


 Cite this: *RSC Adv.*, 2026, 16, 12737

# Ferrite-based materials for anticorrosion: comparative study of $\text{ZnFe}_2\text{O}_4$ , $\text{CuFe}_2\text{O}_4$ , and $\text{SrFe}_{12}\text{O}_{19}$

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Three chitosan ferrite nanoparticles— $\text{ZnFe}_2\text{O}_4$ ,  $\text{CuFe}_2\text{O}_4$ , and  $\text{SrFe}_{12}\text{O}_{19}$ —were synthesized *via* an ultrasound-assisted PEG route, yielding phase-pure products with controlled morphologies. Structural and compositional analyses confirmed phase purity, tailored morphology, and mesoporosity across systems for cubic spinel  $\text{ZnFe}_2\text{O}_4$  and cuprospinel  $\text{CuFe}_2\text{O}_4$ . In contrast,  $\text{SrFe}_{12}\text{O}_{19}$  exhibited coexistence of hexagonal M-type ferrite and rhombohedral  $\alpha\text{-Fe}_2\text{O}_3$ , indicating a multiphase nature. These nanoparticles were incorporated into chitosan-ferrite nanocomposites and evaluated as corrosion inhibitors for carbon steel in 1.0 M HCl *via* potentiodynamic polarization (PDP), electrochemical frequency modulation (EFM), and electrochemical impedance spectroscopy (EIS). All of the techniques revealed concentration-dependent inhibition, with  $\text{ZnFe}_2\text{O}_4$ -based composites consistently demonstrating the highest efficiencies (up to 98.73% by PDP, 94.35% by EFM, and 97.38% by EIS). The inhibition mechanism was identified as mixed-type, primarily affecting the cathodic reaction, supported by causality factors and impedance parameters such as increased  $R_{ct}$  and decreased  $C_{dl}$ . Adsorption modeling showed strong monolayer behavior with spontaneous composite–metal surface interaction, validated by Langmuir fitting and  $\Delta G_{ads}^\circ$  values ( $\sim -28 \text{ kJ mol}^{-1}$ ). These results highlight the performance of ultrasound-engineered ferrite nanocomposites in forming protective films and reducing acid-induced corrosion, underscoring their application potential in advanced coating systems.

 Received 24th October 2025  
 Accepted 22nd February 2026

DOI: 10.1039/d5ra08173d

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## 1. Introduction

Ferrites are a broad class of magnetic oxides with versatile crystal structures, most notably spinel and hexagonal, that have traditionally found use in magnetic recording, permanent magnets, and power electronics. In recent years, however, nanostructured ferrites have emerged as promising anticorrosion materials, particularly when incorporated into protective coatings for metallic substrates. Their chemical inertness, thermal stability, and ability to form passive barrier layers make them ideal candidates for corrosion inhibition in aggressive environments.<sup>1</sup> The nanoscale morphology of ferrites enhances surface reactivity and dispersion within polymeric matrices,

improving coating adhesion and reducing electrolyte permeability.<sup>2</sup>

Spinel ferrites such as  $\text{ZnFe}_2\text{O}_4$  and  $\text{CuFe}_2\text{O}_4$ , and hexagonal ferrites like  $\text{SrFe}_{12}\text{O}_{19}$ , exhibit tailored cation distributions that influence their electrochemical behavior and corrosion resistance. Through composition engineering and controlled synthesis, ferrite nanoparticles can be optimized to suppress anodic and cathodic reactions, promote passivation, and extend the service life of coated metals.<sup>3</sup> These attributes position ferrites as environmentally friendly alternatives to toxic pigments like chromates, offering multifunctional protection in industrial, marine, and infrastructure applications. Zinc ferrite ( $\text{ZnFe}_2\text{O}_4$ ) is a normal spinel ferrite with a cubic crystal structure, exhibiting ferromagnetic behavior and a Néel temperature of approximately 858 K. Beyond its magnetic characteristics,  $\text{ZnFe}_2\text{O}_4$  has gained attention as a promising anticorrosion pigment due to its chemical stability, thermal resistance, and ability to inhibit corrosion when incorporated into protective coatings.<sup>4</sup> The spinel structure, comprising  $\text{Zn}^{2+}$  and  $\text{Fe}^{3+}$  ions distributed over tetrahedral and octahedral sites, contributes to its durability and passivation behavior in aggressive environments. Recent studies have demonstrated that  $\text{ZnFe}_2\text{O}_4$  nanoparticles, when embedded in epoxy or styrene-acrylate matrices,

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enhance the corrosion resistance of coated metal substrates by forming hydroxide layers that suppress electrochemical degradation.<sup>5</sup> Additionally, its nanoscale morphology and high surface area improve pigment dispersion and barrier properties, making  $\text{ZnFe}_2\text{O}_4$  a viable candidate for multifunctional coatings.<sup>6</sup>

Copper ferrite ( $\text{CuFe}_2\text{O}_4$ ) is an inverse spinel ferrite with a tetragonal crystal structure, known for its thermal stability, magnetic properties, and chemical inertness. These attributes make  $\text{CuFe}_2\text{O}_4$  a compelling candidate for anticorrosion coatings, particularly in harsh environments. The unique cation distribution –  $\text{Cu}^{2+}$  ions occupying octahedral sites and  $\text{Fe}^{3+}$  ions distributed across both tetrahedral and octahedral positions – contributes to its structural robustness and passivation behavior. Recent studies have demonstrated that  $\text{CuFe}_2\text{O}_4$  nanoparticles, when incorporated into silicone-based or epoxy resin matrices, significantly enhance the corrosion resistance of coated metal substrates by forming compact barrier layers and promoting hydrophobicity.<sup>7,8</sup> The presence of  $\text{Cu}^{2+}$  ions may also contribute to localized cathodic protection, while the ferrite matrix impedes electrolyte penetration. Furthermore,  $\text{CuFe}_2\text{O}_4$ 's nanoscale morphology and magnetic recoverability offer additional advantages for smart coating systems and multifunctional surface protection.<sup>9</sup>

Strontium hexaferrite ( $\text{SrFe}_{12}\text{O}_{19}$ ) is an M-type hexagonal ferrite known for its high coercivity, thermal stability, and chemical inertness. These properties make it a strong candidate for anticorrosion coatings, especially in environments requiring long-term durability. The magnetoplumbite structure of  $\text{SrFe}_{12}\text{O}_{19}$ , with  $\text{Fe}^{3+}$  ions occupying five distinct crystallographic sites, contributes to its robust lattice and resistance to chemical attack. When incorporated into polymeric matrices such as epoxy or polyaniline composites,  $\text{SrFe}_{12}\text{O}_{19}$  nanoparticles enhance barrier performance by reducing electrolyte permeability and promoting passive layer formation on metal surfaces.<sup>10</sup> Recent studies have shown that  $\text{SrFe}_{12}\text{O}_{19}$ -based nanocomposites exhibit excellent adhesion, low charge-transfer resistance, and high cyclic stability, making them suitable for multifunctional coatings that combine magnetic and protective functions.<sup>10</sup> Additionally, its compatibility with conductive polymers and carbon-based additives allows for tailored electrochemical behavior, further improving corrosion resistance.<sup>11</sup>

Traditionally, the solid-state reaction technique has been widely employed for ferrite synthesis; however, it presents several limitations, including high temperature requirements, large crystallite sizes, and poor compositional homogeneity.<sup>12</sup> To overcome these drawbacks, recent studies have investigated various wet chemical methods for synthesizing ferrite materials such as  $\text{ZnFe}_2\text{O}_4$ ,  $\text{CuFe}_2\text{O}_4$ , and  $\text{SrFe}_{12}\text{O}_{19}$  – notably sol-gel, coprecipitation, and microwave-assisted hydrothermal techniques. Among these, ultrasound-assisted synthesis has emerged as a mild, energy-efficient, and versatile approach for producing high-purity, crystalline, and compositionally homogeneous ferrites. For example, Chen *et al.* synthesized  $\text{ZnFe}_2\text{O}_4@/\text{TiO}_2$  core-shell structures *via* ultrasonic treatment, achieving enhanced phase control and photocatalytic activity.<sup>13</sup>

Meenu *et al.* reported the ultrasound-enabled fabrication of  $\text{CuFe}_2\text{O}_4$ -Ag nanocomposites within hydrogel matrices, demonstrating improved dispersion and dye degradation performance.<sup>14</sup> Similarly, Palomino *et al.* achieved monodisperse  $\text{SrFe}_{12}\text{O}_{19}$  nanoparticles through sonochemical processing, highlighting the method's efficacy for complex hexaferrites.<sup>15</sup> These findings underscore the adaptability of ultrasound-assisted synthesis across both simple binary oxides and structurally intricate spinel and hexaferrite systems.

Herein, we report the synthesis of  $\text{ZnFe}_2\text{O}_4$ ,  $\text{CuFe}_2\text{O}_4$ , and  $\text{SrFe}_{12}\text{O}_{19}$  nanoparticles *via* a versatile ultrasound-assisted polyethylene glycol (PEG) route. This method enabled the formation of phase-pure, crystalline  $\text{ZnFe}_2\text{O}_4$  and  $\text{CuFe}_2\text{O}_4$  ferrites with controlled morphology and dispersion, while  $\text{SrFe}_{12}\text{O}_{19}$  was obtained as a multiphase material comprising dominant hexagonal magnetoplumbite and a minor  $\alpha$ - $\text{Fe}_2\text{O}_3$  phase. The structural characteristics of the synthesized nanoparticles were systematically investigated, and their performance as corrosion inhibitors was evaluated. To comprehensively assess their anticorrosion potential, electrochemical techniques and adsorption modeling were employed, complemented by density functional theory (DFT) calculations to elucidate the molecular interactions and reactivity at the metal-inhibitor interface.

## 2. Experimental Section

### 2.1 Materials

All reagents used were commercially available and directly employed without further purification. Iron(III) nitrate nonahydrate (99%) was purchased from Riedel-deHaen, sodium hydroxide (99%), zinc acetate-2-hydrate (99%) from FARCO, copper(II) acetate monohydrate (99%), strontium nitrate (99%), ethanol (p.a.), polyethylene glycol 6000 (PEG 6000) (99%) from Sigma-Aldrich.

### 2.2 Synthetic procedures

**2.2.1 Synthesis of  $\text{ZnFe}_2\text{O}_4$ ,  $\text{CuFe}_2\text{O}_4$ , and  $\text{SrFe}_{12}\text{O}_{19}$ .** Spinel  $\text{ZnFe}_2\text{O}_4$ ,  $\text{CuFe}_2\text{O}_4$ , and hexaferrite  $\text{SrFe}_{12}\text{O}_{19}$  were synthesized using a PEG-assisted sonochemical precipitation approach. Stoichiometric amounts of  $\text{Fe}(\text{NO}_3)_3 \cdot 9\text{H}_2\text{O}$  (0.33, 0.4, and 0.6 g),  $\text{Zn}(\text{CH}_3\text{COO})_2 \cdot 2\text{H}_2\text{O}$  (0.12 g),  $\text{Cu}(\text{CH}_3\text{COO})_2 \cdot \text{H}_2\text{O}$  (0.1 g), and  $\text{Sr}(\text{NO}_3)_2$  (0.2 g) were individually dissolved in 5 mL of deionized water containing PEG 600 (0.5 g), followed by stirring for 10 min in sealed glass vessels at room temperature. Sodium hydroxide (0.25 g) was then introduced to each solution, and the mixtures were stirred vigorously for an additional 30 min. Each reaction mixture underwent sonication for 3 h in an ultrasonic bath (LUC-405, DAIHAN LABTECH Co. Ltd; 60 kHz, 350 W). The resulting precipitates were separated by centrifugation, thoroughly washed with distilled water, and dried at 100 °C for 3 h. Finally, calcination in air at 500 °C for 3 h yielded phase-pure  $\text{ZnFe}_2\text{O}_4$  and  $\text{CuFe}_2\text{O}_4$ .  $\text{SrFe}_{12}\text{O}_{19}$  required higher thermal treatment and was calcined at 700 °C for 3 h to achieve the desired hexaferrite phase.



### 2.2.2 Synthesis of chitosan/metal oxide nanocomposites.

For the preparation of chitosan/metal oxide nanocomposites, 1 g of chitosan was dissolved in 50 mL of deionized water containing 2.5 mL of 5% acetic acid. The solution was stirred continuously for 4 h until a homogeneous viscous gel was formed. Subsequently, 0.3 g of  $\text{ZnFe}_2\text{O}_4$ ,  $\text{CuFe}_2\text{O}_4$ , or  $\text{SrFe}_{12}\text{O}_{19}$  powder was separately added to the chitosan solution and stirred for 24 h to ensure uniform dispersion. The mixture was then neutralized using 100 mL of 2% NaOH, followed by centrifugation and repeated washing with distilled water. The resulting Ch–Oxide nanocomposites were dried in an oven at 100 °C for 3 h.

### 2.3 Characterization

The phase composition and structural properties of the metal oxide nanoparticles were determined using X-ray diffraction (XRD), performed on a Seifert 3003TT diffractometer with copper  $K\alpha$  radiation as the source.

Transmission Electron Microscopy (TEM), conducted with a JEOL GEM-1010 system, provided high-resolution imaging of nanoparticle morphology. Elemental analysis was carried out concurrently using Energy-Dispersive X-ray spectroscopy (EDX).

The specific surface area and adsorption–desorption characteristics of the sample were assessed at cryogenic temperatures using a Quantachrome instrument (USA), featuring TouchWin software for data acquisition and analysis.

