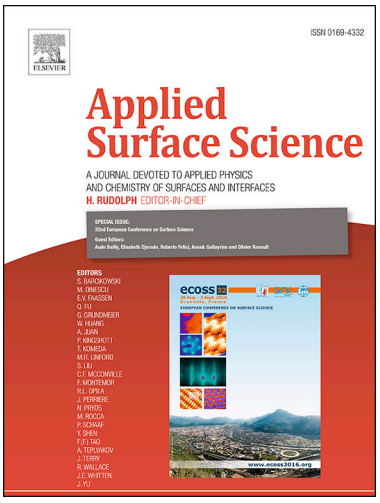

Full Length Article

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Choline based ionic liquids as sustainable corrosion inhibitors on mild steel surface in acidic medium: Gravimetric, electrochemical, surface morphology, DFT and Monte Carlo Simulation studies

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Abstract:

The adsorption tendency of choline based ionic liquids namely, 2-hydroxyethyl-trimethyl-ammonium chloride [Chl][Cl], 2-hydroxyethyl-trimethyl-ammonium iodide [Chl][I] and 2-hydroxyethyl-trimethyl-ammonium acetate [Chl][Ac] on mild steel surface in 1M HCl has been demonstrated using experimental and theoretical approaches. Weight loss analysis showed that inhibition efficiencies of [Chl][Cl], [Chl][I] and [Chl][Ac] increases with their concentrations. The maximum efficiencies of are in the order; [Chl][Cl] (92.04%) < [Chl][I] (96.02%) < [Chl][Ac] (96.59%) at 17.91×10^{-4} M concentration. Electrochemical analyses (OCP, PDP and EIS) data provide good support to the weight loss study and showed that investigated ionic liquids behaved as interfacial and mixed type corrosion inhibitors. The adsorption of [Chl][Cl], [Chl][I] and [Chl][Ac] at mild steel/ 1M HCl (electrolyte) interfaces obeyed the Temkin adsorption isotherm. The adsorption of studied ionic liquids on the metallic surface was further supported by SEM-EDX and AFM methods. DFT and Monte Carlo (MC) Simulations based computational approaches were undertaken to support the experimental findings. DFT studies revealed that [Chl][Cl], [Chl][I] and [Chl][Ac] interact with metallic surface through donor-acceptor interactions in which the anionic parts act as electron donor (HOMO) and cationic parts behaved as electron acceptor (LUMO). The MC simulations study showed that studied ionic liquids adsorb spontaneously on mild steel surface and their effectiveness depends upon nature of anionic moieties. The experimental and theoretical analyses show that investigated the inhibition efficiencies of studied ionic liquids followed the order: [Chl][Cl] < [Chl][I] < [Chl][Ac].

Keywords: Ionic liquids, sustainable corrosion inhibitors, Temkin isotherm, Mixed type corrosion inhibitors, MC simulations, DFT studies.