophobic and electrostatic interactions. Data from adsorption at the air/liquid interface indicate that adsorption is preferred to micellization. The interaction of AA's zwitterionic groups with C₁₄-C₁₆AOS's ionic groups increases C₁₄-C₁₆AOS agglomeration in an aqueous solution. The physicochemical properties, cytotoxicity, and antibacterial activity of tertiary ammonium-acid-based surfactants are highly dependent on the hydrocarbon chain and are unmodified by the polar part of amino acid (leucine or methionine). The toxicity and antimicrobial properties of C₁₂ and C₁₄ alkyl chains were the same but higher against Gram-positive bacteria than BAC as a reference drug in Figure 12.⁶⁵

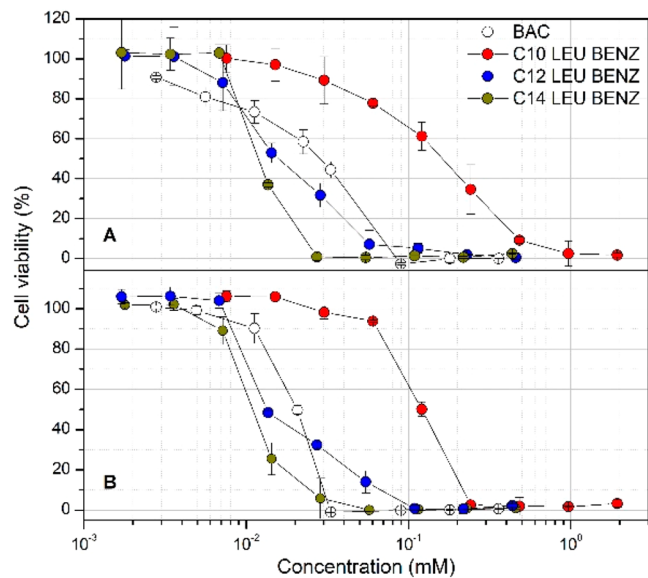


Figure 12. Cell viability (%) of Caco-2 (A) and Calu-3 (B) cell lines after exposure to different concentrations of quaternary ammonium surfactants derived from leucine and methionine and the reference compound BAC. Dots represent the mean, and bars are the standard error ($n = 4$). Reprinted with permission from ref 65. Copyright 2019 Elsevier, Ltd.

7. SURFACTANT–SURFACTANT INTERACTIONS

The surfactant–amino acid interaction is an essential topic of research in biotechnological and pharmaceutical applications. Thermodynamic parameters of surfactant–surfactant aqueous media have important thermodynamic characteristics because they reveal the types of interactions present and facilitate the study and application of these systems.⁶⁶

Researchers presented a novel family of amphiphilic gemini surfactants as gene delivery vehicles, as well as the start of a thorough structure–activity investigation. Preliminary studies indicate that the gemini surfactant along with DOPE may result in the formation of micelles of various sizes and content.³⁸ The surfactant–surfactant interaction affects the

physicochemical properties. Qin et al. studied the change in the surface properties and application performance of mixture of anionic (SLL) and cationic surfactant (gemini quaternary ammonium salt with a hydroxyl group (GC12)).⁶⁷ To assess the behavior of synthetic surfactant qualities at the air–water interface, standard physicochemical parameters of surfactants such as CMC, Kraft temperature, and minimum surface area per molecule (A_{\min}) were evaluated. Researchers have studied corrosion inhibition of different surfaces at different temperatures and pressures; in this work, novel gemini cationic surfactants, DHNMMB and DHNBMBDMB, were synthesized. From the computational study, it was concluded that performance of inhibition was enhanced with the increase in concentration and a decrease in temperature. The C/θ vs C graphs of the linear Langmuir adsorption has a slope close to 1. This shows that the Langmuir isotherm model was followed by both DHNMMB and DHNBMBDMB. Increasing K_{ads} values reveal the high adsorption capacity of DHNMMB and DHNBMBDMB on the CS surface. However, DHNBMBDMB adsorption is more successful than DHNMMB, as shown in Figure 13.⁶⁸

