Effective Protection for Copper Corrosion by Two Thiazole Derivatives in Neutral Chloride Media: Experimental and Computational Study

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Two corrosion inhibitors for copper in neutral NaCl solution, 2-aminobenzothiazole (ABT) and 2-amino-6-bromobenzothiazole (ABBT) were investigated by corrosion experiments and theoretical simulations. The results of weight loss and electrochemical experiments revealed that ABT and ABBT are efficient cathodic inhibitors with excellent inhibition efficiency (ABBT > ABT), which was further confirmed by field emission scanning electronic microscope (FESEM) observation. The adsorption of these molecules on copper surface was found to obey Langmuir adsorption isotherm. Moreover, the quantum chemical calculations and molecular dynamic (MD) simulation were used to investigate inhibition mechanism of studied inhibitors.

Keywords: Corrosion inhibitor, Adsorption, Copper, Electrochemical test, Quantum chemical calculation, Molecular dynamic simulation

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