ECP 2025 Conference

The 4th International Electronic Conference on Processes

20–22 October 2025 | Online

MDPI

EXPERIMENTAL AND IN SILICO STUDY TO EVALUATE THE CORROSION INHIBITION POTENTIAL OF PRAWN SHELL-DERIVED CHITOSAN ON MILD STEEL IN SALINE SOLUTION: EFFECT OF TEMPERATURE AND CONCENTRATION

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INTRODUCTION & AIM

- Corrosion is an electrochemical process which involves the reaction of metal with the components of the adjacent aggressive environment.
- According to a NACE's study, the financial loss due to the corrosion is around 2.5 trillion $ (USD), (Janse van Rensburg, et al. 2019).

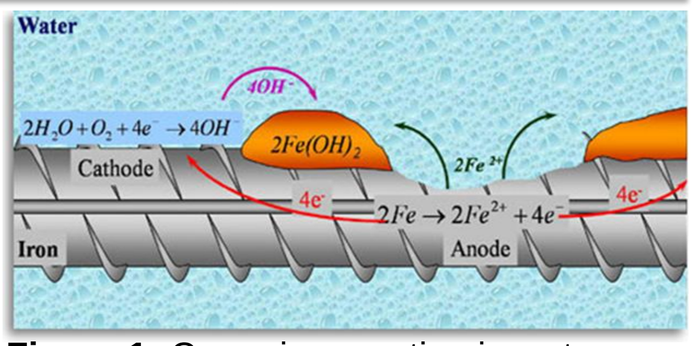


Figure 1: Corrosion reaction in water

- Corrosion inhibitors are added to an environment with the aim of decreasing the corrosion rate of a given material. They contains carbon and hydrogen, together with heteroatoms such as P, N, O, S.
- Prawn shells contains components such as chitosan, protein, minerals and chitin.
- About 20–50% of the dry weight of prawn shell debris is made up of chitin. Synthesized from chitin is chitosan ($C_6H_{11}NO_4$).

- **Aim and Objectives**

To evaluate the corrosion inhibition capacity of prawn shells and its derivative (chitosan) as a green corrosion inhibitor of reinforced concrete structured made of carbon steel in saline environments.

- Determine the functional groups and molecular species exhibited by the inhibitor.
- Determine the localized corrosion resistance of carbon steel in aqueous saline solutions at different temperature ranges (293K, 298K and 303K) and varying inhibitor.
- Perform quantum chemical simulation using Gauss view and molecular dynamics studies using Material studio software 2020.

METHOD

Preparation of chitosan from prawn shells:

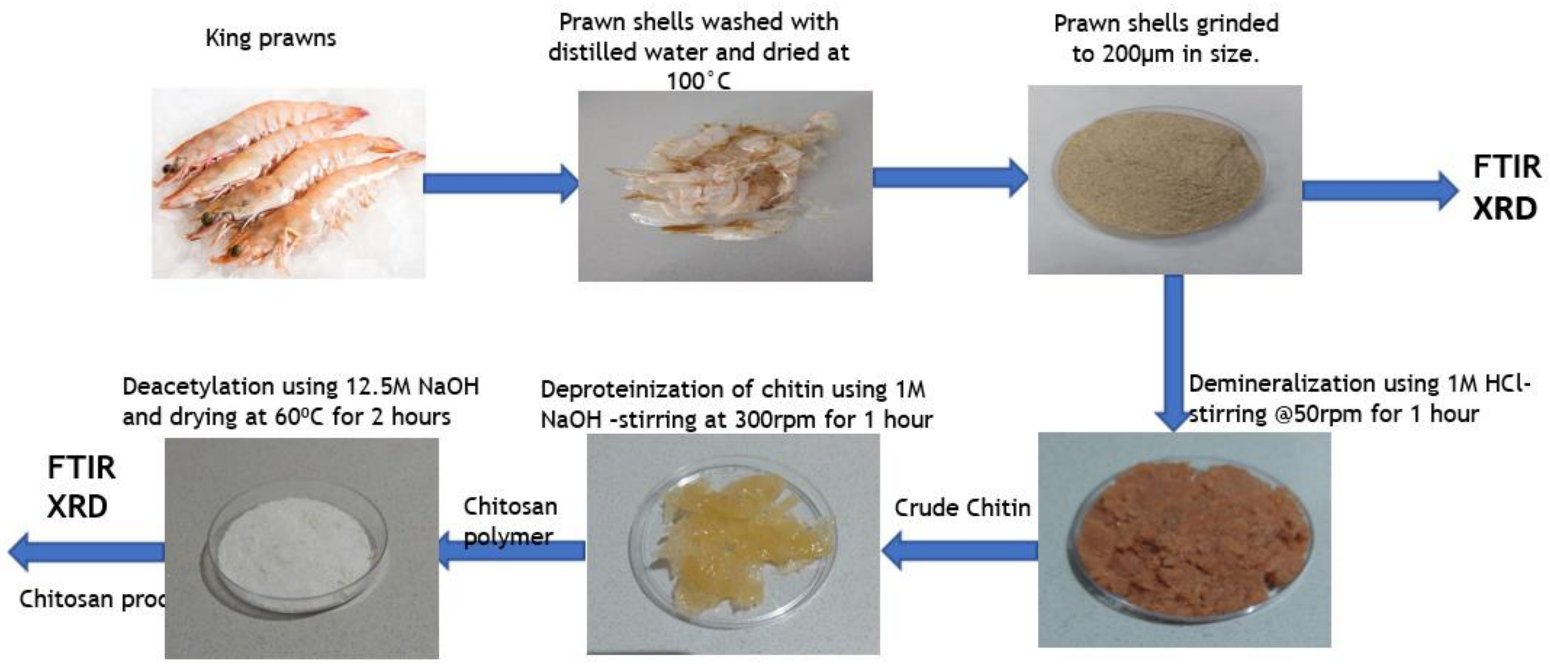


Figure 2: The preparation steps of chitosan from prawn shells

Preparation of carbon steel:

- The coupons for the electrochemical test were 10x10x4 mm in size. The coupons were polished with silicon carbide papers.
- **Preparation of saline solutions:**
- The saline solutions were prepared by using 3.5% NaCl diluted in 1 liter of deionized water. The pH was adjusted by using 1M HCl to pH 6.5, 7.5 and 8.5.

Electrochemical tests: Autolab potentiostat (CR,%IE and Tafel plots)

- Three different environments were created which is simulated marine water.
- Three different inhibitor amounts were used - 2g, 4g, 8g.
- The tests were ran at three different temperatures (293K, 298K and 303K).

Computation studies:

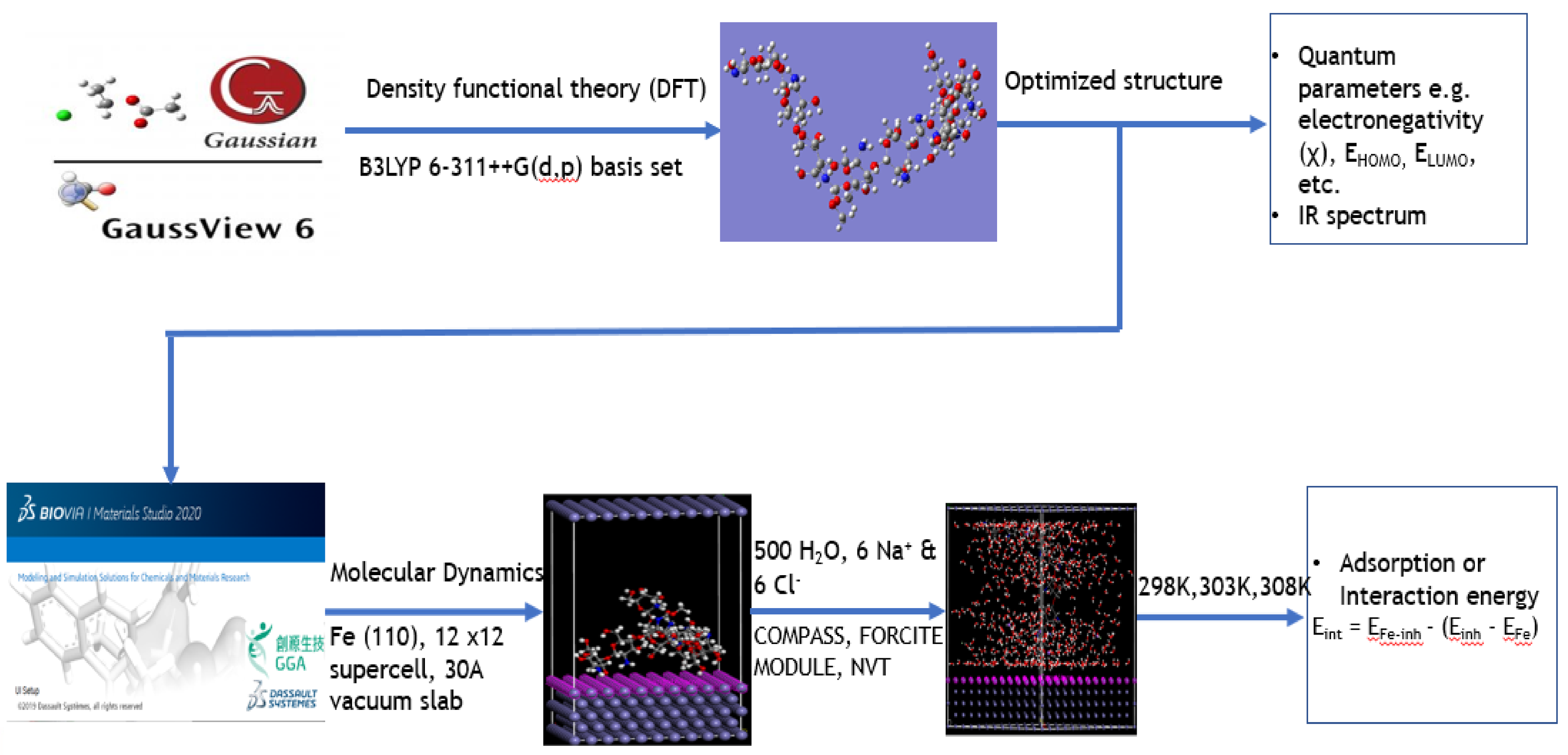


Figure 3: Computation studies

RESULTS & DISCUSSION

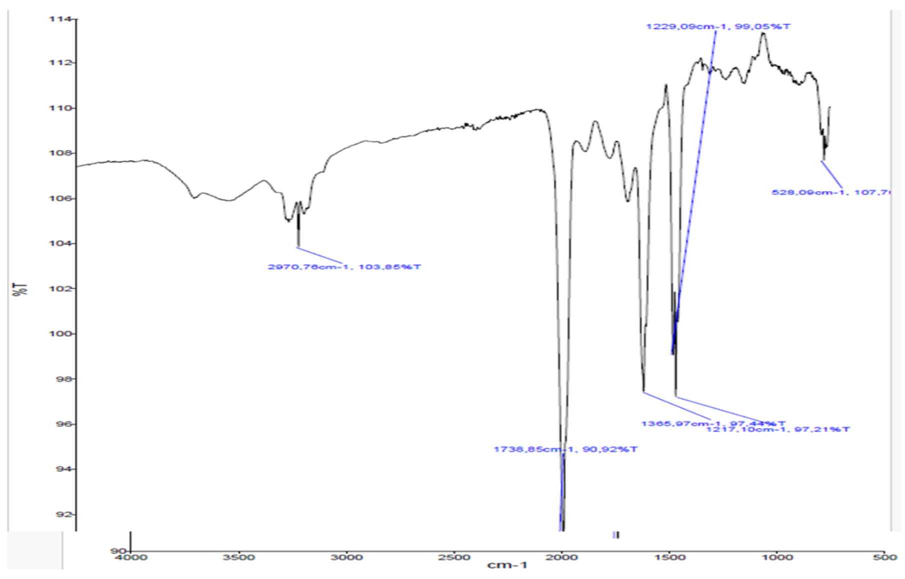


Figure 4: FTIR spectrum of chitosan

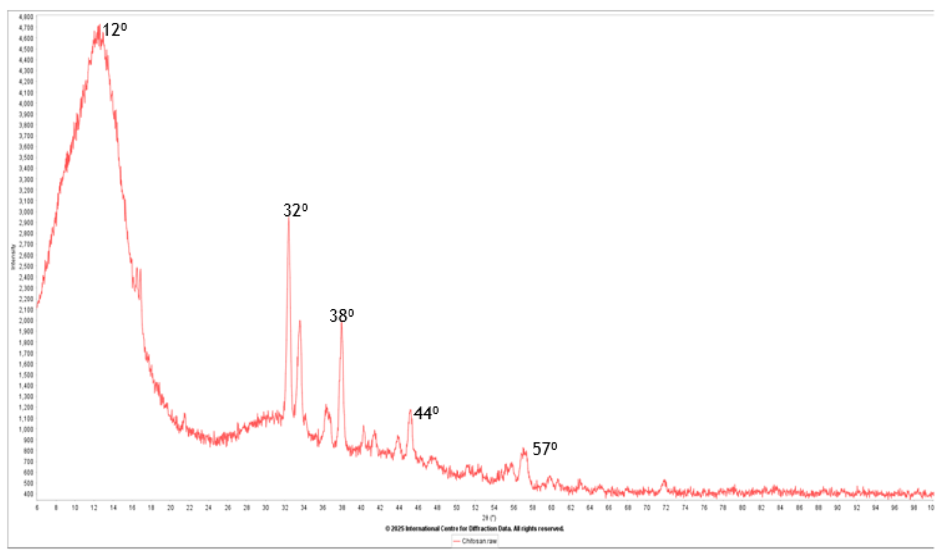


Figure 5: XRD pattern of chitosan

- FTIR shows functional groups located around frequency 3290 as N-H/OH, 2970 C=C/CH, 1738 C=O and 1365 C-N.
- XRD Patterns were located at around 12 and 31° in 2θ and the crystalline peaks at various angles indicates that the sample is both amorphous and crystalline. Estimated mean crystallite size, calculated as 6.90 nm for chitosan representing, CH, N and CO.