### 2.4 Electrochemical measurements

Electrochemical tests were conducted using a Gamry REF600-16084 potentiostat with data processed using Echem Analyst 2 (Framework v7.10.4). A standard three-electrode setup (100 mL capacity) was used, consisting of a polished steel working electrode (1.0  $\text{cm}^2$ ), platinum wire counter electrode, and saturated Ag/AgCl reference electrode. Tests were conducted in 1 M HCl at  $30 \pm 1$  °C, with varying concentrations (40 to 400 ppm) of chitosan/metal oxide nanocomposites. Prior to testing, the working electrode was immersed in the test solution and left to stabilize for 3600 seconds to reach a stable open circuit potential (OCP). Electrochemical Frequency Modulation (EFM) was performed with a foundational frequency of 0.1 Hz, along with multipliers of 2.0 and 5.0, and an amplitude set at 10 mV.<sup>16</sup> The utilization of these parameters facilitated the examination of inhibitor adsorption kinetics and non-faradaic phenomena.<sup>17</sup> Concurrently, Electrochemical Impedance Spectroscopy (EIS) was executed at the open circuit potential (OCP) employing a 10 mV alternating current (AC) signal across a frequency spectrum ranging from 100 kHz to 0.01 Hz. Potentiodynamic polarization (PDP) was carried out by scanning the potential  $\pm 250$  mV with respect to OCP at a scan rate of 0.5  $\text{mV s}^{-1}$ . Inhibition efficiency was calculated from the following equations:<sup>18</sup>

$$\eta_{\text{P,EFM}}\% = 100 \left( 1 - \frac{i_{\text{corr}}^{\text{inh}}}{i_{\text{corr}}^{\text{blank}}} \right) \quad (1)$$

### 2.5 Theoretical methodology and methods

Plane-wave Kohn–Sham density functional theory (KS-DFT) calculations with pure PBEPBE exchange–correlation functional,<sup>19</sup> implemented into Quantum Espresso program package, version 7.1,<sup>20</sup> were used to optimize the geometries of the NPs. The van der Waals correction (DFT-D) was applied to realistically represent van der Waals forces in KS-DFT calculations.<sup>21</sup> The plane-wave energy cut-off was set to 75 Ry for the zinc-containing system and 45 Ry for all other systems. Due to the accuracy limitations of pure functionals, the global reactivity parameters and partial atomic charges were deliberately obtained *via* hybrid density functional theory (HDFT). The M11 exchange–correlation *meta*-GGA functional was hereby used.<sup>22</sup> To solve d-element-containing compositions, we employed the Stuttgart/Dresden effective core potentials. The dispersive attraction was included inherently.<sup>23,24</sup> The convergence criterion within the self-consistent field procedure was set to  $10^{-7}$  hartree. The implicit solvent water was used because the simulated NPs are expected to neutralize corrosion promoters in their aqueous environment. The partial atomic electrostatic charges were derived by fitting the HDFT-derived electrostatic potential in the system using the Merz–Kollman algorithm. The HDFT calculations were conducted in Gaussian'09D.<sup>25</sup> The reported calculations were carried out using an implicit water model, which represents the solvent as a matterless polarizable continuum at effectively low ionic strength. In particular, the 1 M HCl environment of the corrosion experiments is not hereby explicitly modeled. No hydronium cations and no chloride anions are present. Thereby no electric double layer is formed at the metal/solution interface. The modeled inhibitor is treated in its neutral form. In tun, under the strongly acidic experimental conditions it is expected to exist predominantly in protonated and fractionally ion-paired states. As a consequence, the computed electronic descriptors and adsorption-related properties should be regarded as qualitative indicators of the intrinsic reactivity of the inhibitor molecules. A fully quantitative description of the 1 M HCl medium requires explicit treatment of  $\text{H}^+/\text{H}_3\text{O}^+$  and  $\text{Cl}^-$ , high ionic strength, and interfacial charging, which is beyond the current scope.

## 3. Results and discussion

### 3.1 Morphology, crystallinity, and porosity of ferrite nanoparticles

Powder X-ray diffraction (XRD) analysis was employed to assess the phase composition and purity of the synthesized samples, as illustrated in Fig. 1. The diffraction pattern of  $\text{ZnFe}_2\text{O}_4$  matched perfectly with the reference data (JCPDS Card No. 01-082-1042), confirming the formation of cubic spinel zinc ferrite without any detectable secondary phases or impurity peaks. Similarly, the XRD pattern of  $\text{CuFe}_2\text{O}_4$  revealed that the dominant phase was cuprospinel, with all diffraction angles corresponding to the standard card [JCPDS No. 034-0425], and no evidence of extraneous crystal phases. Notably, no peak splitting, broadening, or asymmetry-typically associated with tetragonal distortion-was observed in the diffraction pattern.



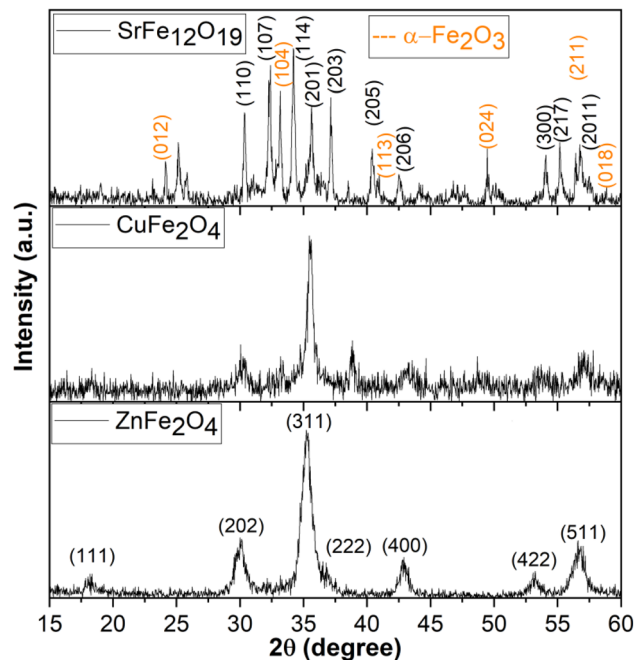


Fig. 1 XRD patterns recorded for the  $\text{ZnFe}_2\text{O}_4$ ,  $\text{CuFe}_2\text{O}_4$ , and  $\text{SrFe}_{12}\text{O}_{19}$  samples.

Detailed peak analysis of  $\text{SrFe}_{12}\text{O}_{19}$  indicated that the majority of reflections aligned with the hexagonal space group  $P6_3/mmc$ , while a subset of peaks matched the rhombohedral space group  $R\bar{3}c$ . This coexistence of reflections suggests the presence of two distinct crystalline phases within the synthesized material. Specifically, the lattice planes (110), (112), (107), (114), (201), (203), (205), (206), (300), (217), (2011), (220), and (2013) are characteristic of M-type hexaferrites with a hexagonal structure (JCPDS Card No. 79-1411). The second phase, attributed to  $\alpha\text{-Fe}_2\text{O}_3$  with rhombohedral symmetry, is evidenced by peaks at (012), (113), (024), (211), (018), and (224), corresponding to the  $R\bar{3}c$  space group (JCPDS Card No. 33-0664). By comparing the integrated intensities of the  $\alpha\text{-Fe}_2\text{O}_3$  reflections to those of the dominant  $\text{SrFe}_{12}\text{O}_{19}$  peaks, the  $\alpha\text{-Fe}_2\text{O}_3$  phase was estimated to constitute approximately 11 wt% of the total crystalline content. The average crystallite size of the synthesized composite materials was calculated using Scherrer's equation (eqn (2)):

$$D = \frac{k\lambda}{\beta \cos \theta} \quad (2)$$

where  $D$  = crystallite size,  $k$  = shape factor,  $\lambda$  = wavelength of X-ray,  $\beta$  = (FWHM) full width at half maximum of the peak in radians,  $\theta$  = Bragg diffraction angle. The estimated crystallite sizes were approximately 11.70 nm for  $\text{ZnFe}_2\text{O}_4$ , 15.80 nm for  $\text{CuFe}_2\text{O}_4$ , and 38.00 nm for  $\text{SrFe}_{12}\text{O}_{19}$ .

The elemental composition of the synthesized  $\text{ZnFe}_2\text{O}_4$ ,  $\text{CuFe}_2\text{O}_4$ , and  $\text{SrFe}_{12}\text{O}_{19}$  samples was evaluated using energy dispersive X-ray spectroscopy (EDX). As shown in Fig. 2, the spectra confirm the presence of the respective constituent elements: Zn, Cu, Sr, Fe, and O, consistent with the expected stoichiometry of each ferrite system. Importantly, no extraneous impurity bands were detected in any of the spectra, affirming

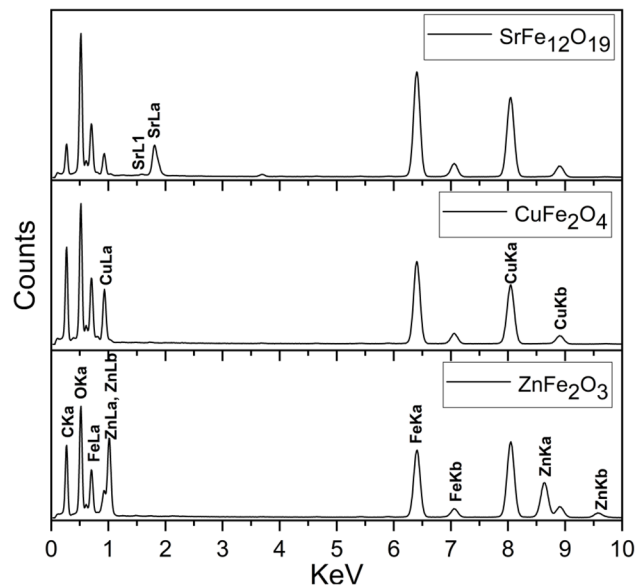


Fig. 2 EDX spectra recorded for the  $\text{ZnFe}_2\text{O}_4$ ,  $\text{CuFe}_2\text{O}_4$ , and  $\text{SrFe}_{12}\text{O}_{19}$  samples.

the phase purity of the synthesized samples. Minor C peaks were observed, attributed to the carbon support film used in the TEM sample preparation, and are not indicative of contamination from synthesis.

The TEM was conducted to investigate the morphology, crystallite dimensions, and agglomeration behavior of the synthesized ferrite samples (Fig. 3).  $\text{ZnFe}_2\text{O}_4$  nanoparticles (Fig. 3a) exhibit predominantly spherical to quasi-spherical morphologies, with diameters ranging from  $\sim 5$  to 20 nm and a notable concentration within the 10–15 nm range. Individual crystallites frequently assemble into chain-like and flower-shaped polycrystalline aggregates with average sizes of  $\sim 100$ –120 nm, formed through oriented attachment and surface energy minimization.  $\text{CuFe}_2\text{O}_4$  nanoparticles (Fig. 3b) display nearly spherical to faceted morphologies, reflecting shape anisotropy likely influenced by local growth conditions. Primary particle sizes measure  $\sim 10$ –30 nm, while TEM images reveal densely packed clusters with average dimensions of  $\sim 120$ –140 nm, suggesting stronger agglomeration compared to  $\text{ZnFe}_2\text{O}_4$ . This clustering is likely driven by magnetic dipole interactions, which promote particle–particle attraction and reduce dispersion.  $\text{SrFe}_{12}\text{O}_{19}$  particles (Fig. 3c) exhibit plate-like and slightly elongated morphologies, with occasional faceted edges. These features align with the intrinsic hexagonal magnetoplumbite structure, where anisotropic growth along specific crystallographic axes dominates. Particle sizes span  $\sim 30$ –80 nm, and the relatively well-defined edges suggest high crystallinity. However, the presence of a secondary  $\alpha\text{-Fe}_2\text{O}_3$  phase, confirmed by XRD, indicates that the observed morphology may also include interspersed hematite crystallites. Hematite typically forms smaller, pseudo-plate or granular particles that can adhere to or embed within the larger hexaferrite plates, subtly altering surface texture and particle boundaries. As a result, the morphology of  $\text{SrFe}_{12}\text{O}_{19}$  should be



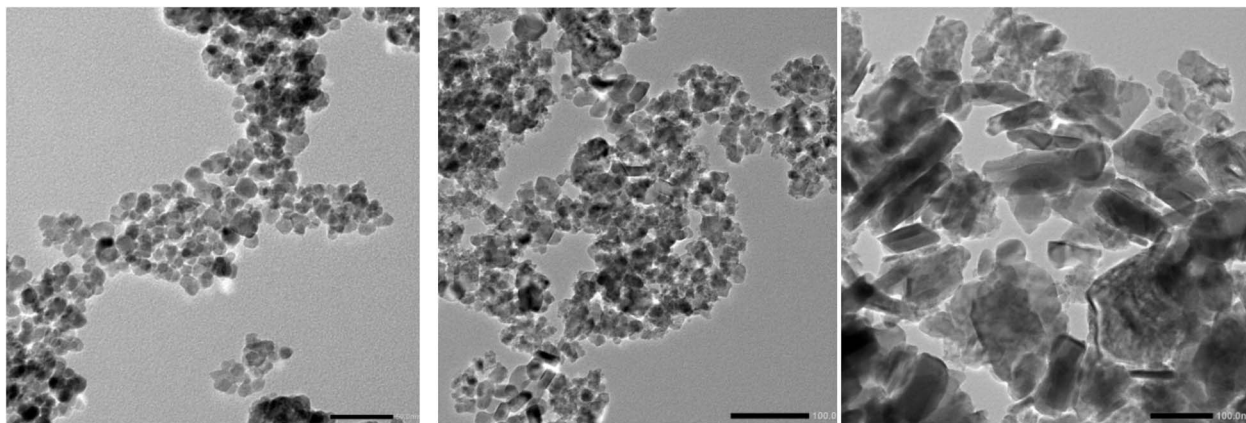


Fig. 3 TEM images of  $\text{ZnFe}_2\text{O}_4$  (left),  $\text{CuFe}_2\text{O}_4$  (middle) and  $\text{SrFe}_{12}\text{O}_{19}$  (right) NPs.

understood as a composite of dominant hexaferrite plates with embedded or attached hematite crystallites, a structural complexity that may influence surface accessibility, particle-particle interactions, and ultimately electrochemical behavior.<sup>26</sup> Overall, TEM analysis confirms distinct morphological characteristics across the ferrite systems: moderate agglomeration in  $\text{ZnFe}_2\text{O}_4$ , stronger clustering in  $\text{CuFe}_2\text{O}_4$ , and relatively uniform

dispersion in  $\text{SrFe}_{12}\text{O}_{19}$ . The hierarchical structures observed are expected to play a critical role in determining surface accessibility, pigment packing, and electrolyte diffusion, thereby influencing inhibition efficiency and overall coating performance. Furthermore, the particle sizes observed through TEM analysis were found to be in good agreement with the