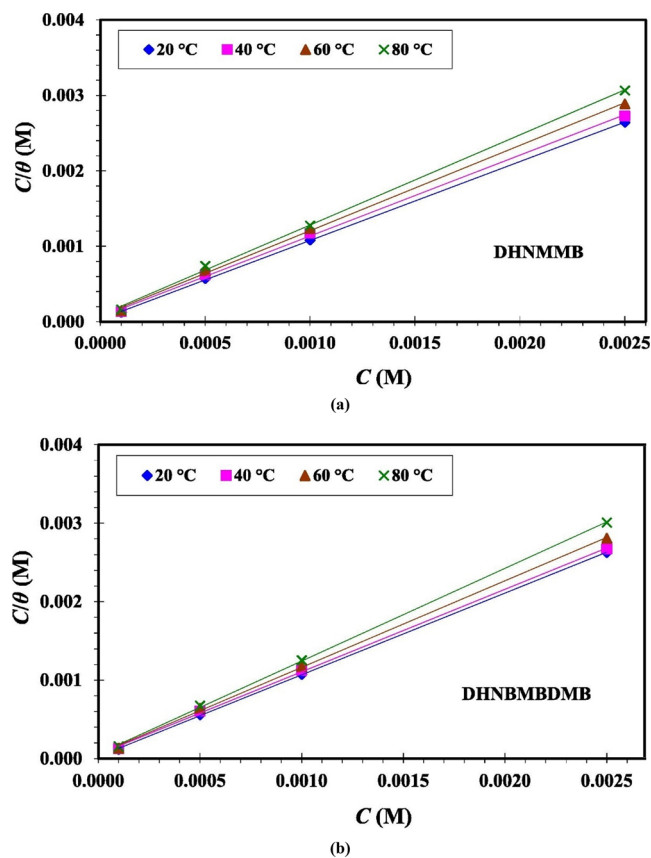


Figure 13. Langmuir isotherm adsorption model of different concentrations of (a) DHNMMB and (b) DHNBMBDMB on the CS surface in 5% HCl at different temperatures. Reprinted with permission from ref 68. Copyright 2022 Elsevier, Ltd.

Nima et al. synthesized a cationic sugar-based surfactant [*N,N,N*-trimethyl-2-oxo-2-(((2*R*,3*S*,4*S*,*S**R*)-3,4,5-trihydroxy-6-(tetradecyloxy)tetrahydro-2*H*-pyran-2yl)methoxy)ethan-1-aminiumiodide], and with the help of a computational study, the size, shape, and aggregation number of the micelle were evaluated using the DFT (B3LYP/6-311G) approach.⁶⁹

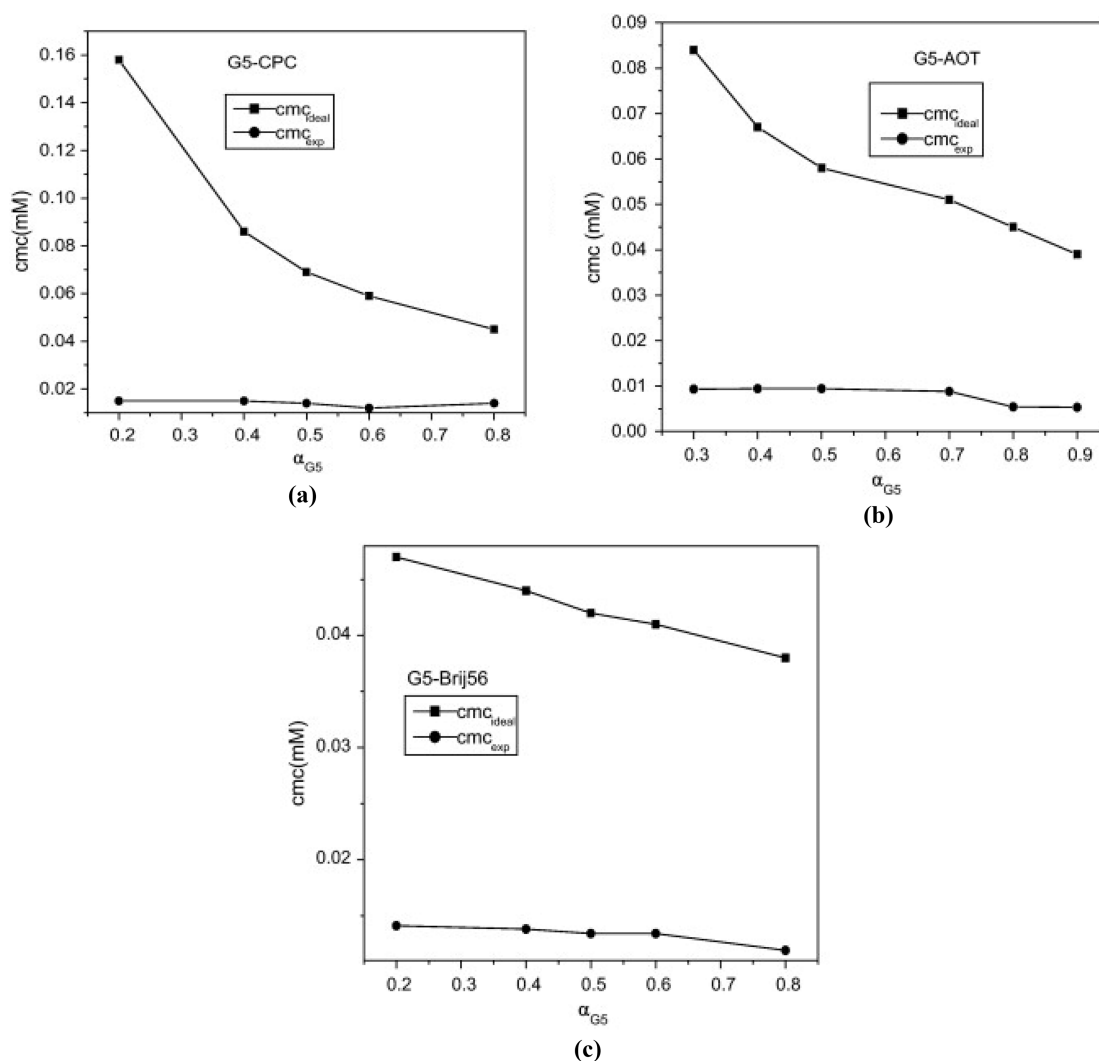


Figure 14. Plots of CMC and the stoichiometric mole fractions of (a) G5-CPC, (b) G5-AOT, and (c) G5-Brij56. Reprinted with permission from ref 72. Copyright 2011, Elsevier, Ltd.

