Electrochemical and Computational Investigations on the Corrosion Inhibition of X65 Steel by 2-Phenylbenzimidazole in H₂SO₄ Solution

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In this work, we studied 2-phenylbenzimidazole (PBI) as a corrosion inhibitor for X65 steel in H₂SO₄ medium. The inhibition performance of PBI for X65 steel were studied using weight loss, electrochemical experiments, surface analysis and computational modelings. The results indicate that PBI has a superior anti-corrosion performance and belongs to modest cathodic-type corrosion inhibitor. The adsorption behavior of PBI molecule on steel conforms to Langmuir adsorption model. The adsorption type is a combination of physical and chemical adsorption. SEM morphology analysis can prove inhibition performance of PBI. DFT calculation and molecular dynamics simulations have revealed active adsorption sites and adsorption configuration of PBI molecule on Fe substrate.

Keywords: Corrosion, X65 steel, Acid inhibitor, Electrochemistry, Weight loss

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