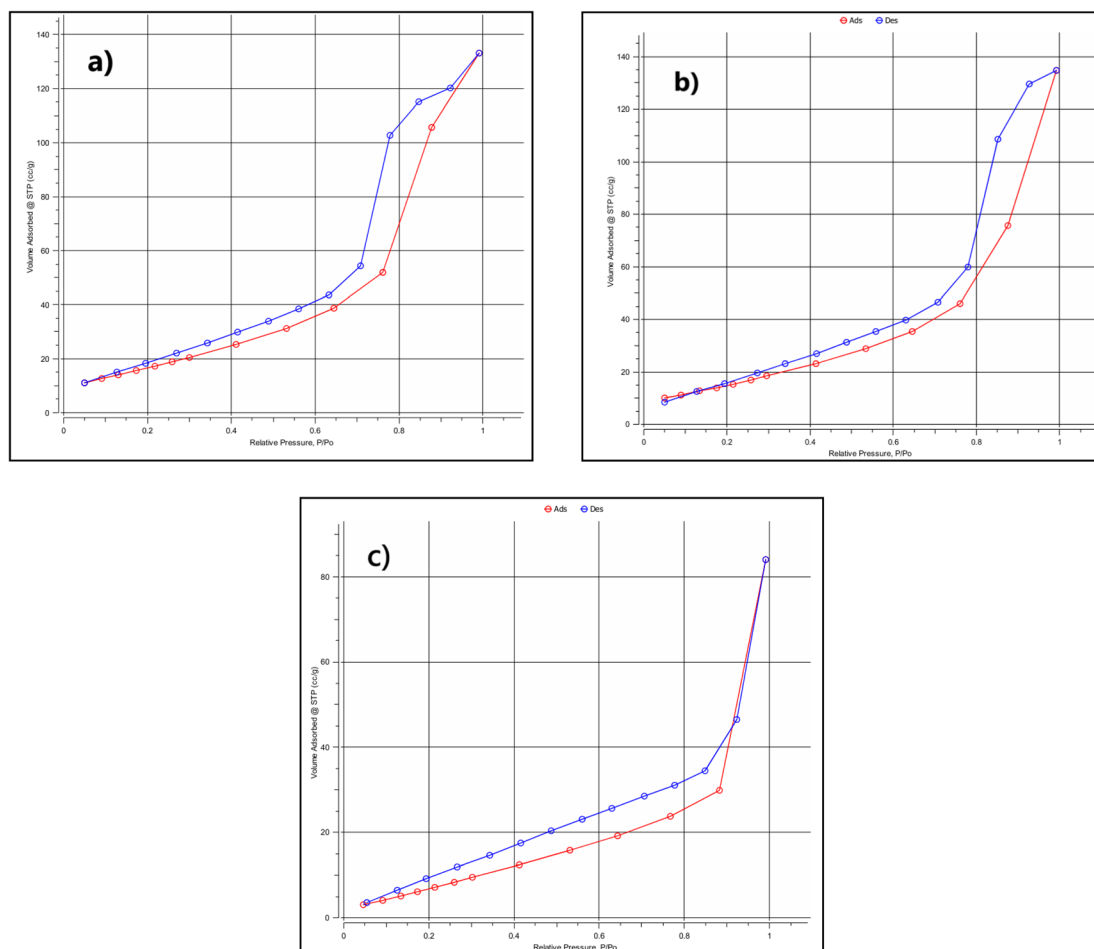


Fig. 4  $\text{N}_2$  adsorption–desorption of the of (a)  $\text{ZnFe}_2\text{O}_4$ , (b)  $\text{CuFe}_2\text{O}_4$  and (c)  $\text{SrFe}_{12}\text{O}_{19}$  samples.



crystallite sizes estimated from XRD data, supporting the reliability of the measurements.

The  $N_2$  adsorption-desorption isotherms of  $ZnFe_2O_4$ ,  $CuFe_2O_4$ , and  $SrFe_{12}O_{19}$  uniformly exhibit type IV profiles with H3 hysteresis loops, consistent with mesoporous structures containing slit-like pores formed *via* particle agglomeration (Fig. 4). These hysteresis loops, arising from the divergence between adsorption and desorption branches, affirm the presence of interconnected pore networks that facilitate capillary condensation and surface accessibility—key factors in optimizing coating performance. In all systems, initial uptake at low relative pressures ( $P/P_0 < 0.3$ ) corresponds to monolayer adsorption, followed by a steep increase near  $P/P_0 \approx 0.8$ – $0.9$  associated with capillary condensation in mesopores.

For  $ZnFe_2O_4$ , the BET surface area was measured at  $65.8 \text{ m}^2 \text{ g}^{-1}$ , which, although lower than some reported maxima – such as the  $78.9 \text{ m}^2 \text{ g}^{-1}$  for  $ZnFe_2O_4$  obtained *via* ultrasound-assisted synthesis using glucose precursors<sup>27</sup> – remains comparatively high and exceeds many values reported for conventional synthesis routes. For instance, Jadhav *et al.* reported a BET value of only  $2.27 \text{ m}^2 \text{ g}^{-1}$  for  $ZnFe_2O_4$  prepared by a sol-gel auto-combustion method using urea as a chelating agent.<sup>28</sup> Similarly, Tomina *et al.* obtained a BET surface area of approximately  $26 \text{ m}^2 \text{ g}^{-1}$  for  $ZnFe_2O_4$  synthesized *via* a precipitation method assisted by citric acid as a capping agent.<sup>29</sup> The slightly reduced surface area observed in our study is attributed to particle agglomeration evident in TEM images, which limits external surface exposure and pore accessibility. Nevertheless, the material exhibits a well-developed mesoporous structure, and the achieved surface area is sufficient to support its intended anticorrosion application.

$CuFe_2O_4$  displayed a BET surface area of  $54.1 \text{ m}^2 \text{ g}^{-1}$ , which lies within the broad literature range ( $9$ – $160 \text{ m}^2 \text{ g}^{-1}$ ) and is higher than several values reported for conventional methods such as thermal decomposition ( $18.2 \text{ m}^2 \text{ g}^{-1}$ ) or precipitation ( $24.1 \text{ m}^2 \text{ g}^{-1}$ ).<sup>30</sup> The relatively small BJH-derived average pore diameter of  $1.93 \text{ nm}$ , though lower than the typical  $4$ – $8 \text{ nm}$  range, is consistent with slit-like mesopores indicated by the H3 hysteresis loop. This discrepancy is explained by synthesis-specific factors—rapid nucleation, restricted grain growth, and magnetic dipole-driven clustering—that reduce interparticle spacing and limit pore expansion. Larger mesopores reported in literature generally arise from template-assisted or high-temperature calcination routes, which differ significantly from the present synthesis conditions.<sup>31–33</sup>

$SrFe_{12}O_{19}$  exhibited a BET surface area of  $41.7 \text{ m}^2 \text{ g}^{-1}$  and a BJH pore size of  $1.92 \text{ nm}$ . While the nearly identical pore size values for  $CuFe_2O_4$  and  $SrFe_{12}O_{19}$  appear statistically unusual, they are more likely artifacts of the BJH method, which assumes cylindrical pore geometry and is less accurate for slit-like or irregular pores.<sup>34</sup> In  $SrFe_{12}O_{19}$ , the low pore volume ( $0.12 \text{ cm}^3 \text{ g}^{-1}$ ) and plate-like morphology suggest minimal mesoporosity, with the measured pore size reflecting surface voids or edge effects rather than intrinsic pore structure.<sup>35</sup>

Correlation between TEM and BET analyses confirms that particle agglomeration plays a decisive role in reducing surface area compared to literature maxima. TEM revealed moderate

Table 1 Textural properties derived from BET and BJH analyses

Pore radius (nm)	Pore volume ( $\text{cm}^3 \text{ g}^{-1}$ )		
	$ZnFe_2O_4$	$CuFe_2O_4$	$SrFe_{12}O_{19}$
1.92	0.0085	0.0105	0.0076
2.58–2.59	0.0207	0.0232	0.0150
3.72–3.76	0.0454	0.0444	0.0246
6.51–6.72	0.1596	0.1067	0.0365
56–71	0.2036	0.2014	0.1242

clustering in  $ZnFe_2O_4$ , stronger aggregation in  $CuFe_2O_4$ , and relatively uniform dispersion in  $SrFe_{12}O_{19}$ . These morphological traits directly influenced BET values, as agglomeration reduces accessible surface area and narrows pore distributions, consistent with prior reports.

To provide quantitative insight, representative BJH adsorption pore volume data points are presented in Table 1. These values highlight the evolution of pore volume across different regimes:  $ZnFe_2O_4$  and  $CuFe_2O_4$  exhibit higher pore volumes and narrower distributions, consistent with their dispersed nanoparticle morphologies, whereas  $SrFe_{12}O_{19}$  shows broader pores and lower overall volume, in agreement with its aggregated plate-like structure. Although  $ZnFe_2O_4$ ,  $CuFe_2O_4$ , and  $SrFe_{12}O_{19}$  were synthesized under identical ultrasound-assisted PEG conditions, the observed differences in BET surface area and pore size distribution arise from the intrinsic crystallographic structures, cation chemistry, and agglomeration tendencies of each ferrite system.  $ZnFe_2O_4$ , with its cubic spinel framework, favors quasi-spherical crystallites that assemble into moderate aggregates, yielding relatively high surface area. In contrast,

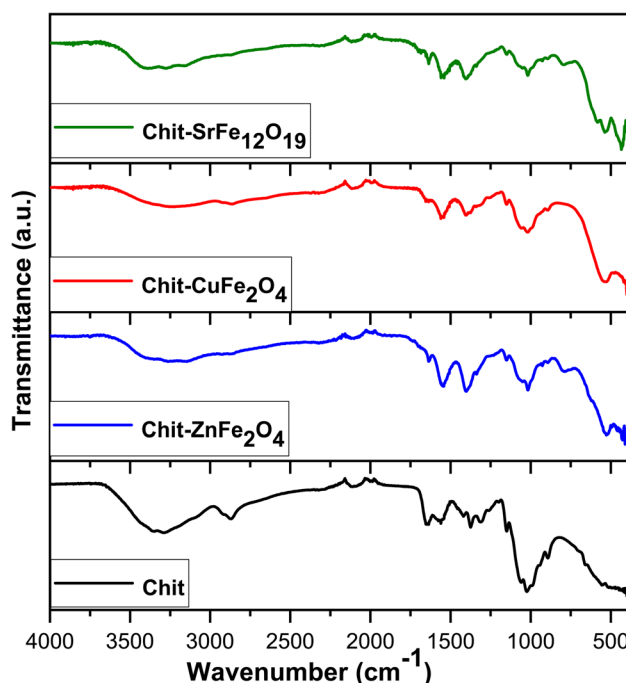


Fig. 5 FTIR spectra of Chit, Chit- $ZnFe_2O_4$  NPs, Chit- $CuFe_2O_4$  NPs, Chit- $SrFe_{12}O_{19}$  NPs.



$\text{CuFe}_2\text{O}_4$  exhibits stronger magnetic dipole interactions that promote clustering, thereby reducing accessible surface area and narrowing pore dimensions.  $\text{SrFe}_{12}\text{O}_{19}$ , dominated by anisotropic plate-like growth and the coexistence of  $\alpha\text{-Fe}_2\text{O}_3$ , shows minimal mesoporosity and lower pore volume due to structural packing constraints. Thus, the textural properties are not solely determined by external synthesis parameters but by the interplay between synthesis conditions and material-specific growth mechanisms. These differences in morphology and porosity directly influence pigment dispersion, interfacial bonding, and electrolyte diffusion, thereby shaping the anti-corrosion performance of the resulting nanocomposites.<sup>24,25</sup>

FTIR analysis was performed to investigate the chemical interactions between chitosan and ferrite nanoparticles in the synthesized composites: **Chit- $\text{ZnFe}_2\text{O}_4$** , **Chit- $\text{CuFe}_2\text{O}_4$** , and **Chit-**

**$\text{SrFe}_{12}\text{O}_{19}$**  (Fig. 5). The spectra were recorded in the range of  $4000\text{--}400\text{ cm}^{-1}$  and compared with pure chitosan (Chit) to identify characteristic functional groups and confirm successful incorporation of ferrite phases. All samples exhibited a broad absorption band around  $3400\text{ cm}^{-1}$ , corresponding to the stretching vibrations of hydroxyl (O-H) and amine (N-H) groups, which are intrinsic to the chitosan backbone. The bands near  $2900\text{ cm}^{-1}$  were attributed to C-H stretching vibrations of aliphatic groups. A prominent peak around  $1650\text{ cm}^{-1}$  was observed in all samples, associated with the amide I (C=O) stretching vibration. Notably, this band showed slight shifts in the ferrite-modified samples, indicating possible interactions between chitosan's carbonyl groups and the metal ions of the ferrite nanoparticles. In the fingerprint region, distinct bands appeared between  $500$  and  $600\text{ cm}^{-1}$  in the **Chit-**

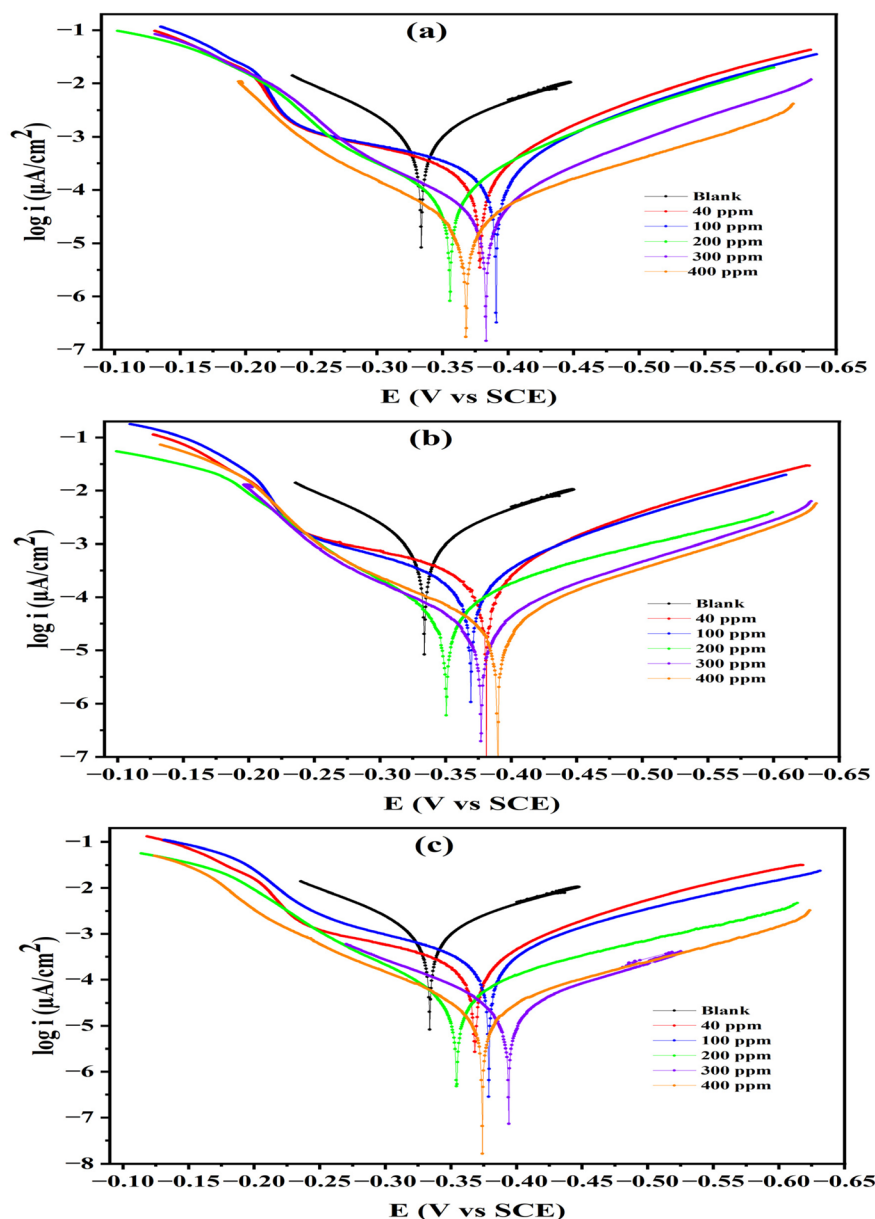


Fig. 6 Potentiodynamic polarization curves for the corrosion of carbon steel in 1.0 M HCl in absence and presence of different concentrations of (Chit- $\text{SrFe}_{12}\text{O}_{19}$  (a), Chit- $\text{CuFe}_2\text{O}_4$  (b) and Chit- $\text{ZnFe}_2\text{O}_4$  (c) composites at  $30\text{ }^\circ\text{C}$ .