The synergetic effect of anionic surfactant (SMS) and cationic surfactant 12-3-12 and a DTAB surfactant in mixed micelles has been studied.⁷⁰ Experiments on the impact of gemini surfactants (GS) were conducted at various concentrations from 0 to $3000 \times 10^{-5} \text{ mol dm}^{-3}$. The results of the experiments revealed that a twin-headed GS medium, even at [16-*s*-16] lower than CMC, is more effective than an aqueous medium and CTAB in accelerating and catalyzing the reaction of Glu and Nin. Their operational skills at each concentration are as follows: 16-4-16 > 16-5-16 > 16-6-16. The influence of different gemini on the rate constant is efficiently handled using a pseudophase model for the activity of the micelle. Gemini can be regarded as a more cost-effective and ecologically friendly surfactant because of the modest amounts utilized in trial runs.⁷¹

The micelle formation and surface studies of the binary mixture prepared using cationic gemini pentanediyl-1,5-bis(dimethylcetylammmonium bromide) (G5, 16-5-16) with conventional cationic part (CPC) were explored. The findings revealed that the analytically obtained CMC values of different binary combinations of G5-AOT, G5-CPC, and G5-Brij56 are smaller than the ideal CMC given by the Clint equation, indicating a dismissive divergence from the ideal behavior in

the mixed micelle production seen in Figure 14. The intensity of a contact has a significant impact on micellar solubilization; less interaction improves solubilization.⁷⁷

Molecular dynamics (MD) simulations were used to investigate the mechanisms and interfacial behaviors of pure and binary mixtures of cationic surfactant (DTAC) and anionic surfactant (AES) at the oil–water interface. The observations indicated that the sulfate groups of AES molecules could approach DTAC molecules in mixed surfactants, lowering repulsion between the molecules. The interactions between headgroups in DTAC molecules result in superior molecular interfacial behaviors that enhanced the arrangement of the AES molecule. Furthermore, it was shown that the quantity of ethylene oxide (EO) groups in AES molecules had a significant impact on contact behavior.⁷³

From Figure 15, it was observed that the peak value for the EO3 system is 6.74, which was higher than that of the EO5 and EO7 systems. The pattern was obtained upon further addition of the EO moiety that increased the steric hindrance and does not promote the production of a thick surfactant layer.⁷³ Another study looked at the rheological and aggregation properties of the EDAB/SDS solution. The EDAB/SDS system exhibits higher viscosity and superior viscoelasticity

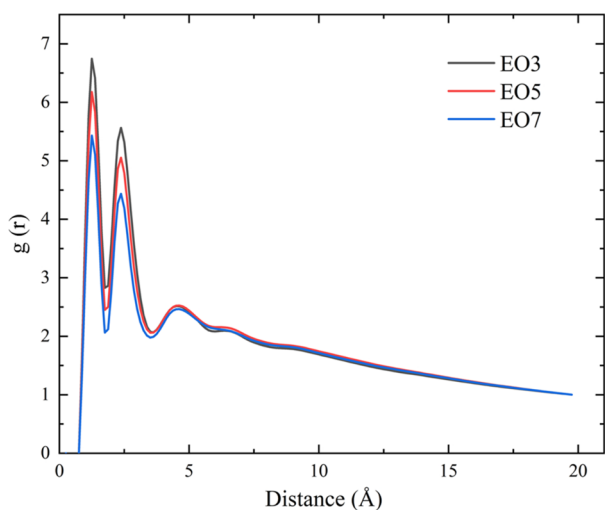


Figure 15. RDF profiles between surfactants with different EO group numbers. Reprinted with permission from ref 73. Copyright 2022 Elsevier, Ltd.

compared to that of the single EDAB system at the same concentration. As the temperature, NaCl concentration, and pH are increased, the rheological behavior of the EDAB/SDS system increases and then drops. When compared to EDAB alone, the EDAB/SDS system provides significant benefits. Lower surfactant concentrations can improve the viscoelastic behavior and aggregation of surfactant solutions in the combined system.⁷⁴

8. CORROSION INHIBITION

Recently, the corrosion of materials is one of the leading issues in the metal industry. Researchers in industrial engineering, electrochemistry, and chemistry are concerned about the degradation of steel-based parts caused by environmental conditions during their usage in acid solutions. Several strategies for protecting steel from acid corrosion have been developed by researchers and industrial engineers, including coating, oxidation, and corrosion inhibition. Among these strategies, inhibition-based protection is the most cost-effective method and environmentally friendly. A novel hexafunctional epoxy polymer was synthesized and tested as a corrosion inhibitor of E24 Carbon Steel (CS) (1.0 M HCl) using gravimetric measurements, electrochemical impedance spectroscopy (EIS), and MD simulations. Furthermore, with the ideal concentration (10^{-3} M) of the epoxy polymer HGTMDAE, the EIS has a higher inhibitory efficiency of 95%. Furthermore, the polarization results show that this macromolecular binder functions as a mixed inhibitor. By adsorption, the epoxy polymer produced a protective layer on the surface of the E24 CS.⁷⁵ Rachid et al. studied the corrosion inhibition of the epoxy polymer named *S,S*-diglycidyl *O,O'*-dicarbonyldithioate of bisphenol A (DGDCBA) in 1.0 M HCl on E24 CS with varying concentrations employing a gravimetric and electrochemical method that shows that the efficiency increases with the increase in concentration. Furthermore, the presence of aromatic rings and heteroatoms in this polymer facilitates the adsorption on the surface of the metal substrate. Moreover, the results obtained from DFT studies and MD simulation show good agreement with the experimental work.⁷⁶ An epoxy resin (triglycidyl ether tribisphenol A of ethylene- TGETBBAE) as a corrosion

