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Experimental and theoretical investigations of some pyrazolo-pyrimidine derivatives as corrosion inhibitors on copper in sulfuric acid solution

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Abstract: The anticorrosion performance of three pyrazolo-pyrimidine derivatives, namely, 4-amino pyrazolo-pyrimidine (APP), 4-hydroxy pyrazolo-pyrimidine (HPP), and 4-mercapto pyrazolo-pyrimidine (MPP) on copper in 0.5 M H₂SO₄ solution have been investigated using electrochemical, surface analysis, as well as theoretical techniques. The results indicate that these inhibitors have largely inhibited the corrosion of copper and the inhibition efficiency increased with increasing concentration. Moreover, the inhibitors adsorb on copper surface following Langmuir adsorption isotherm. XPS analysis were performed for describing the bonding characteristics between inhibitors and copper substrate. Furthermore, DFT and molecular dynamics simulation calculations were applied to further explain the anti-corrosion mechanism.

Keywords: A. Copper; B. Corrosion inhibitor; C. pyrazolo-pyrimidine; D. Modelling studies

1. Introduction

Copper and its alloys have been applied to nearly the whole industrial field, such as electronics, machinery, transportation and chemical industries [1]. As everyone knows, pickling is generally utilized to prevent further oxidation and corrosion after a period work of metal. Copper surface is vulnerable to corrosion by aggressive ions during pickling [2-4]. Hence, it is indispensable to explore methods to protect copper from corrosion. The most effective technique is the application of corrosion inhibitors to metals thereby minimizing the acid attack, which has been a practically accepted method [5-8].

It is reported that lots of organic compounds containing conjugated double bonds, groups with heteroatoms (N, S, O, etc.), and polar functional groups can be served as corrosion inhibitors [9-12]. In our previous work, we have investigated the impact of alkyl chain length on the inhibition ability of some benzotriazole derivatives [13], and we also found that halogen atoms can enlarge the inhibition properties of organics [14]. Undoubtedly, it is very necessary to keep

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