**ZnFe<sub>2</sub>O<sub>4</sub>**, **Chit-CuFe<sub>2</sub>O<sub>4</sub>**, and **Chit-SrFe<sub>12</sub>O<sub>19</sub>** spectra, which were absent in pure chitosan. These bands are characteristic of metal–oxygen (Fe–O) stretching vibrations and confirm the presence of ferrite phases within the chitosan matrix. The variation in peak positions and intensities among the different composites reflects the influence of the specific metal ions (Sr<sup>2+</sup>, Cu<sup>2+</sup>, Zn<sup>2+</sup>) on the structural configuration and bonding environment. Overall, the FTIR results demonstrate successful integration of ferrite nanoparticles into the chitosan matrix and suggest chemical interactions between the polymer and the ferrite surfaces, which may influence the electrochemical behavior observed in subsequent EIS measurements.

### 3.2 Electrochemical measurements

**3.2.1 Potentiodynamic polarization (PDP).** The electrochemical behavior of carbon steel (CS) in 1.0 M HCl solution in the absence and presence of different concentrations (40, 100, 200, 300, and 400 ppm) of the synthesized **Chit-ZnFe<sub>2</sub>O<sub>4</sub>**, **Chit-CuFe<sub>2</sub>O<sub>4</sub>**, and **Chit-SrFe<sub>12</sub>O<sub>19</sub>** nanocomposites was investigated systematically by potentiodynamic polarization (PDP) measurements. The resulting polarization curves (Fig. 6a–c) and the extracted electrochemical parameters (Table 2) clarify the corrosion kinetics and inhibition efficiency of the composites being studied. Examination of the PDP curves indicates that addition of the chitosan–ferrite composites considerably changes the corrosion behavior of CS relative to the uninhibited acid solution. The corrosion current density ( $i_{\text{corr}}$ ) drops considerably with increasing inhibitor concentration for all three composites (Table 2). This implies a considerable reduction of the overall corrosion rate, validating the effectiveness of these materials as corrosion inhibitors.<sup>36–38</sup> At the same time, the inhibition efficiency ( $\eta_{\text{p}}\%$ ) derived from the  $i_{\text{corr}}$  values (by using the formula given in the Experimental section) improves with concentration to arrive at impressive figures of 98.13%,

98.55%, and 98.73% for **Chit-SrFe<sub>12</sub>O<sub>19</sub>**, **Chit-CuFe<sub>2</sub>O<sub>4</sub>**, and **Chit-ZnFe<sub>2</sub>O<sub>4</sub>**, respectively, at the highest concentration of 400 ppm. The corrosion potential ( $E_{\text{corr}}$ ) shows variation in response to the addition and concentration of inhibitors. That is, for **Chit-ZnFe<sub>2</sub>O<sub>4</sub>** and **Chit-CuFe<sub>2</sub>O<sub>4</sub>**,  $E_{\text{corr}}$  exhibits a slight shift towards more negative (cathodic) potentials as the concentration is increased, showing a notable influence on the cathodic reaction (e.g., hydrogen evolution).<sup>39,40</sup> However, the shift for **Chit-SrFe<sub>12</sub>O<sub>19</sub>** is relatively less. The Tafel slopes ( $\beta_{\text{a}}$  and  $\beta_{\text{c}}$ ) generally exhibit close value to that of the blank sample, with minor deviations based on the concentration and nature of the inhibitor. The results suggest that the inhibition mechanism probably has a mixed-type nature, having a primary influence on the cathodic process without significantly altering the inherent reaction mechanisms.<sup>41,42</sup> The higher efficiency of **Chit-ZnFe<sub>2</sub>O<sub>4</sub>**, followed by **Chit-CuFe<sub>2</sub>O<sub>4</sub>** and **Chit-SrFe<sub>12</sub>O<sub>19</sub>**, is in accordance with the expected trends based on the textural properties and intrinsic characteristics of the ferrite nanoparticles.<sup>43</sup> The significant surface area and mesoporosity of ZnFe<sub>2</sub>O<sub>4</sub> nanoparticles are expected to favor greater adsorption and better spreading of the inhibitor over the metal interface, thus forming a more efficient protective film.<sup>44</sup> Though CuFe<sub>2</sub>O<sub>4</sub> has a lower surface area, its spinel structure and redox properties are likely to be responsible for its high inhibition efficiency. In spite of having the lowest surface area and pore volume, SrFe<sub>12</sub>O<sub>19</sub> still manifests excellent inhibition, which can be related to its unique plate-like morphology and the chemical stability imparted by its hexagonal structure, possibly providing effective barrier coverage.<sup>45</sup>

The PDP data validate that the chitosan–ferrite nanocomposites synthesized are good corrosion inhibitors for carbon steel in 1.0 M HCl. The inhibition efficiency is concentration-dependent, and the activity order (**Chit-ZnFe<sub>2</sub>O<sub>4</sub>**  $\geq$  **Chit-CuFe<sub>2</sub>O<sub>4</sub>** > **Chit-SrFe<sub>12</sub>O<sub>19</sub>** at higher concentrations) aligns with the physicochemical characteristics of the ferrite

Table 2 Electrochemical parameters for carbon steel dissolution in 1.0 M HCl solution containing different concentrations of the (Chit-SrFe<sub>12</sub>O<sub>19</sub>, Chit-CuFe<sub>2</sub>O<sub>4</sub> and Chit-ZnFe<sub>2</sub>O<sub>4</sub>) composites obtained from polarization measurements at 30 °C<sup>a</sup>

Inhibitor name	Conc. (ppm)	$E_{\text{corr}}$ vs. SCE (mV)	$i_{\text{corr}}$ ( $\mu\text{A cm}^{-2}$ ) $\pm$ SD	$\beta_{\text{a}}$ (mV dec <sup>-1</sup> )	$-\beta_{\text{c}}$ (mV dec <sup>-1</sup> )	$k$ (mpy)	$\theta$	$\eta_{\text{p}}\%$
Blank	—	−333.7	1579.00 $\pm$ 11.04	104.1	136.4	721.5	—	—
<b>Chit-SrFe<sub>12</sub>O<sub>19</sub></b>	40	−378.6	349.30 $\pm$ 7.99	202.9	113.3	159.6	0.7788	77.88
	100	−390.9	245.30 $\pm$ 7.12	173.7	105.9	112.1	0.8446	84.46
	200	−355.7	94.46 $\pm$ 5.35	79.49	99.65	43.16	0.9402	94.02
	300	−383.1	38.03 $\pm$ 4.52	73.72	96.14	17.38	0.9759	97.59
	400	−367.9	29.59 $\pm$ 2.29	83.32	121.3	13.52	0.9813	98.13
<b>Chit-CuFe<sub>2</sub>O<sub>4</sub></b>	40	−381.0	339.70 $\pm$ 6.52	183	183	155.2	0.7849	78.49
	100	−369.2	225.00 $\pm$ 7.77	131.3	117.3	102.8	0.8575	85.75
	200	−350.6	75.80 $\pm$ 4.85	82.29	141.9	34.63	0.9520	95.20
	300	−377.0	35.36 $\pm$ 4.87	90.66	115	16.16	0.9776	97.76
	400	−389.7	22.82 $\pm$ 3.11	76.86	103.4	10.43	0.9855	98.55
<b>Chit-ZnFe<sub>2</sub>O<sub>4</sub></b>	40	−368.2	313.40 $\pm$ 6.45	168.7	115.1	143.2	0.8015	80.15
	100	−378.6	216.40 $\pm$ 6.29	103.2	116.1	98.87	0.8630	86.30
	200	−354.2	53.92 $\pm$ 4.34	75.38	134.3	24.64	0.9659	96.59
	300	−394.0	34.68 $\pm$ 2.15	102.5	129.3	15.85	0.9780	97.80
	400	−373.9	20.05 $\pm$ 2.03	78.01	119	9.161	0.9873	98.73

<sup>a</sup>  $E_{\text{corr}}$  is the corrosion potential;  $i_{\text{corr}}$  is the corrosion current density;  $\beta_{\text{a}}$  and  $\beta_{\text{c}}$  are Tafel constants for both anode and cathode;  $k$ , is the corrosion rate;  $\theta$ , is the surface coverage;  $\eta_{\text{p}}$ , is the inhibition efficiency.



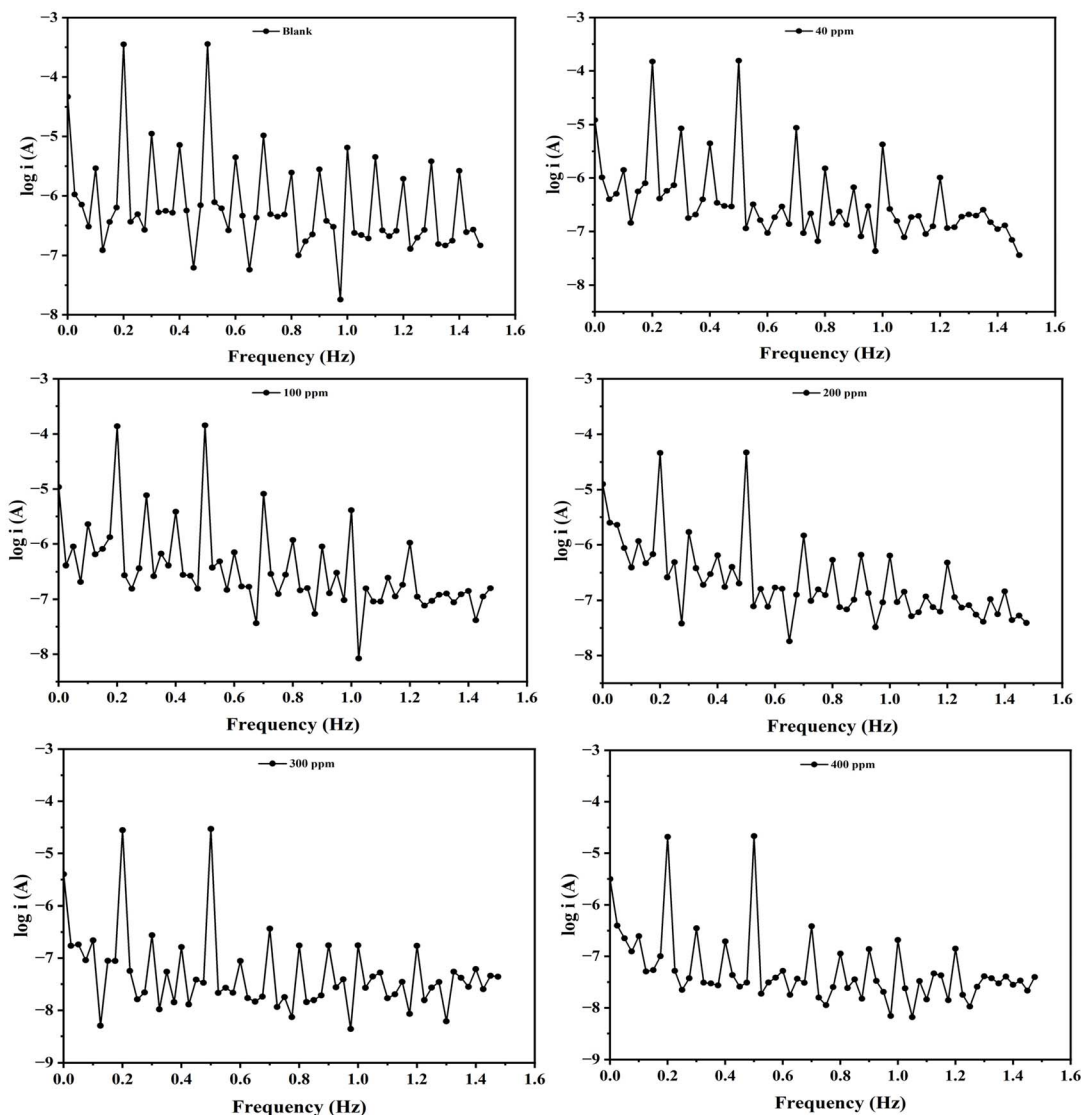


Fig. 7 Intermodulation spectra for carbon steel in 1.0 M HCl in absence and presence of different concentrations from Chit-ZnFe<sub>2</sub>O<sub>4</sub> composite at 30 °C.

nanoparticles incorporated. The inhibition process seems to be through the adsorption of a protective layer onto the steel surface, inhibiting anodic dissolution and, more pronouncedly, the cathodic evolution of hydrogen.