inhibitor was used for CS in aggressive solutions (1.0 M HCl) at different concentrations on using weight loss (WL) measurement and the EIS approach. DFT (B3LYP) studies were used to optimize the overall Fe-TGETBAE complex geometry. LanL2DZ was chosen as the basis set for this difficult optimization study, and the calculation was carried out in the Gaussian 09 program. The RDF of O and C atoms, given in Figure 16, reveals that the bond lengths of Fe–O (a)

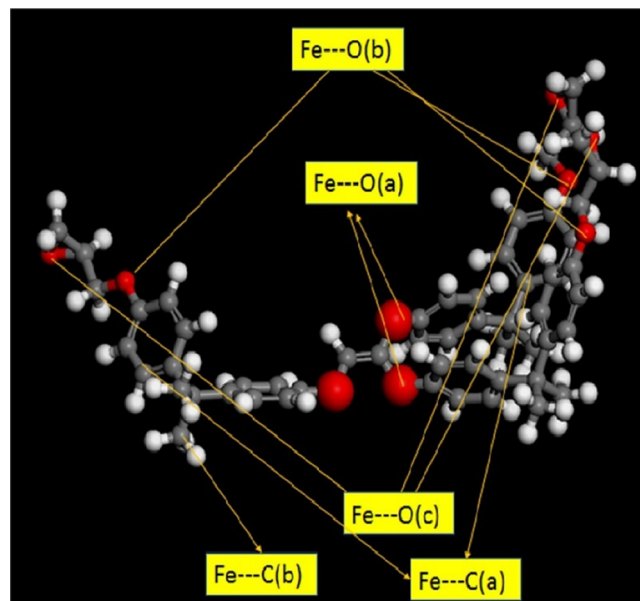


Figure 16. RDF of TGETBAE epoxy polymer on the Fe(110) surface. Reprinted with permission from ref 77. Copyright 2020 Elsevier, Ltd.

(2.6 Å), Fe–O (b) (2.9 Å), and Fe–C (b) (2.7 Å) are all less than 3.5 Å. Furthermore, the bond lengths of Fe–O (c) (4 Å) and Fe–C (a) (7.2 Å) exceed 3.5 Å. Finally, the findings demonstrate the maximum adsorption ability of the TGETBAE inhibitor utilized to adsorb and, more importantly, to prevent the metal from corrosion.⁷⁷

Using computation studies, phosphorus polymer pentaglycidyl ether pentabisphenol A of phosphorus (PGEPPAP) was evaluated as corrosion inhibition for CS. The greater inhibition efficiencies for PDP, EIS, and WL tests at 10^{-3} M PGEPPAP polymer concentration are 94.18%, 91.79%, and 91.3%, respectively.⁷⁸ In one literature report, the quantum parameter performance of two newly synthesized multifunctional polymeric architectures was examined: triglycidyl ether ethylene of bisphenol A (TGEEBA) and hexaglycidyl ethylene of methylene dianiline (HGEEBA) (HDEMMA).⁴⁴ As promising anticorrosive coatings, triglycidyl ether triethoxy triazine (TGETET) was incurred by the 1,6-diamino hexane (DAH), and 4,4-diaminodiphenylmethane (DDM) curing epoxy resins were studied. TGETET/DAH and TGETET/DDM have greater protection efficiency (for EIS and PC) as compared to a 3.5% NaCl solution alone.⁷⁹ The anticorrosive behavior of CS in [1 M] HCl medium was examined using a novel derivative epoxy polymer, 2,4,6-tris(4-(2-(4-(2-methoxy oxiran)phenyl)propan-2-yl)phenoxy)-1,3,5-triazine (EPT).⁸⁰ Using methylene dianiline as a curing agent and natural phosphate as an inorganic filler, the five epoxy polymers, triglycidyl ether tribisphenol A of ethylene (TGETBAE), hexaglycidyl trimethylene dianiline of ethylene (HGTMDAE), pentaglycidyl ether pentaphenoxy of phosphorus (PGEPPP),

