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# Experimental and theoretical insights into copper corrosion inhibition by protonated amino-acids

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The effects of cysteine (Cys) and L-methionine (L-Met) on copper corrosion inhibition were examined in 1 M HNO<sub>3</sub> solution for short and long exposure times. Potentiodynamic polarization (PDP) and electrochemical impedance spectroscopy (EIS) were used. The EIS determined the potential for zero charges of copper (PZC) in the inhibitor solution. SEM and AFM have been used to study material surfaces. Energy-dispersive X-ray spectroscopy (EDS) was used to identify surface elemental composition. DFT and molecular dynamics simulations explored the interaction between protonated amino acids and aggressive media anions on a copper (111) surface.

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## 1. Introduction

Copper, with a reddish-orange color, is the fifth most common metal in the earth's crust which allows it to be used in a wide variety of industrial applications and also in everyday life, such as industrial equipment, marine industries, power station, coinages, electricity, desalination plants, fabrication of heat exchangers, tubes, cooling towers, water treatment, and electronics and many more.<sup>1–9</sup> This metal is preferred in all these applications because of favorable properties like high electrical and thermal conductivity,<sup>10</sup> mechanical workability, malleability, and resistance to atmospheric and chemical agents. In

addition to all these properties, copper has antimicrobial activity. Copper is a relatively noble metal. Copper dissolves in severe environments regardless of the application location. Although passive protective oxide film formation provides the appearance that copper is resistant to corrosion under some circumstances or in the atmosphere,<sup>11</sup> copper oxidizes rapidly in certain situations and generates a layer of copper oxides and/or hydroxides on its surface. The nature of this film depends on the medium's composition. Despite this self-protective film, this metal may undergo corrosion in acid medium or industrial environments containing chloride, sulfate, or nitrate ions. Nitric acid is an oxidizing acid whose oxidizing capacity depends on its concentration. Oxygen in nitric acid adds to the acceleration of copper surface corrosion.<sup>12</sup> The nitric acid reaction of copper gives hydrogen used to reduce nitric acid to different products.<sup>13–16</sup> Most metals are known to react with nitric acid and form compounds rich in hydrogen (NH<sub>3</sub> or NH<sub>2</sub>OH). Likewise, noble metals like silver and copper generate oxygen-rich molecules (NO<sub>2</sub>, NO, or HNO<sub>2</sub>).<sup>1,17–20</sup>

Understanding the corrosion process aims to discover techniques for limiting or preventing the metal's reactivity to its surroundings. Organic inhibitor chemicals have recently been shown to be the most efficient and feasible strategy for achieving this objective. Organic inhibitors,<sup>21,22</sup> comprising nitrogen, oxygen, and/or sulfur atoms and aromatic rings, are potent and commonly employed to preserve copper and its alloys.<sup>23–28</sup> Due to their toxicity, however, the use of some inhibitors has been banned in many nations and regions. In this context, some of our research examines the applicability of non-toxic, inexpensive, healthy, ecologically friendly, and efficient corrosion inhibitors. Amino acids are non-toxic, biodegradable, and environmentally benign molecules, relatively

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