**3.2.2 Electrochemical frequency modulation (EFM).** In order to get more information about the inhibition mechanism of corrosion and confirm the PDP results, Electrochemical Frequency Modulation (EFM) measurements were made. EFM is a non-destructive DC method that superimposes two small-amplitude sine waves, producing intermodulation products with amplitudes and phases dependent on the corrosion current density ( $i_{\text{corr}}$ ) and Tafel parameters, without the need for previous knowledge of  $\beta_a$  and  $\beta_c$  to interpret data.<sup>46,47</sup> The intermodulation spectra recorded for carbon steel in 1.0 M HCl solution, in the absence and presence of different concentrations (40, 100, 200, 300, 400 ppm) of Chit-ZnFe<sub>2</sub>O<sub>4</sub>, Chit-CuFe<sub>2</sub>O<sub>4</sub>, and Chit-SrFe<sub>12</sub>O<sub>19</sub>, are shown in Fig. 7, S1, S2 and

tabulated in Table 3. The spectra generally exhibit current density responses at different frequencies, including the base frequencies ( $f_1, f_2$ ) and their combinations (e.g.,  $2f_1, 2f_2, f_1 + f_2, f_1 - f_2$ ).<sup>48,49</sup> The amplitude of these responses is directly related to the corrosion activity. EFM-derived causality factors (CF-2 and CF-3) compare measured intermodulation currents to theoretical, with ideal values of CF-2  $\approx$  2.0 and CF-3  $\approx$  3.0.<sup>50</sup> The blank solution values (CF-2 = 1.574, CF-3 = 3.465) were near ideal, confirming the validity of the EFM measurements.<sup>51</sup> With chitosan-ferrite composites addition, CF-2 and CF-3 varied around their theoretical values. These changes signify the composites affect interfacial electrochemical processes beyond simple physical blocking, suggesting kinetic modifications or complex layer formation. Examination of the EFM data shows that there are drastic changes in the corrosion behavior with the addition of inhibitors. The calculated  $i_{\text{corr}}$  values (Table 3) show a steady reduction with increasing concentration of the inhibitors for



**Table 3** Electrochemical kinetic parameters obtained by EFM technique for carbon steel in the absence and presence of various concentrations of (Chit-SrFe<sub>12</sub>O<sub>19</sub>, Chit-CuFe<sub>2</sub>O<sub>4</sub> and Chit-ZnFe<sub>2</sub>O<sub>4</sub>) composites in 1.0 M HCl at 30 °C<sup>a</sup>

Inhibitor name	Conc. (ppm)	$i_{\text{corr}}$ ( $\mu\text{A cm}^{-2}$ ) $\pm$ SD	$\beta_a$ (mV dec <sup>-1</sup> )	$\beta_c$ (mV dec <sup>-1</sup> )	CF-2	CF-3	$k$ (mpy)	$\theta$	$\eta_{\text{EFM}}\%$
Blank	—	739.3 $\pm$ 5.18	124.2	162.0	1.574	3.465	337.80	—	—
<b>Chit-SrFe<sub>12</sub>O<sub>19</sub></b>	40	437.3 $\pm$ 5.37	137.6	216.5	1.861	2.601	199.80	0.4085	40.85
	100	307.7 $\pm$ 6.29	84.9	100.0	2.008	3.114	140.60	0.5838	58.38
	200	193.5 $\pm$ 5.42	100.6	115.6	1.883	3.368	88.40	0.7383	73.83
	300	67.0 $\pm$ 3.04	111.1	120.6	1.873	2.950	30.62	0.9094	90.94
	400	59.2 $\pm$ 3.65	117.4	140.2	2.224	3.198	27.04	0.9199	91.99
<b>Chit-CuFe<sub>2</sub>O<sub>4</sub></b>	40	334.8 $\pm$ 6.44	115.9	247.2	2.022	2.492	153.00	0.5471	54.71
	100	302.3 $\pm$ 5.99	132.1	158.8	1.869	2.129	138.10	0.5911	59.11
	200	88.9 $\pm$ 4.07	110.0	138.6	1.840	2.059	40.60	0.8798	87.98
	300	64.4 $\pm$ 3.99	114.3	148.7	1.830	3.721	29.42	0.9129	91.29
	400	53.8 $\pm$ 2.22	138.6	147.8	1.489	3.640	24.60	0.9272	92.72
<b>Chit-ZnFe<sub>2</sub>O<sub>4</sub></b>	40	327.2 $\pm$ 5.35	115.9	194.6	1.975	3.616	149.50	0.5574	55.74
	100	261.4 $\pm$ 5.57	103.8	162.2	1.973	2.422	119.40	0.6464	64.64
	200	75.9 $\pm$ 3.76	100.4	127.6	2.483	3.520	34.67	0.8974	89.74
	300	61.5 $\pm$ 2.11	137.5	151.9	1.906	2.811	28.10	0.9168	91.68
	400	41.8 $\pm$ 2.64	124.9	144.3	1.824	2.366	19.10	0.9435	94.35

<sup>a</sup>  $E_{\text{CORR}}$  is the corrosion potential;  $i_{\text{CORR}}$  is the corrosion current density;  $\beta_a$  and  $\beta_c$  are Tafel constants for both anode and cathode;  $k$ , is the corrosion rate;  $\theta$ , is the surface coverage;  $\eta_{\text{EFM}}$ , is the inhibition efficiency.

the three nanocomposites, similar to those found in PDP measurements. This is a clear indication of the ability of the chitosan–ferrite composites to minimize the corrosion rate of carbon steel in the acidic medium.<sup>52</sup> At the same time, the inhibition efficiency ( $\eta_{\text{EFM}}\%$ ), calculated from the  $i_{\text{CORR}}$  values, rises with concentration. Interestingly, at the highest concentration examined (400 ppm), inhibition efficiencies of 91.99%, 92.72%, and 94.35% were achieved for **Chit-SrFe<sub>12</sub>O<sub>19</sub>**, **Chit-CuFe<sub>2</sub>O<sub>4</sub>**, and **Chit-ZnFe<sub>2</sub>O<sub>4</sub>**, respectively. EFM-derived Tafel constants ( $\beta_a$  and  $\beta_c$ ) (Table 3) are also informative. For chitosan–ferrite composites,  $\beta_c$  and  $\beta_a$  values exhibit slight changes relative to the blank. The variations of  $\beta_a$  and  $\beta_c$  indicate that the inhibitors affect the kinetics of both the anodic dissolution and, more pronouncedly, the cathodic reduction process.<sup>53,54</sup> The EFM data validates the efficacy of the synthesized chitosan–ferrite nanocomposites as corrosion inhibitors for carbon steel in 1.0 M HCl. The inhibition efficiency is concentration-dependent, in the order **Chit-ZnFe<sub>2</sub>O<sub>4</sub>** > **Chit-CuFe<sub>2</sub>O<sub>4</sub>** > **Chit-SrFe<sub>12</sub>O<sub>19</sub>** at high concentrations, which is in agreement with the trends in PDP and is consistent with the physicochemical characteristics of the included ferrite nanoparticles. The EFM measurements also indicate a mixed-type inhibition mechanism with prevailing influence on the cathodic process.

**3.2.3 Electrochemical impedance spectroscopy (EIS).** EIS is useful for understanding the interfacial processes and resistive and capacitive behavior of the electrode–electrolyte system.<sup>55,56</sup> The EIS data were fitted to a modified equivalent circuit, which comprises solution resistance ( $R_s$ ), film resistance ( $R_f$ ) and film capacitance ( $CPE_f$ ), charge transfer resistance ( $R_{ct}$ ), and double-layer capacitance ( $CPE_{dl}$ ) (inset of Fig. 8). Low  $\chi^2$  values ( $<10^{-3}$ ) indicate good agreement between the experimental data and the fitted equivalent circuit model.<sup>57</sup> The utilization of Constant Phase Elements (CPE) rather than pure capacitors explains the non-ideal behavior and surface heterogeneity widely encountered in corrosion systems.<sup>58,59</sup> The representative Nyquist and

Bode plots for carbon steel in 1.0 M HCl with chitosan–ferrite nanocomposites are displayed in Fig. 8. Examination of Nyquist plots (Fig. 8a–c) shows drastic modification of impedance response with the addition of chitosan–ferrite nanocomposites. The blank solution shows one capacitive loop with a comparatively small diameter, which signifies low polarization resistance and high corrosion activity.<sup>60</sup> However, with the addition of chitosan–ferrite nanocomposites, the diameter of the capacitive loop increases considerably and increases with increasing concentration of the inhibitor. This directly signifies an increase in overall impedance of the system and represents the inhibitive effect of the composite.<sup>61</sup> The loop shape further indicates the presence of more than one time constant, which corroborates the proposed equivalent circuit with both a film and a charge transfer resistance. The Bode plots (magnitude and phase angle, Fig. 8d–f) also complement these observations. The impedance magnitude ( $|Z|$ ) at low frequencies rises significantly with chitosan–ferrite nanocomposites concentration, reinforcing the increased barrier properties.<sup>62</sup> The phase angle plots exhibit a shift to more negative angles in the intermediate frequency range with increasing inhibitor concentration, pointing towards increasingly capacitive interfacial behavior and the formation of the protective film.<sup>63,64</sup> The EIS parameters derived from fitting experimental data using the equivalent circuit are listed in Table 4. The solution resistance ( $R_s$ ) is relatively constant for all measurements, as can be expected for a fixed concentration of the electrolyte. One of the main observations is the large increase in charge transfer resistance ( $R_{ct}$ ) with increasing inhibitor concentration for all three composites. For example, for **Chit-ZnFe<sub>2</sub>O<sub>4</sub>**,  $R_{ct}$  rises from 19.05  $\Omega \text{ cm}^2$  for the blank to 646.42  $\Omega \text{ cm}^2$  at 400 ppm. This large increase in  $R_{ct}$  indicates a decrease in the rate of the charge transfer process (corrosion reaction), demonstrating the efficiency of the chitosan–ferrite nanocomposites.<sup>65</sup> At the same time, the double-layer capacitance ( $C_{dl}$ , calculated from  $CPE_{dl}$ )



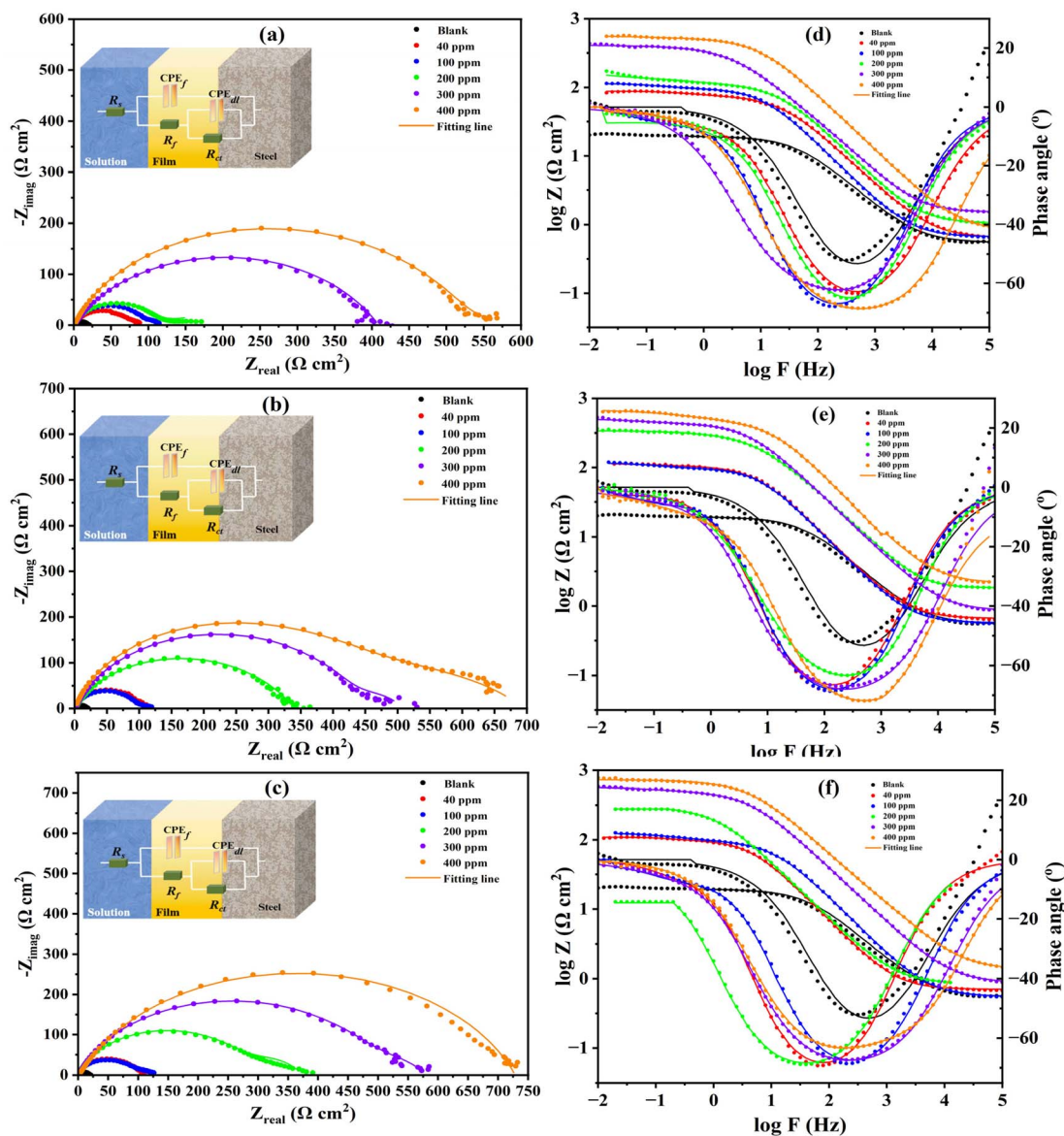


Fig. 8 Nyquist plots, Bode and phase angle plots for steel in 1.0 M HCl solution without and with different concentrations of (Chit-SrFe<sub>12</sub>O<sub>19</sub> (a and d), Chit-CuFe<sub>2</sub>O<sub>4</sub> (b and e) and Chit-ZnFe<sub>2</sub>O<sub>4</sub> (c and f) composites at 30 °C.