PGEPBAP, and decaglycidyl pentamethylene dianiline of phosphorus (DGPMDAP) were formulated. By adjusting the components of the reaction mixture (resin/hardener) and the amount of natural phosphate, the research group has reported the synthesis of thermo setting composite films. Incorporating 5% natural phosphorus (NP) and cured by methylene dianiline (MDA) as the charge improved the protective efficacy of composites of TGETBAE/MDA/NP, PGEPBAP/NP/MDA, HGTMDA/NP/MDA, PGEPPP/NP/MDA, and DGPMDAP/MDA/NP.⁸¹ Authors compared the corrosion activity of TGETET/DDM and TGETET/DAH with both experimental and theoretical methods and concluded that TGETET/DDM has a high protective efficiency compared to that of TGETET/DAH in 3.5% NaCl solution.⁸² Hssisou et al. developed a chitosan-based inhibitor and studied the corrosion inhibition performance of COS-g-Glu for steel in HCl medium.⁸³ A new compound, epoxy prepolymer diglycidyl amino benzene (DGAB), was synthesized and identified by FTIR NMR spectroscopy as a corrosion inhibitor for CS in 1.0 M HCl medium at 298 K using WL and EIS techniques. The results showed that its inhibition efficacy increases with concentration. The acquired values from the weight loss, polarization, and EIS approach all agreed reasonably well with the computational results.⁸⁴ The purpose of this study was to look into the corrosion behavior of carbon steel (CS) in HCl and H₂SO₄ solutions (1 M HCl and 0.5 M H₂SO₄) in the presence of a newly synthesized macromolecular epoxy resin called N₂,N₄,N₆-tris(2-(oxiran-2-yl methoxy)ethyl)-N₂,N₄,N₆-tris(oxiran-2-yl methyl)-2.4.6-triamine-1 (ERT).⁸⁵

Amino acids have shown corrosion inhibition in hostile environments. Amino acids are one of the most intriguing classes of chemicals that produce high inhibitory efficacy. Inhibitors must also be ecologically benign and safe for people. Amino acids are found insignificant parts of the human body, making them a suitable candidate for corrosion inhibitors. Furthermore, amino acids are easily acquired with a high degree of purity, are fairly or sparingly soluble in aqueous solutions, and are affordable.⁸⁶ Recently, amino acids have been thoroughly investigated as potential corrosion inhibitors for brass, iron, and copper in a various conditions. Steel corrosion releases ions that are hazardous to health and can trigger inflammation in the human body.⁸⁷ As a result, it is critical to reduce corrosion of stainless steel (SS) implants and identify inhibitors that will not harm your health and can be used safely. Milosev et al. evaluated the influence of certain amino acids on the corrosion process of copper in 0.5 M HCl solution, and the researchers used the DFT/B3LYP calculations (6-311G basis set) combined with MD simulations. On the one side, alanine and leucine significantly enhanced the corrosion rate, while the inhibitory effectiveness of the remaining amino acids was boosted at 10 mM. The theoretical investigation, on the other hand, did not support the involvement of the amine group's nitrogen atom in the adsorption process of protonated amino acid derivatives, since the NH₃⁺ molecule was orientated outward from the metal substrate into the solution.⁸⁸

cysteine (50%) > histidine ≈ arginine (25%)
> threonine ≈ tyrosine ≈ tryptophan (12%)
> methionine (10%) > glycine (3%) at 10 mM

The investigation of amino acids (lysine and threonine) on the corrosion inhibition process on stainless steel has been performed via exploring or through EIS, atomic force microscopy (AFM), and quantum calculations for the studies. To improve the inhibitory performance, surfactants were used with amino acid to modify the surface, making it easier for L-lysine to bind to the electrode surface which gives facile adsorption of L-lysine on the surface of the electrode. The resistance of charge transfer increases in the appearance of amino acid, but after pretreatment with SDS solution, there is an increase in the generation of coating on the CS surface, according to EIS measurements.⁸⁹ The potential of glutamine (Gln) and its derivative compounds as inhibitors for the anticorrosive behavior of iron was evaluated using DFT calculations. The transformation of Gln upon integration into dipeptides was studied. The inhibition activity of dipeptides has been reported to improve as the number of reaction centers has increased. Theoretically, peptides are much more likely to bind on the surface of iron, indicating that these moieties are extremely useful in corrosion inhibition applications.⁹⁰ To further understand the inhibitory synergistic impact of two environmentally friendly and sustainable amino acids (L-histidine, L-cysteine) and thiourea on the corrosion of N80 CS in a CO₂ atmosphere, electrochemical testing and surface analysis were conducted. These findings demonstrate that the inhibitory efficacy of L-histidine/L-cysteine and thiourea may be enhanced by a synergistic combination, resulting in exceptional inhibitory synergism.⁹¹

The inhibitory activity of di- and tripeptides increases as the number of reaction sites increases in the molecular structure. For the adsorption of short peptides and Cys onto the surfaces of Fe, the adsorption energies (E_{ads}) were calculated. It was discovered that tripeptides were adsorbed onto these substrates via chemical adsorption. Within the protonated forms, the absolute E_{ads} values between these inhibitors on the examined metal surface increased. The peptides' ability to adsorb onto the surface of the Fe was the best, suggesting that their inhibitory efficacy is the maximum theoretically.⁹² Ganjoo et al. conducted an experimental and in silico investigation of sodium cocoyl glycinate (SCG) on mild steel (M.S.) as the corrosion inhibitor in the HCl medium. WL and electrochemical studies reveal that enhancing SCG concentration less or around 0.2864 mM increases the inhibitory efficacy. This occurs due to the well-known aggregating feature of the surfactant, which causes dimers and multimolecular cluster together at the metal/electrolyte interface when the surfactant concentration is at or above the CMC.⁹³

