Mild Steel Corrosion Inhibition by Furocoumarin Derivatives in Acidic Media

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The development of natural-based corrosion inhibitors has increasingly become an important research objective. Herein, we report the potential use of two natural furocoumarins namely, Bergamottin (FC-C) and Isopimpinellin (FC-M) for the corrosion protection of mild steel (MS) in 1.0 M HCl. Corrosion inhibitory activities of two compounds were evaluated using gravimetric, electrochemical, scanning electron microscope (SEM) and computational techniques. Electrochemical results disclosed that the two compounds could effectively control the dissolution rate of mild steel in acidic medium through physicochemical adsorption following Langmuir adsorption model. Potentiodynamic polarization curves indicated that the furocoumarin molecules could be classified as mixed-type inhibitors by preventing anodic metal dissolution and cathodic hydrogen evolution reaction. Density functional theory (DFT) and molecular dynamics (MD) simulations were carried out to describe electronic properties of two furocoumarins and their interaction with Fe(110) surface.

Keywords: Mild steel; Corrosion inhibition; HCl; Furocoumarin; Molecular dynamic; DFT.

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