decreases noticeably with increasing inhibitor concentration (e.g., from 406.90  $\mu\text{F cm}^{-2}$  for the blank to 28.39  $\mu\text{F cm}^{-2}$  for **Chit-ZnFe<sub>2</sub>O<sub>4</sub>** at 400 ppm). The decrease in  $C_{dl}$  is usually explained by the adsorption of inhibitor molecules on the metal surface, decreasing the effective area for charge transfer and/or thickening the electrical double layer by forming an adsorbed layer.<sup>66–69</sup> The inhibition efficiency as determined using the EIS data  $\eta_z\%$  (based on  $[R_p = R_{ct} + R_f]$  values using the formula given in the Experimental section) follows the expected trend and increases with the concentration of the chitosan–ferrite nanocomposites. At the highest concentration examined (400 ppm), inhibition efficiencies of 97.16%, 97.29%, and 97.38% for **Chit-SrFe<sub>12</sub>O<sub>19</sub>**, **Chit-CuFe<sub>2</sub>O<sub>4</sub>**, and **Chit-ZnFe<sub>2</sub>O<sub>4</sub>**, respectively, were achieved. Such high efficiencies are a strong indication of the formation of efficient protective layers. Also, the surface

coverage values ( $\theta$ ) tend towards unity (0.9738 for **Chit-ZnFe<sub>2</sub>O<sub>4</sub>** at 400 ppm), reflecting almost complete surface coverage by the inhibitor film at the highest concentration. The EIS data also enables the examination of the properties of the film formed itself. The resistance of the film ( $R_f$ ) is seen to increase appreciably with chitosan–ferrite nanocomposites concentration (e.g., from 13.90  $\Omega \text{ cm}^2$  for **Chit-ZnFe<sub>2</sub>O<sub>4</sub>** at 40 ppm to 79.91  $\Omega \text{ cm}^2$  for **Chit-ZnFe<sub>2</sub>O<sub>4</sub>** at 400 ppm), reflecting the formation of a resistive barrier layer. The values of film capacitance ( $C_f$ ) are typically lower than  $C_{dl}$ , in line with the formation of a thicker, more dielectric layer than the electric double layer.<sup>70</sup> The EIS findings validate that the prepared chitosan–ferrite nanocomposites are good inhibitors for the corrosion of carbon steel in 1.0 M HCl through the formation of protective films. The inhibition efficiency is concentration-dependent for all



Table 4 EIS parameters for corrosion of steel in 1.0 M HCl in the absence and presence of different concentrations of (Chit-SrFe<sub>12</sub>O<sub>19</sub>, Chit-CuFe<sub>2</sub>O<sub>4</sub> and Chit-ZnFe<sub>2</sub>O<sub>4</sub>) composites at 30 °C<sup>a</sup>

Inhibitor	Conc. (ppm)	CPE <sub>r</sub>					CPE <sub>dl</sub>					R <sub>p</sub> (R <sub>f</sub> + R <sub>ct</sub> )	θ	η <sub>i</sub> %	
		R <sub>s</sub> (Ω cm <sup>2</sup> )	R <sub>f</sub> (Ω cm <sup>2</sup> )	Y <sub>0i</sub> (μΩ <sup>-1</sup> s <sup>n</sup> cm <sup>-2</sup> )	n <sub>1</sub>	C <sub>f</sub> (μF cm <sup>-2</sup> )	R <sub>ct</sub> (Ω cm <sup>2</sup> )	Y <sub>0d</sub> (μΩ <sup>-1</sup> s <sup>n</sup> cm <sup>-2</sup> )	n <sub>2</sub>	C <sub>dl</sub> (μF cm <sup>-2</sup> )	Chi squared (χ <sup>2</sup> )				
Blank	—	0.5409	—	—	—	—	19.05	736.27	0.8780	406.90	9.04 × 10 <sup>-3</sup>	19.05	—	—	—
Chit-SrFe <sub>12</sub> O <sub>19</sub>	40	0.6385	9.17	694.30	0.8789	346.00	79.56	689.00	0.8049	340.83	3.78 × 10 <sup>-4</sup>	88.73	0.7853	78.53	—
	100	0.6649	16.55	520.40	0.8429	214.53	97.31	384.60	0.8717	237.14	6.29 × 10 <sup>-4</sup>	113.86	0.8327	83.27	—
	200	1.0340	42.03	213.70	0.8338	83.53	113.55	221.60	0.8627	123.32	9.21 × 10 <sup>-4</sup>	155.58	0.8775	87.75	—
	300	1.5000	56.40	116.90	0.8328	42.65	350.40	174.70	0.8627	111.98	3.39 × 10 <sup>-4</sup>	406.80	0.9532	95.32	—
Chit-CuFe <sub>2</sub> O <sub>4</sub>	400	0.8146	63.90	63.75	0.8131	17.99	607.93	126.00	0.8712	86.17	1.76 × 10 <sup>-4</sup>	671.83	0.9716	97.16	—
	40	0.6408	12.62	607.50	0.8999	353.38	95.83	475.50	0.8819	314.43	8.62 × 10 <sup>-4</sup>	108.45	0.8243	82.43	—
	100	0.5712	17.20	516.30	0.8466	219.36	97.37	384.30	0.9227	291.83	7.14 × 10 <sup>-4</sup>	114.57	0.8337	83.37	—
	200	1.8370	44.08	144.10	0.9155	90.34	294.12	206.30	0.8624	131.90	2.67 × 10 <sup>-4</sup>	338.20	0.9437	94.37	—
Chit-ZnFe <sub>2</sub> O <sub>4</sub>	300	0.9596	59.55	87.82	0.9999	87.77	412.10	164.00	0.8716	110.28	4.14 × 10 <sup>-3</sup>	471.65	0.9596	95.96	—
	400	0.8649	69.84	47.81	0.8518	17.73	633.66	108.60	0.8532	68.52	1.50 × 10 <sup>-4</sup>	703.50	0.9729	97.29	—
	40	0.7041	13.90	571.50	0.8599	259.94	95.27	401.80	0.8999	279.50	9.57 × 10 <sup>-4</sup>	109.17	0.8255	82.55	—
	100	0.5518	28.28	276.00	0.8408	110.12	96.30	291.50	0.8747	174.72	6.50 × 10 <sup>-4</sup>	124.58	0.8471	84.71	—
200	0.8497	45.56	119.40	0.8254	39.63	321.55	199.10	0.8750	134.44	3.98 × 10 <sup>-4</sup>	367.11	0.9481	94.81	—	
300	0.8728	62.18	64.99	0.7994	16.30	510.86	142.40	0.8713	96.70	7.07 × 10 <sup>-4</sup>	573.04	0.9668	96.68	—	
400	1.3630	79.91	17.17	0.8087	3.61	646.42	47.50	0.8713	28.39	2.98 × 10 <sup>-4</sup>	726.33	0.9738	97.38	—	

<sup>a</sup> R<sub>s</sub> = solution resistance, R<sub>ct</sub> = charge transfer resistant, Y<sub>0i</sub>, n = constant phase elements, C<sub>dl</sub> = double layer capacitance, θ = surface coverage, η<sub>i</sub> = inhibition efficiency.

composites, with **Chit-ZnFe<sub>2</sub>O<sub>4</sub>** having the highest efficiency, followed by **Chit-CuFe<sub>2</sub>O<sub>4</sub>** and **Chit-SrFe<sub>12</sub>O<sub>19</sub>**. The EIS measurements establish that the inhibition process is through the formation of a resistive film (rise in R<sub>f</sub>) that suppresses both electrolyte access and charge transfer (rise in R<sub>ct</sub>), resulting in a notable decrease in corrosion. The surface area and morphology are the key physicochemical attributes of the individual ferrite nanoparticles that determine the overall composite inhibition performance.

**3.2.4 Adsorption considerations.** The degree of surface coverage (θ) gained from the electrochemical measurements (PDP, EFM, EIS) isotherm data fitted in several theoretical adsorption models, such as Langmuir, Freundlich, Temkin, Frumkin, Flory-Huggins, and El-Awady. The parameters and correlation coefficients (R<sup>2</sup>) for the different adsorption models are summarized in Table 5. The analysis of the various isotherm models indicates that the Langmuir model fits the adsorption data best, with the largest correlation coefficients (R<sup>2</sup> values close of 1 were determined) for all three composites.<sup>71</sup> The linearized Langmuir plot (Fig. 9) of **Chit-ZnFe<sub>2</sub>O<sub>4</sub>**, **Chit-CuFe<sub>2</sub>O<sub>4</sub>** and **Chit-SrFe<sub>12</sub>O<sub>19</sub>**, shows excellent linearity of R<sup>2</sup> values of 0.9996, 0.9997, and 0.9995, respectively. The Langmuir model assumes monolayer adsorption of modest no interaction between the adsorbed species on a homogeneous surface with a finite number of identical sites. By using the linear plot of C/θ versus C, intercept provide the reciprocal of K<sub>ads</sub>.<sup>72</sup> The K<sub>ads</sub> values calculated from the Langmuir model were 0.0782 M<sup>-1</sup>, 0.0727 M<sup>-1</sup> and 0.0537 M<sup>-1</sup>, for **Chit-ZnFe<sub>2</sub>O<sub>4</sub>**, **Chit-CuFe<sub>2</sub>O<sub>4</sub>**, and **Chit-SrFe<sub>12</sub>O<sub>19</sub>**, respectively. The corresponding standard free energy of adsorption (ΔG<sub>ads</sub><sup>o</sup>) was calculated using the expression: ΔG<sub>ads</sub><sup>o</sup> = -RT ln(10<sup>6</sup> × K<sub>ads</sub>), wherein R is the gas constant, T is the absolute temperature in degrees Kelvin (303 K), and 10<sup>6</sup> ppm is the water concentration.<sup>73</sup> The resulting ΔG<sub>ads</sub><sup>o</sup> values of -28.38 kJ mol<sup>-1</sup>, -28.20 kJ mol<sup>-1</sup>, and -27.44 kJ mol<sup>-1</sup> were for **Chit-ZnFe<sub>2</sub>O<sub>4</sub>**, **Chit-CuFe<sub>2</sub>O<sub>4</sub>**, and **Chit-SrFe<sub>12</sub>O<sub>19</sub>**, respectively. The negative values indicate that the adsorption process is spontaneous.<sup>74</sup> The magnitude of ΔG<sub>ads</sub><sup>o</sup> values from -20 to -40 kJ mol<sup>-1</sup> indicates the adsorptive process involved physical adsorption (physisorption, that is, by electrostatic interaction) and chemical adsorption (chemisorption, which can be thought of as charge sharing or transfer) involving the chitosan-ferrite nanocomposites and the metal surface.<sup>75</sup> The higher fit of the Langmuir model for all three composites provides solid evidence that the chitosan-ferrite composites form a monolayer on the carbon steel surface. The order of calculated K<sub>ads</sub> and the magnitudes of ΔG<sub>ads</sub><sup>o</sup> (**Chit-ZnFe<sub>2</sub>O<sub>4</sub>** > **Chit-CuFe<sub>2</sub>O<sub>4</sub>** > **Chit-SrFe<sub>12</sub>O<sub>19</sub>**) correlated well with the achieved inhibition efficiencies and the physico-chemical properties of the ferrite nanoparticles.

### 3.3 Global reactivity parameters

The standard set of global reactivity descriptors provides a practical framework for assessing the fundamental characteristics of chemical compounds under study.<sup>76</sup> These parameters are valuable for comparing structures and drawing essential insights into their chemical reactivity and



Table 5 Adsorption isotherms models of the inhibitors with values of  $R^2$ , slopes, intercepts,  $K_{\text{ads}}$ , and  $\Delta G_{\text{ads}}$  obtained by using data from electrochemical measurements<sup>a</sup>

Adsorption isotherm model	Linear form equation	Technique	Inhibitor	Slope	Intercept	$R^2$	$K_{\text{ads}} \text{ M}^{-1}$	$\Delta G_{\text{ads}} \text{ kJ mol}^{-1}$
Freundlich	$\log \theta = \log K + 1/n \log C$	PDP	Chit-SrFe <sub>12</sub> O <sub>19</sub>	0.10810	-0.28294	0.97877	0.5213	-33.16
			Chit-CuFe <sub>2</sub> O <sub>4</sub>	0.10535	-0.27330	0.97736	0.5330	-33.22
			Chit-ZnFe <sub>2</sub> O <sub>4</sub>	0.09774	-0.25275	0.95955	0.5588	-33.34
Langmuir	$\frac{c}{\theta} = \frac{1}{K} + c$	EFM	Chit-SrFe <sub>12</sub> O <sub>19</sub>	0.89962	73.84235	0.99019	0.0135	-23.97
			Chit-CuFe <sub>2</sub> O <sub>4</sub>	0.94619	49.12175	0.98715	0.0204	-24.99
			Chit-ZnFe <sub>2</sub> O <sub>4</sub>	0.94931	42.64592	0.99396	0.0234	-25.35
		EIS	Chit-SrFe <sub>12</sub> O <sub>19</sub>	0.99261	18.61154	0.99769	0.0537	-27.44
			Chit-CuFe <sub>2</sub> O <sub>4</sub>	0.99553	13.76444	0.99916	0.0727	-28.20
			Chit-ZnFe <sub>2</sub> O <sub>4</sub>	0.99480	12.78497	0.99938	0.0782	-28.38
		PDP	Chit-SrFe <sub>12</sub> O <sub>19</sub>	0.97828	16.02054	0.99950	0.0624	-27.82
			Chit-CuFe <sub>2</sub> O <sub>4</sub>	0.97708	14.85207	0.99967	0.0673	-28.01
			Chit-ZnFe <sub>2</sub> O <sub>4</sub>	0.97858	13.40201	0.99960	0.0746	-28.27
Frumkin	$\log \frac{\theta}{(1-\theta)C} = \log K + 2a\theta$	PDP	Chit-SrFe <sub>12</sub> O <sub>19</sub>	1.18111	-2.10323	0.40612	$7.8844 \times 10^{-3}$	-22.60
			Chit-CuFe <sub>2</sub> O <sub>4</sub>	1.46607	-2.31054	0.51726	$4.8917 \times 10^{-3}$	-21.40
			Chit-ZnFe <sub>2</sub> O <sub>4</sub>	1.74358	-2.51981	0.58694	$3.0213 \times 10^{-3}$	-20.19
Temkin	$\theta = -\frac{1}{2a} \ln C - \frac{1}{2a} \ln K$	PDP	Chit-SrFe <sub>12</sub> O <sub>19</sub>	10.28473	-4.24152	0.97753	0.6621	-33.76
			Chit-CuFe <sub>2</sub> O <sub>4</sub>	10.49258	-4.50646	0.97792	0.6508	-33.72
			Chit-ZnFe <sub>2</sub> O <sub>4</sub>	10.97046	-5.02587	0.95867	0.6325	-33.65
Flory-Huggins	$\log \left( \frac{\theta}{c} \right) = \log K + n \log(1-\theta)$	PDP	Chit-SrFe <sub>12</sub> O <sub>19</sub>	0.72422	-1.36808	0.92221	$4.2847 \times 10^{-2}$	-26.87
			Chit-CuFe <sub>2</sub> O <sub>4</sub>	0.69302	-1.36228	0.94004	$4.3423 \times 10^{-2}$	-26.90
			Chit-ZnFe <sub>2</sub> O <sub>4</sub>	0.68194	-1.33621	0.93478	$4.6110 \times 10^{-2}$	-27.05
El-Awady	$\log \left( \frac{\theta}{1-\theta} \right) = \log K + y \log c$	PDP	Chit-SrFe <sub>12</sub> O <sub>19</sub>	1.24518	-1.57383	0.93477	0.054457	-27.47
			Chit-CuFe <sub>2</sub> O <sub>4</sub>	1.31841	-1.67360	0.94854	0.053777	-27.44
			Chit-ZnFe <sub>2</sub> O <sub>4</sub>	1.33708	-1.65761	0.94447	0.057581	-27.61

<sup>a</sup>  $R^2$  = regression correlation coefficient,  $K$  = binding constant,  $\theta$  = surface coverage,  $c$  = concentration.