Researchers synthesized two nonionic surfactants and studied their application on the acid corrosion by empirical and computational methods on carbon steel (CS). The heterogeneous resistance behavior occurs in polarization data, and their existence on the CS was elucidated with the Langmuir model through chemisorption. AFM, scanning electron microscopy (SEM), and energy-dispersive X-ray spectroscopy (EDX) methods were used to indicate the existence of an organic protective layer on the surface of CS. DFT calculations and MC calculations were used to analyze the inhibitory action at molecular level. Figure 17 represents the interaction of the inhibitor on Fe (110) to investigate the adsorption process.⁹⁴

Dagdag et al. studied the inhibition of corrosion of tetra-functionalized aniline for CS in 1 M HCl medium using PDP, SEM, PP, DFT studies, and MD simulations approaches. In

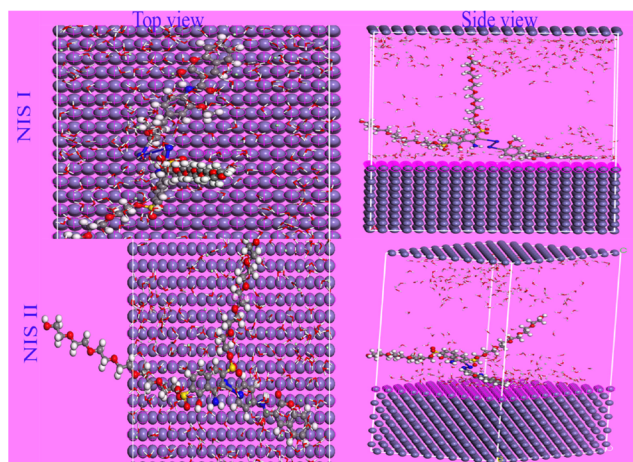


Figure 17. Molecular simulations for the most favorable modes of adsorption obtained for the investigated inhibitors on the Fe(110) surface, side and top view. Reprinted with permission from ref 94. Copyright 2022 Elsevier, Ltd.

Figure 18, the graph was plotted for adsorption energy and temperature that shows most of the molecule has interacted through N and O molecules. The results revealed that AA2 showed a high efficiency of 91.3% at 10^{-3} M, and it behaves as a cathodic type of inhibitor.⁹⁵

Another researcher studied the influence of concentration and temperature on the corrosion inhibition of amino acids (Trp and His) on SABIC Fe in 0.5 M HCl solution. According to their research, the inhibitory efficacy increases on increasing concentrations of amino acids and decreases with rising temperature. DFT calculations results demonstrated that Trp is more efficient than the His molecule, which is compatible with the experimental data. The Trp has a higher energy than the His based on Monte Carlo simulation, and this finding is consistent with the practical outcome. As illustrated in **Figure 19**, the Trp adsorbs horizontally on the Fe(110) surface via the indole ring, whereas the His adsorbs via the imidazolium ring.⁹⁶ In **Table 1**, the research group have tabulated the different amino acid studies on corrosion using various metal surfaces.

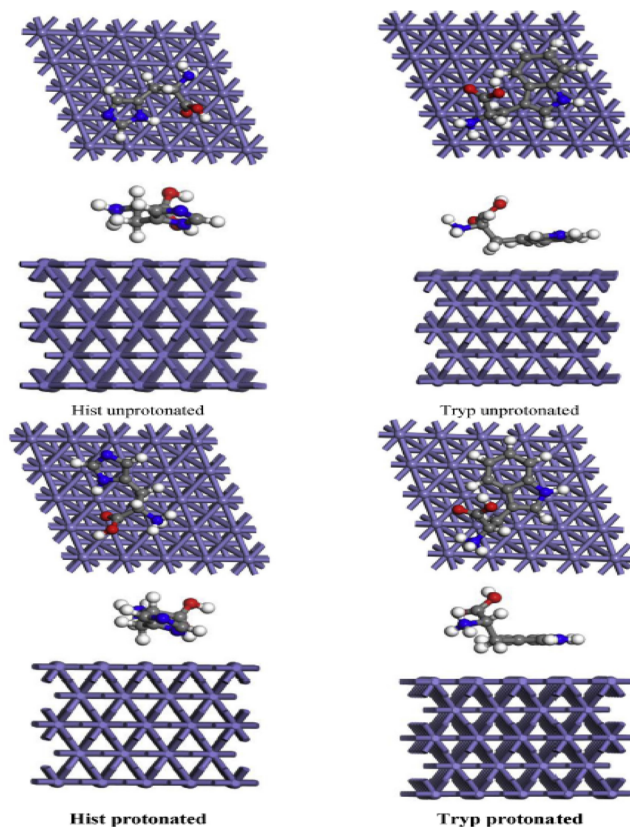


Figure 19. Top and side view of adsorption of His and Tryp on Fe(110). Reprinted with permission from ref 96. Copyright 2022 Elsevier, Ltd.

