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Interaction of newly synthesized dipeptide Schiff bases with mild steel surface in aqueous HCl: Experimental and theoretical study on thermodynamics, adsorption and anti-corrosion characteristics

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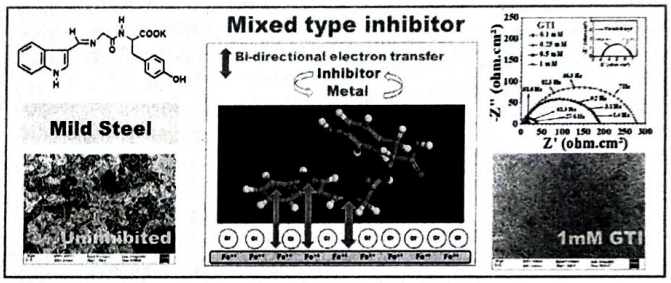
HIGHLIGHTS

- Dipeptide Schiff bases act as cathodic inhibitors for mild steel in aqueous HCl.
- The aromatic ring in the dipeptide backbone provides best inhibitory effect.
- DFT study interconnects electronic properties with inhibitory performance.
- Planar orientation of Schiff bases on metal surface is predicted by MD simulation and DFTB + calculation.
- Inhibitor to metal change transfer is proposed comparing PDOS curves for bonded and non-bonded inhibitor.

GRAPHICAL ABSTRACT



ARTICLE INFO

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ABSTRACT

Adsorption behavior and anti-corrosion propensity of three newly synthesized dipeptide Schiff bases are investigated using mild steel submerged in aqueous 1 M HCl. Electrochemical techniques (potentiodynamic polarization and electrochemical impedance spectroscopy) as well as gravimetric method are employed to ascertain the effect of concentration, temperature and immersion time on corrosion inhibition performance of the inhibitors. It is revealed that the Schiff base condensed between glycyl-L-tyrosine and indole-3-carboxaldehyde (GTI) imparts better inhibitory effect (greater than 98% inhibition efficiency) than those condensed between the same aldehyde and glycyl glycine (GGI) or glycyl-L-glutamine (GGMI). Thermodynamic parameters are evaluated employing Langmuir adsorption isotherm model to explain the mechanism of adsorption of inhibitor molecules on mild steel. Additional π-electron density of the aromatic moiety present in GTI seems to be responsible behind it. MD simulation study reveals almost parallel orientation of inhibitor molecules with respect to the metal surface. Interaction energy enumerated through MD simulation matches exactly with inhibitory trend. Following DFTB + calculation, charge transfer from the inhibitor to metal surface is established. Scanning electron microscopy images provide visual support to the effective corrosion inhibition by dipeptide Schiff bases.

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