البحث السابع

ɪnsight Into the Inhibition Performance of Thiosemicarbazones as Efficient Inhibitors for Copper in Acidic Environment: Combined Experimental and Computational Investigations

Abstract

The corrosion resistance of copper makes it a popular material. Despite this, the Cu metal is prone to corrosion, and pitting corrosion is frequently observed which leads to application restrictions. In this work, we devolved three efficient corrosion inhibitor types of thiosemicarbazone derivatives namely, (2*E*,2′*E*)- 2,2′-(1,4-phenylenebis(methanylylidene))bis(N-benzylhydrazine-1-carbothioamide) (BBCT), (2*E*,2′*E*)- 2,2′-(1,4-phenylenebis (methanylylidene))bis(N-allylhydrazine-1-carbothioamide) (BACT) and (*E*)- 2-(5-azido-2-hydroxybenzylidene)-*N*-benzylhydrazine-1-carbothioamide (HBCT)that can inhibit the copper corrosion in 0.5 M sulfuric acid. The chemical structure of these materials were confirmed by FT-IR, HRMS,1HNMR and 13CNMR spectroscopic techniques. Moreover, their inhibition performance were evaluated by using various electrochemical techniques *i.e*. potentiodynamic polarization, AC impedance method, along with the density functional theory (DFT) and Monte Carlo (MC) simulations. The maximum inhibition efficiency (η) obtained by electrochemical techniques was 98.37% at 298 K for 150 ppm BBCT. The synthesized compounds were adsorbed *via* Langmuir adsorption model with physiochemical adsorption as inferred from the standard free energy (ΔG°_{ads}) values and the favorable performance was ascribed to the formation of BBCT adsorption films on the surface of the copper. Finally, the experimental results were correlated with the theoretical calculations using DFT theory which revealed the interaction between the assembled compounds and the copper surface.

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