9. CHALLENGES

In recent years, surfactants have been increasingly used to enhance the transportability of “hard to deliver” pharmaceuticals as a result of medical progress. However, concerns over the safety of surfactants have been brought to focus by its sudden popularity. Numerous chemicals, solvents, and catalysts (often metals) are released into the environment during the synthesis of various surfactants, posing a threat to both

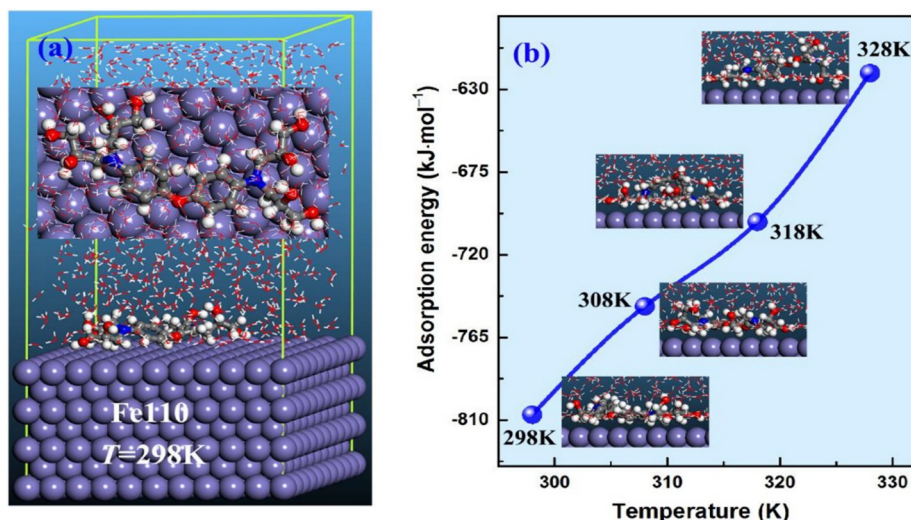


Figure 18. (a) Equilibrium configuration of AA2 adsorbed on the Fe(110) surface. (b) Dependence of adsorption energy on the temperature for the adsorbed AA2 molecule on Fe(110). Reprinted with permission from ref 95. Copyright 2020 Elsevier, Ltd.

Table 1. Various Amino Acids/Surfactants for Corrosion Inhibition

| no. | amino acid–surfactant/surfactant–surfactant | material | computational studies | concentration | ref |
|-----|--|------------|---|--------------------------------------|-----|
| 1 | tryptophan (Tryp) and histidine (His) | SABIC Fe | MS, PDP, EIS, DFT, and MC simulation | 0.5 M HCl | 96 |
| 2 | benzotriazole (BTAH) | L245 steel | chemical adsorption, electrochemical test | 0.5 M H ₂ SO ₄ | 97 |
| 3 | phospho-zwitterionic gemini surfactant | steel | AFM, XPS | 1.0 M aggressive HCl | 98 |
| 4 | CTAB and NLS | M.S. | SEM, EIS, PP | 3.5% NaCl solution | 99 |
| 5 | gemini surfactant (12-B-12) | CS | DFT and MD simulations | 0.01 mM seawater | 100 |
| 6 | BFIS and SFIS | CS | PP, EIS | 1 M HCl | 101 |
| 7 | MET, CYS, and SDBS | 316 L SS | FTIR, SEM, EIS | 0.5 M NaCl solution | 102 |
| 8 | glycine, CTAG, and OTAG | Fe | corrosion inhibition | 5% HCl | 103 |
| 9 | sodium <i>N</i> -dodecyl asparagines (AS), sodium <i>N</i> -dodecylhistidine (HS), and sodium <i>N</i> -dodecyltryptophan (TS) | CS | potentiodynamic polarization and EIS | 0.5 M NaCl and 0.5 M NaOH | 104 |
| 10 | Arg, Gln, Asn, Met, Cys, Ser, | CS | PP and EIS | 0.5 M H ₂ SO ₄ | 105 |
| 11 | leucine, phenyl alanine, and methionine | CS | PP and EIS | 1 M HCl | 106 |
| 12 | CHOGS-8, CHOGS-12, and CHOGS-16 cyclohexane-1,4-diyl bis(2-chloroacetate) | CS | PP, EIS, SEM, EDX | 15% HCl | 107 |
| 13 | CTAB and SDS | M.S. | PP | 2 M HCl | 108 |
| 14 | L-histidine, SDS, and CTAB | mild CS | PP, EIS, AFM, SEM | 0.1 M H ₂ SO ₄ | 109 |
| 15 | L-tryptophan | CS | DFT studies, adsorption isotherms | 1 M HCl | 110 |