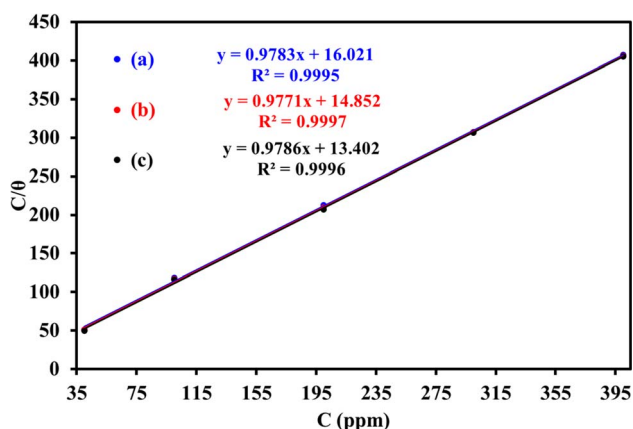


Fig. 9 The Langmuir adsorption model for (Chit-SrFe<sub>12</sub>O<sub>19</sub>) (a), Chit-CuFe<sub>2</sub>O<sub>4</sub> (b) and Chit-ZnFe<sub>2</sub>O<sub>4</sub> (c) composites on the steel surface in 1.0 M HCl using data obtained from PDP measurements at 30 °C.

thermodynamic stability. The descriptors are derived from the electronic structure of the molecule, specifically the energies of the highest occupied (HOMO) and lowest unoccupied (LUMO) molecular orbitals.<sup>77</sup> The ionization potential is defined as the minimum energy needed to remove the highest-energy electron from an isolated molecule. The electron affinity describes the accommodation of an excess electron corresponding to the LUMO energy. Molecular electronegativity is calculated as follows:

$$\chi = -\frac{1}{2}(E_{\text{HOMO}} + E_{\text{LUMO}}). \quad (3)$$

The electronic chemical potential equals:

$$\mu = \frac{1}{2}(E_{\text{HOMO}} + E_{\text{LUMO}}). \quad (4)$$

The chemical hardness and chemical softness originate from the ionization potential,  $I$ , and electron affinity,  $A$ :

$$\eta = \frac{1}{2}(I - A); \quad S = \frac{1}{2}(A - I). \quad (5)$$

The system's electrophilicity index equals:

$$\omega = \frac{1}{2}\mu^2\sigma. \quad (6)$$

In this work, the DFT calculations were used to characterize the intrinsic electronic structure of representative chitosan/ferrite fragments in aqueous environment, rather than to reproduce individual electrochemical observables. Global reactivity descriptors, band gap, chemical hardness/softness, and electronegativity together with population analysis quantify the tendency of the respective units to donate and accept charge and identify the most nucleophilic and electrophilic regions that are expected to interact with the steel surface and aggressive ionic species. These quantities are defined for isolated molecular units. The inhibitor formulations studied were



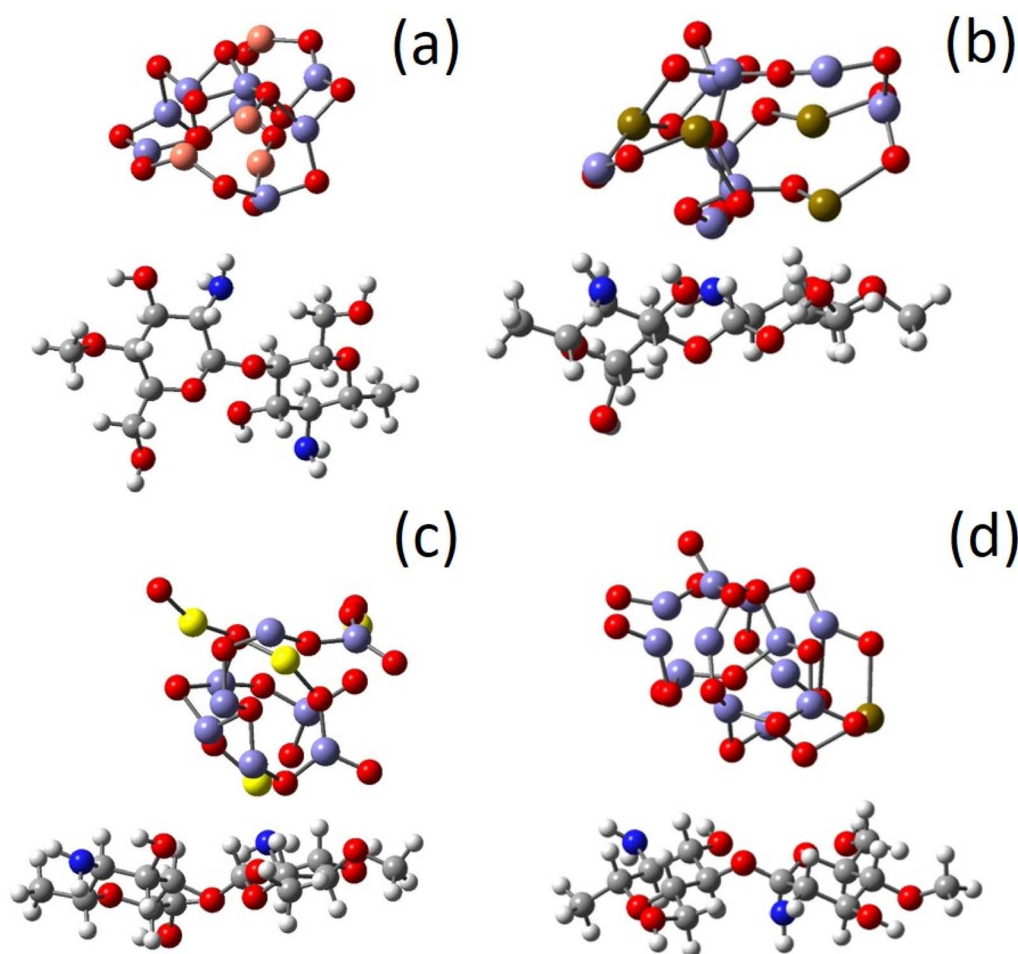
**Table 6** Global reactivity parameters – ionization potential, electron affinity, electronegativity, and electronic chemical potential – for the NP + chitosan systems

Nanoparticle	Ionization potential, eV	Electron affinity, eV	Electronegativity, eV	Electronic chemical potential, eV
CuFe <sub>2</sub> O <sub>4</sub>	9.003	4.397	2.303	−2.303
ZnFe <sub>2</sub> O <sub>4</sub>	7.734	3.541	2.096	−2.096
SrFe <sub>2</sub> O <sub>4</sub>	7.553	3.116	2.218	−2.218
SrFe <sub>12</sub> O <sub>19</sub>	9.111	4.386	2.363	−2.363

unrevealed to be chemically similar, so the numerical variation in the computed band gaps and hardness values is relatively small compared with the experimental scatter of the electrochemical data. To recapitulate, no formal regression between global reactivity descriptors and impedance or polarization parameters was attempted. Instead, the DFT results are interpreted qualitatively and comparatively.

Table 6 presents a set of parameters determined for the computed systems composed of the NPs and chitosan monomer (Fig. 10). SrFe<sub>12</sub>O<sub>19</sub> (9.111 eV) and CuFe<sub>2</sub>O<sub>4</sub> (9.003 eV) have the highest IP values, meaning it is harder to remove an electron

from these systems compared to ZnFe<sub>2</sub>O<sub>4</sub> (7.734 eV) and SrFe<sub>2</sub>O<sub>4</sub> (7.553 eV). This indicates slightly stronger electron binding in SrFe<sub>12</sub>O<sub>19</sub> and CuFe<sub>2</sub>O<sub>4</sub>.<sup>78</sup> It is consistent with the observed electronic stabilization. CuFe<sub>2</sub>O<sub>4</sub> (4.397 eV) and SrFe<sub>12</sub>O<sub>19</sub> (4.386 eV) have the highest EA values, reflecting their ready acceptance of the electron. ZnFe<sub>2</sub>O<sub>4</sub> and SrFe<sub>2</sub>O<sub>4</sub> show lower affinities, suggesting less tendency toward reduction. SrFe<sub>12</sub>O<sub>19</sub> (2.363 eV) and CuFe<sub>2</sub>O<sub>4</sub> (2.303 eV) are more electronegative than ZnFe<sub>2</sub>O<sub>4</sub> (2.096 eV). This observation indicates a stronger electron-attracting capability of the structure. Electronic chemical potential ( $\mu$ ) is, expectedly, negative in all cases.



**Fig. 10** The optimized structures of CuFe<sub>2</sub>O<sub>4</sub> nanoparticle + chitosan (a), SrFe<sub>2</sub>O<sub>4</sub> nanoparticle + chitosan (b), ZnFe<sub>2</sub>O<sub>4</sub> nanoparticle + chitosan (c), SrFe<sub>12</sub>O<sub>19</sub> nanoparticle + chitosan (d). The copper atoms are rosy, the strontium atoms are brown, the iron atoms are violet, the zinc atoms are yellow, the oxygen atoms are red, the carbon atoms are grey, and the hydrogen atoms are white.



**Table 7** Global reactivity parameters – global chemical softness, global chemical hardness, electrophilicity index, and band gap – computed for the investigated systems

NP	Global chemical softness, $\text{eV}^{-1}$	Global chemical hardness, eV	Electrophilicity index, eV	Band gap, eV
$\text{CuFe}_2\text{O}_4$	0.217	2.303	1.152	4.606
$\text{ZnFe}_2\text{O}_4$	0.239	2.096	1.048	4.193
$\text{SrFe}_2\text{O}_4$	0.225	2.218	1.109	4.437
$\text{SrFe}_{12}\text{O}_{19}$	0.212	2.363	1.181	4.725

Herewith,  $\text{SrFe}_{12}\text{O}_{19}$  has the most negative  $\mu$ , and therefore must gain extra electron density to decrease the potential energy.

Table 7 summarizes additional global reactivity descriptors. Hardness reflects resistance to charge transfer.  $\text{SrFe}_{12}\text{O}_{19}$  (2.363 eV) and  $\text{CuFe}_2\text{O}_4$  (2.303 eV) are the hardest species, while  $\text{ZnFe}_2\text{O}_4$  (2.096 eV) is the softest. This suggests  $\text{ZnFe}_2\text{O}_4$  is more chemically reactive due to easier charge redistribution.<sup>79</sup> Global chemical softness is inversely related to hardness. Thus,  $\text{ZnFe}_2\text{O}_4$  ( $0.239 \text{ eV}^{-1}$ ) is the softest (most polarizable and reactive). On the contrary,  $\text{SrFe}_{12}\text{O}_{19}$  is the hardest ( $0.212 \text{ eV}^{-1}$ ) out of the investigated set. Note that the observed differences are fairly modest.

Electrophilicity index reflects the system's ability to accept electrons. Values are all in the range 1.05–1.18 eV.  $\text{CuFe}_2\text{O}_4$  and  $\text{SrFe}_{12}\text{O}_{19}$  appeared to be slightly more electrophilic. This observation aligns with their high electron affinities discussed above.  $\text{SrFe}_{12}\text{O}_{19}$  exhibits the widest band gap (4.725 eV), making it relatively insulating and least conductive. Whereas  $\text{ZnFe}_2\text{O}_4$  has the narrowest band gap (4.193 eV), making it relatively electronically active in terms of possible semiconductor behavior. Yes, the analysis of the global reactivity parameters confirms that all four systems exhibit similar performance in the context of their chemical activities against a corrosion promoter.

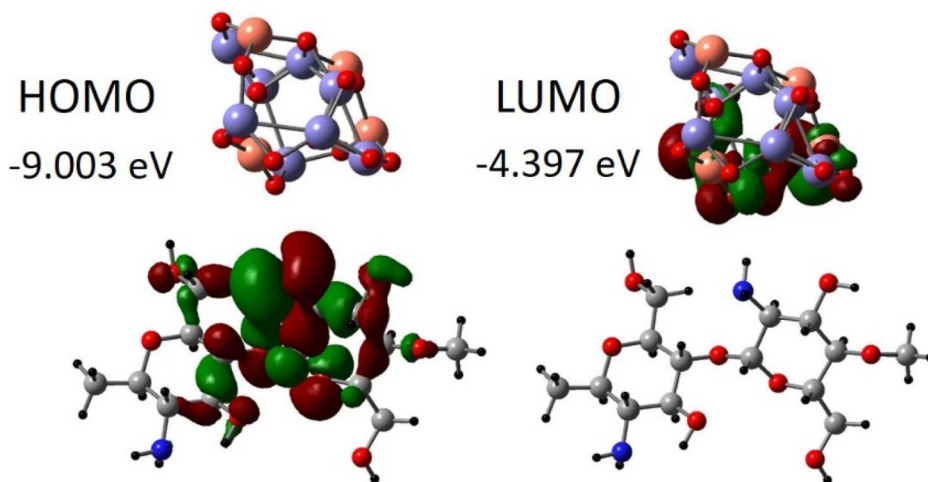
The spatial distribution of the frontier molecular orbitals was analyzed (Fig. 10–12). The analysis revealed distinct

localization patterns depending on the nanoparticle's composition. In the  $\text{CuFe}_2\text{O}_4$  + chitosan system (Fig. 11), the HOMO ( $E_{\text{HOMO}} = -9.003 \text{ eV}$ ) is localized on the organic chitosan fragment, while the LUMO ( $E_{\text{LUMO}} = -4.397 \text{ eV}$ ) is centered on the inorganic nanoparticle. This indicates that chitosan acts as an electron donor, and the copper nanoparticle acts as an acceptor.<sup>80,81</sup>

In contrast, the picture changes for the zinc and strontium systems. In both  $\text{ZnFe}_2\text{O}_4$  + chitosan (Fig. 12) and  $\text{SrFe}_2\text{O}_4$  + chitosan (Fig. 13), both orbitals—the HOMO ( $E_{\text{HOMO}} = -7.734 \text{ eV}$  and  $-7.553 \text{ eV}$ , respectively) and the LUMO ( $E_{\text{LUMO}} = -3.541 \text{ eV}$  and  $-3.116 \text{ eV}$ , respectively)—are localized predominantly on the inorganic nanoparticle core. In the strontium system, a minor contribution to the HOMO is observed on the nitrogen atom of chitosan. This distribution demonstrates that in these systems, the nanoparticle itself serves as both the donor and acceptor center, governing its interaction mechanism with the metal surface. The observed differences in orbital localization are consistent with the calculated global reactivity parameters and confirm the distinct nature of the inhibitory action of the investigated composites.

