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Azoles molecules as potential corrosion inhibitors: A DFT study.

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Abstract: Corrosion is an undesirable process that affects several areas of industrial activity, especially the oil industry, resulting in huge economic losses. Although it is not possible to completely avoid the corrosion process there are ways to inhibit it. Organic heterocyclic compounds containing nitrogen atoms are commonly used as corrosion inhibitors. Those inhibitors can adhere to a metal surface to form a protective film against corrosive agents in the environment [1]. Azoles and particularly their derivatives are known as efficient corrosion inhibitors [2].

With the advances in computational chemistry and the development of new algorithms, theoretical methods have been used to investigate the inhibition mechanism and to design new and environment friendly molecules with potential to corrosion inhibition. Most of the theoretical calculations try to correlate structural properties with the inhibition efficiency of an isolated molecule. Since the interaction with the metallic surface is not taken into account, these calculations do not provide a full picture of the inhibition mechanism. Some recent studies considered the adsorption of the inhibitor on a metallic surface by performing calculations within the framework of the density functional theory (DFT) under periodic boundary conditions providing significant understanding about the corrosion inhibition mechanism [3,4].The aim of the present study is to analyze the nature of the interaction of four azole molecules – imidazole, imidazoline, imidazolidine and pyrrolidine – with the (001) iron surface in gas phase, in order to verify whether these molecules are potential corrosion inhibitors and how the inhibition process takes place.

The calculations were performed using DFT under periodic boundary conditions with a plane wave basis set and ultrasoft pseudopotentials. We used the Generalized Gradient Approximation (GGA) functional of Perdew, Burke and Ernzerhof (PBE) [5] implemented in the PWSCF code of the Quantum Espresso suite of programs [6]. Several initial orientations of the molecules relative to the surface, parallel,

perpendicular and tilted, as well as the binding sites, *hollow* and *top*, have been considered.

In their neutral forms pyrrolidine and imidazole exhibit good potential as corrosion inhibitors, pyrrolidine being more strongly adsorbed than imidazole, imidazoline and imidazolidine on the Fe(001) surface. Considering all the possible orientations, the four molecules showed preference to interact with a *top* iron atom of the surface, with pyrrolidine and imidazole interacting preferably with an iron atom of the surface through the *pyridine-like* nitrogen atom, while imidazoline and imidazolidine molecules adsorb tilted to the surface to interact with two iron atoms. The process of adsorption of the molecules showed to be quite different and clearly ditacted by the molecular structure of the azole. Also, the differences in the strength of interaction of the molecules with the surface, are directly related to the way that they bind to the surface.

Key-words: Corrosion inhibition, azoles, iron surface, periodic DFT calculations

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