terrestrial and aquatic ecosystems. Additionally, various undesirable byproducts are linked to the manufacturing of these compounds. As a result, the idea of amino acid–surfactant interactions emerged, emphasizing the use of safer, more eco-friendly alternatives that pose no threat to human health and the environment but nevertheless provide adequate protection even when used in dilute solutions.¹¹¹ In addition, most amino-acid-based surfactants are expensive, thus, using them for extraction would not be a practical or economical option. The use of surfactants for extraction is also severely limited since most of them are poisonous and not eco-friendly but lack purity issues. On the approach to widespread application, surfactant flooding must first overcome significant obstacles in managing of generated fluids. Surfactants and polymers (P) in liquid have resulted in highly tight oil-in-water (O/W) emulsions, producing major issues in surface oil/water separation, despite the large reduction in the water cut of produced liquid and the rise in oil output.¹¹² The application of surfactants has a drying and irritating impact on the skin with prolonged usage and may even cause permanent harm. The regular physiological processes of the human body are disrupted once surfactants enter the body and harm the action of enzymes. Sodium dodecyl benzenesulfonate (SDBS) has been linked to skin absorption, shrinkage, liver damage, and other persistent symptoms, as well as teratogenic and carcinogenic effects.¹¹³ Nevertheless, several amino-acid-based surfactants are studied as inhibitors in corrosion systems for different metals and alloys in different electrolytes. Literature study suggested that amino acid based surfactants are promising corrosion inhibitors in NaCl, H₂SO₄, HCl, and other electrolytes.¹¹⁴

10. FUTURE PERCEPTIVE

Researchers will be better equipped to optimize structures, perhaps yielding an ideal surfactant that may enhance scientific, economical, and industrial application and expand or boost local companies in the field of corrosion. The pH of amino acid based surfactants may be adjusted to fine-tune their solution, interfacial, and rheological characteristics. The application of amino acid based surfactants is expected to

rise in the next years, providing a stable environment for ongoing study and patenting efforts in this area. The created surfactants encourage towards the frontier of formulation using surfactants derived amino acids. It might improve the quality of our disinfection and other applications, which would be beneficial for protecting both our healthcare facilities and our natural ecosystems. Since these relationships involve people directly, it is important to have a thorough comprehension of them and perform studies about them.¹¹⁵

11. CONCLUSION

The interactions between surfactants and amino acids have been an important topic for different researchers in past and present time due to their diverse applications and great significance to humanity. Various research groups have investigated the effect of cosolvents, temperature, and pH, chain length of the surfactant on CMC, structure, binding ability, and thermodynamic parameters. Amino acids, dipeptides, and surfactants interact through ionic–ionic and ionic–hydrophilic interactions and with the tail part through hydrophobic–hydrophobic interactions. These interactions also become hydrophobic with an increase in the concentration of surfactants. At low pH, amino acids become cationic, and at high pH, they behave as zwitterions. When the pH is below the isoelectric point, the amino acid has a positive charge and binds strongly to the surfactant. The interactions between amino acids and surfactants are hydrophobic when they possess the same charge but become hydrophobic and electrostatic when they have opposite charges. Aqueous methanol solution increases the CMC of anionic surfactant, while ethane and propane decrease the CMC of anionic SDS. Cosolvents, dimethyl sulfoxide (DMSO) and *N,N*-dimethylformamide (DMF), result in the increase of CMC. Consequently, the solubility of the hydrocarbon chain increases in the presence of DMSO in an aqueous medium. In this review manuscript, the application of amino acids and surfactants was studied, and the studies performed at different temperature and pressure on various metal surfaces revealed that they act as efficient corrosion inhibitors. From the computational study, the performance of inhibition was

improved with an increase in concentration as well as with decrease in temperature. An understanding of the factors that affect the micellization property of various surfactants will enable researchers in optimization studies, which may in turn give an ideal surfactant that may improve scientific, economic, and industrial applications as well as increase or boost local businesses in this area. It may also produce better disinfectant, safe guarding our environment and healthcare institutions. Therefore, it is necessary to have a clear understanding of these interactions and also explore research on them as they are associated directly with human beings.

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Notes

The authors declare no competing financial interest.

ABBREVIATION

DMSO, dimethyl sulfoxide; DMF, *N,N*-dimethylformamide; HAE, hexadecyl alcohol ethoxylate; DOPE, dioleoylphosphatidylethanolamine; CPC, cetylpyridinium chloride; G5, 16-5-16-sodium bis(2ethylhexylsulfosuccinate); SLL, sodium lauroyl lactate; LAD, dodecylglutamic acid; STAB, stearyltrimethylammonium bromide; CTAB, cetyltrimethylammonium bromide; CAPB, cocamidopropyl betaine; C₁₆A₂₅, hexadecyl

poly[oxyethylene] alcohol; SLSar, sodium lauroyl sarcosinate; CAHS, cocoamidopropyl hydroxysultaine; TEA, 2,2',2''-nitrilotriethanol; PGEPPAP, phosphorus polymer pentaglycidyl ether pentabispheol A of phosphorus; NP, natural phosphorus; MDA, methylene dianiline; TGETBAE, triglycidyl ether tribispheol A of ethylene; HGTMDA, hexaglycidyl trimethylene dianiline of ethylene; PGEPPP, pentaglycidyl ether pentaphenoxy of phosphorus; DGPMMA, decaglycidyl pentamethylene dianiline of phosphorus; DGAB, diglycidyl amino benzene; ERT, *N*₂,*N*₄,*N*₆-tris(2-(oxiran-2-yl methoxy)-ethyl)-*N*₂,*N*₄,*N*₆-tris(oxiran-2-yl methyl)-2.4.6-triamine-1; EPT, 2,4,6-tris(4-(2-(4-(2-methoxy oxiran) phenyl) propan-2-yl) phenoxy)-1,3,5-triazine

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