### 3.4 Electrostatic potential charges

Computed electrostatic potential (ESP) charges and Hirshfeld charges for the investigated NPs are collected in Tables 8 and 9 correspondingly. In the system  $\text{SrFe}_2\text{O}_4$  + chitosan, the ESP



**Fig. 11** The HOMO and LUMO distribution in  $\text{CuFe}_2\text{O}_4$  nanoparticle + chitosan. The copper atoms are rosy, the iron atoms are violet, the oxygen atoms are red, the carbon atoms are grey, the nitrogen atoms are blue and the hydrogen atoms are black.



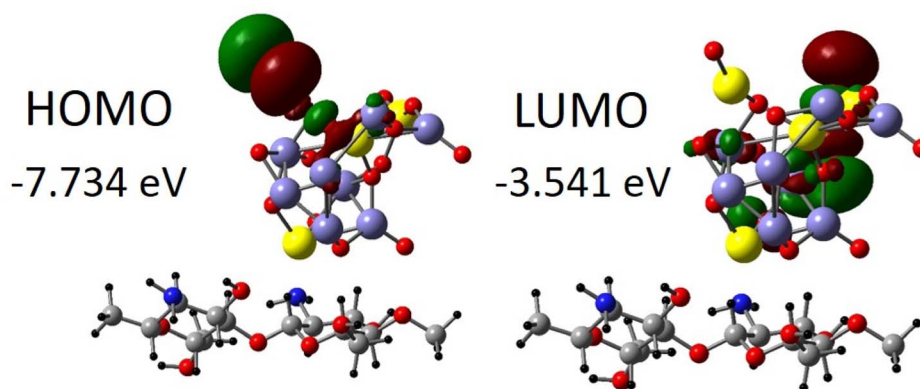


Fig. 12 The HOMO and LUMO distribution in  $\text{ZnFe}_2\text{O}_4$  nanoparticle + chitosan. The zinc atoms are yellow, the iron atoms are violet, the oxygen atoms are red, the carbon atoms are grey, the nitrogen atoms are blue and the hydrogen atoms are black.

charges on Sr are  $+1.526e$ ,  $+1.615e$ ,  $+1.619e$ , and  $+1.254e$  on the atom closest to the OH group of chitosan. The nearest oxygen in this OH group carries a charge of  $-0.675e$ . Compared to  $-1.143e$  on the oxygen of the other OH group. The distance between the closest Sr and O atoms is 262 pm. On the Fe nanoparticle, the charges are  $+0.699e$ ,  $+0.778e$ ,  $+0.921e$ ,  $+0.955e$ ,  $+1.073e$ ,  $+1.638e$ , and  $+0.484e$ . The Fe atom closest to the nitrogen of chitosan is nearly neutral,  $+0.093e$ . The corresponding N atom carries a charge of  $+0.296e$ . The distance between the nearest Fe and N atoms is 207 pm. The charges on the oxygen atoms of the NP range from  $-0.613e$  to  $-1.527e$ .

The ESP charges on the Zn atoms in the system with  $\text{ZnFe}_2\text{O}_4$  nanoparticle are  $+1.267e$ ,  $+1.330e$ , and  $+1.462e$ . The closest Zn atom to the nitrogen of chitosan carries a charge of  $+1.372e$ . For

the Fe atoms in the nanoparticle, the charges are  $+1.134e$ ,  $+1.135e$ ,  $+1.293e$ ,  $+1.341e$ ,  $+1.378e$ ,  $+1.470e$ , and  $+1.652e$ , with the Fe nearest to the hydrogen of chitosan's -OH group, having a charge of  $+1.181e$ . The hydrogen in this -OH group carries a charge of  $-0.517e$ , whereas the hydrogen in the remote -OH group, farther from the nanoparticle, has a charge of  $+0.580e$ . The Fe...H distance between the closest atoms is 249 pm. The oxygen atom with a charge of  $-1.164e$  competes with Fe for the interaction with the same H, as evidenced by a shorter O-H distance of 197 pm. The charges on the oxygen atoms within the nanoparticle range from  $-0.597e$  to  $-1.629e$ .

The ESP charges on the Cu atoms in the  $\text{CuFe}_2\text{O}_4$  nanoparticle are  $+0.786e$ ,  $+1.078e$ ,  $+1.152e$ , and  $+1.370e$ . The charges on the Fe atoms are  $+1.064e$ ,  $+1.142e$ ,  $+1.178e$ ,  $+1.241e$ ,  $+1.242e$ ,

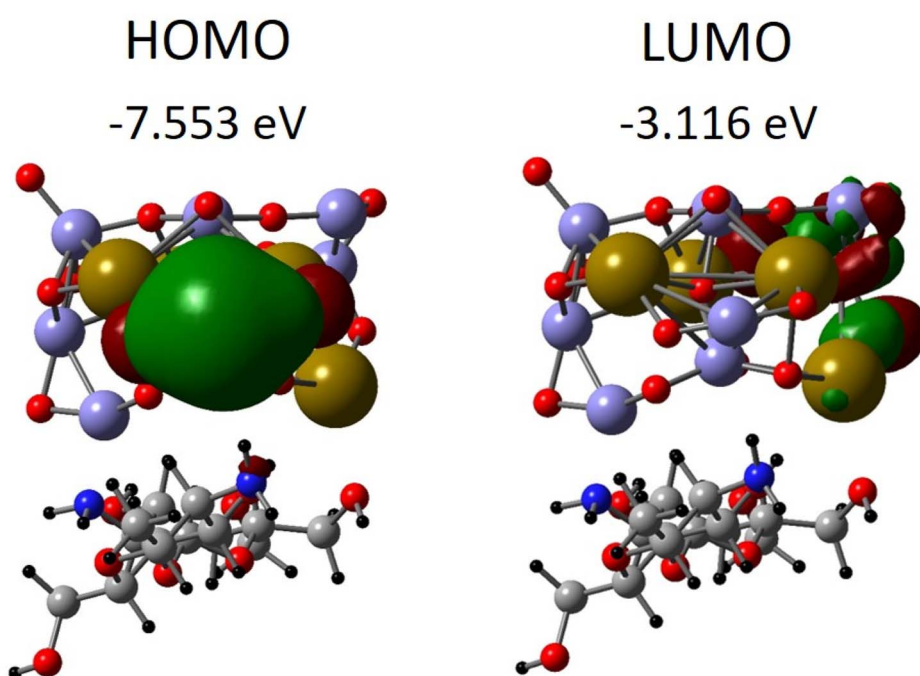


Fig. 13 The HOMO and LUMO distribution of  $\text{SrFe}_2\text{O}_4$  nanoparticle + chitosan. The strontium atoms are brown, the iron atoms are violet, the oxygen atoms are red, the carbon atoms are grey, the nitrogen atoms are blue and the hydrogen atoms are black.

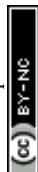


Table 8 Electrostatic potential charges (e) computed for the investigated nanoparticles

SrFe <sub>2</sub> O <sub>4</sub>		
Sr	Fe	O
+1.619	+0.093	-0.188
+1.615	+1.073	-0.882
+1.254	+0.955	-0.613
+1.526	+0.921	-1.352
	+0.778	-1.527
	+1.638	-0.880
	+0.484	-1.021
	+0.699	-0.820
		-0.906
		-0.621
		-0.799
		-0.841
		-0.954
		-0.970
		-0.559
		-0.614
ZnFe <sub>2</sub> O <sub>4</sub>		
Zn	Fe	O
+1.330	+1.134	-1.029
+1.372	+1.135	-1.136
+1.267	+1.652	-1.026
+1.462	+1.293	-0.597
	+1.341	-0.942
	+1.181	-0.745
	+1.378	-1.629
	+1.470	-0.876
		-1.221
		-0.947
		-1.164
		-1.048
		-0.672
		-1.121
		-0.862
		-1.066
CuFe <sub>2</sub> O <sub>4</sub>		
Cu	Fe	O
+1.370	+1.284	-0.895
+1.152	+1.241	-0.699
+0.786	+1.284	-0.841
+1.078	+1.178	-0.944
	+1.142	-0.809
	+1.323	-0.847
	+1.242	-0.749
	+1.064	-1.210
		-0.893
		-0.849
		-0.854
		-1.033
		-0.817
		-1.002
		-1.084
		-0.680

Table 9 Hirshfeld charges (e) computed for the investigated nanoparticles

SrFe <sub>2</sub> O <sub>4</sub>		
Sr	Fe	O
+0.532	+0.171	-0.303
+0.457	+0.401	-0.371
+0.521	+0.217	-0.254
+0.502	+0.413	-0.365
	+0.457	-0.263
	+0.579	-0.342
	+0.075	-0.447
	+0.418	-0.414
		-0.295
		-0.282
		-0.350
		-0.330
		-0.316
		-0.483
		-0.308
		-0.319
ZnFe <sub>2</sub> O <sub>4</sub>		
Zn	Fe	O
+0.241	+0.398	-0.385
+0.505	+0.441	-0.366
+0.518	+0.506	-0.285
+0.592	+0.754	-0.325
	+0.667	-0.315
	+0.358	-0.422
	+0.237	-0.967
	+0.897	-0.356
		-0.418
		-0.382
		-0.324
		-0.322
		-0.378
		-0.508
		-0.332
		-0.404
CuFe <sub>2</sub> O <sub>4</sub>		
Cu	Fe	O
+0.673	+0.529	-0.412
+0.607	+0.458	-0.314
+0.526	+0.404	-0.376
+0.596	+0.426	-0.411
	+0.351	-0.350
	+0.458	-0.415
	+0.377	-0.354
	+0.448	-0.334
		-0.373
		-0.362
		-0.378
		-0.369
		-0.294
		-0.462
		-0.315
		-0.338



+1.284e, +1.284e, and +1.323e. The charges on the oxygen atoms of the nanoparticle range from  $-1.002e$  to  $-0.699e$ , with the oxygen closest to the  $-NH_2$  group of chitosan carrying a charge of  $-0.817e$ . The corresponding atoms of this  $-NH_2$  group exhibit charges of +0.616e (H),  $-1.311e$  (N), and +0.485e (H). For comparison, the charges on a different  $-NH_2$  group amount to  $-1.059e$  (N), +0.449e (H), and +0.389e (H). The smallest distance between the NP (O site) and chitosan (H site) is 230 pm. The wide distribution of the ESP charges on the  $SrFe_{12}O_{19}$  NP is exemplified by +1.488e on the Sr atom and +0.293e to +1.308e on the Fe atoms. The oxygen atoms in the nanoparticle possess charges varying from  $-0.068e$  to  $-0.867e$ . The Sr is closest to the chitosan molecule, with distances to its hydrogen atoms amounting to 463 pm and 493 pm.

## 4. Conclusion

This study demonstrates the successful synthesis of  $ZnFe_2O_4$ ,  $CuFe_2O_4$ , and  $SrFe_{12}O_{19}$  nanoparticles *via* an ultrasound-assisted PEG route, yielding morphologically tailored ferrites with mesoporous characteristics. XRD analysis confirmed single-phase formation for  $ZnFe_2O_4$  and  $CuFe_2O_4$ , while  $SrFe_{12}O_{19}$  exhibited coexistence of hexagonal M-type ferrite and rhombohedral  $\alpha$ - $Fe_2O_3$ , indicating a multiphase nature. Incorporation into chitosan-based nanocomposites enabled high-performance corrosion inhibition of carbon steel in acidic media, with inhibition efficiencies exceeding 98% at optimal concentration. The comprehensive electrochemical evaluation—spanning PDP, EFM, and EIS techniques—confirmed a mixed-type inhibition mechanism, predominantly impacting the cathodic process. Increased charge transfer resistance, reduced double-layer capacitance, and near-complete surface coverage underscore the formation of resistive protective films. Adsorption analyses supported spontaneous, monolayer composite-metal interactions with both physisorptive and chemisorptive contributions. Among the systems, **Chit-ZnFe<sub>2</sub>O<sub>4</sub>** exhibited the highest inhibition efficiency, attributed to its favorable textural properties and interfacial activity. These results validate the use of ultrasound-engineered ferrites as multifunctional additives for corrosion-resistant coatings and highlight their potential in advanced material formulations.

## Author contributions

T. A., M. O., F. A.: conceptualization, methodology, investigation, synthesis, writing – original draft, resources. M. A. B., A. M. A., M. A. A.: electrochemical analysis, writing – review & editing, validation, visualization, data curation. N. A. A., V. V. C.: computational methodology, software, writing – original draft.

## Conflicts of interest

The authors hereby declare no financial interests and professional connections that might bias the interpretations of the obtained results.

## Data availability

The data supporting this article have been included in the publication.

Supplementary information (SI) is available. See DOI: <https://doi.org/10.1039/d5ra08173d>.

## Acknowledgements

The authors are thankful to the Deanship of Graduate Studies and Scientific Research at the University of Bisha for supporting this work through the Fast-Track Research Support Program. The results of the work were obtained using the computational resources of Peter the Great Saint-Petersburg Polytechnic University Supercomputing Centre (<https://www.spbstu.ru/>). This work was also supported by the Deanship of Scientific Research, Vice Presidency for Graduate Studies and Scientific Research, King Faisal University, Saudi Arabia [Grant No. KFU260913]. During the preparation of this work the author(s) used QUILBOT to improve readability and language of the work. After using this tool/service, the author(s) reviewed and edited the content as needed and took(s) full responsibility for the content of the publication.

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