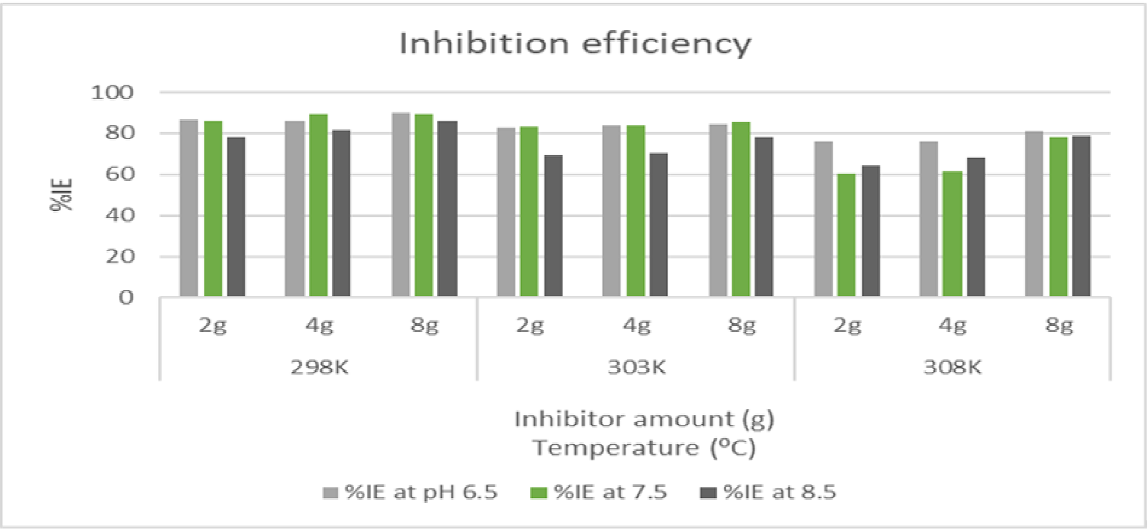


Figure 6: Inhibition efficiencies at different temperatures and inhibitor amount

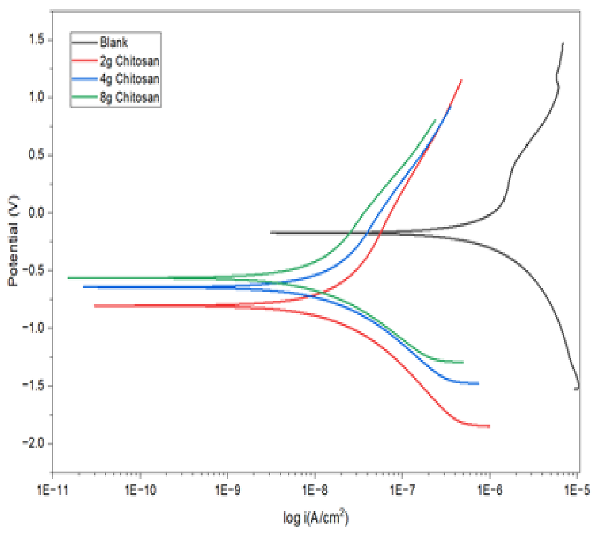
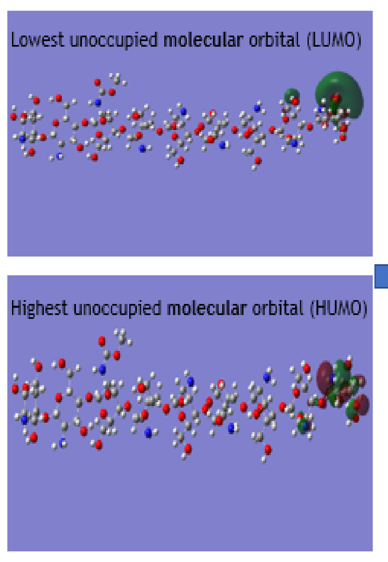


Figure 7: Tafel plots for pH 6.5 at 298K

From Figure 6, the corrosion rate tend to increase as the temperature increases, and the corrosion rate tend to decrease as the inhibitor amount increases. The more saline the solution is the higher the corrosion rate.

The chitosan as proven to be a mixed type inhibitor as the plots move to both the anodic and cathodic side, as shown in Figure 7.



(a) Chitosan optimized structure

S. No	Quantum paramaters	Chitosan
1	Molecular formula	(CnHnNOx
2	Energt (RB3LYP) (hartee)	-5622.59
3	EHOMO	-0.238
4	ELUMO	-0.026
6	ΔE (ev)	0.224
7	Dipole moment (µ)	2.67
8	Ionization affinity (A)	0.026
9	Electronegativity (χ)	0.513
10	Chemical hardness	0.487
11	Chemical softness	0.2435
12	Electronic energy (EE)	5622.59
13	Plorisation (α) (a.u)	893.943

(b) Quantum parameters

Figure 8: (a) Optimized structures-LUMO &HUHO, (b) Quantum parameters

Table 1: Interaction energies at different temperatures

Temperature (K)	Fe+Solution energy	Chitosan energy (kcal/mol)	Total energy (kcal/mol)	Interaction (kcal/mol)
298	-82832.185	422.613	-82611.367	-201.795
303	-82762.112	424.698	-82465.589	-128.175
308	-82775.035	494.375	-82393.571	-112.911

- From the computational studies chitosan has demonstration to have a good adsorption capacity.

CONCLUSION

- Chitosan from prawn shells was characterized by the use of the XRD and FTIR. The results shows the presence of essential molecules which are contributing to the corrosion inhibition.
- Results from the electrochemical tests gave the highest inhibition efficiency of 90%.
- The quantum studies through DFT calculations shows parameters that supports the experimental and theoretical data. Molecular dynamics shows good interaction between the iron, solution and inhibitor, showing that indeed chitosan can be employed as a green corrosion inhibitor.

FUTURE WORK / REFERENCES

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