Theoretical investigation on the mechanism of corrosion inhibition of the (001) iron surface by imidazole and imidazoline: a surface coverage study.

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INTRODUCTION

Organic heterocyclic compounds containing nitrogen atoms are commonly used as corrosion inhibitors[1]. Those inhibitors can adhere to a metal surface to form a protective film against corrosive agents in the environment. However, the mechanism of inhibition is not well understood yet. In the current work, we applied density functional theory (DFT) under periodic boundary conditions to evaluate the surface coverage of four organic heterocyclic compounds and predict a potential formation of a protective film on the (001) iron surface.

COMPUTATIONAL DETAILS

The calculations were performed within the DFT (Density Functional Theory) 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)[3] implemented in the PWSCF code of the Quantum Espresso[4] suite of programs. The coverage was carried out varying from 2 to 6 the number of adsorbed molecules.

RESULTS AND DISCUSSION

For imidazole the highest surface coverage was achieved with four molecules adsorbed per unit cell, giving rise to a tetrameric structure (-1.62 eV) (Figure 1, left). For imidazoline, the highest coverage is achieved with only two molecules adsorbed, resulting in a dimeric structure (-2.68 eV) (Figure 1, right). The new structures (imidazole tetramer and imidazoline dimer), interact more strongly with the (001) iron surface than the respective monomers (-1.53 eV and -0.93 eV, respectively). These results can be understood as a cooperative effect that occurs during the adsorptions, leading to the formation of a film.

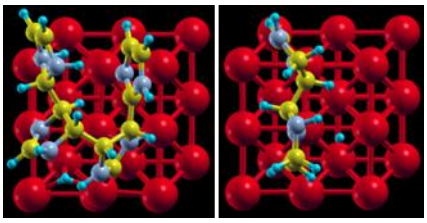

Figure 1. Structures yielded from the surface coverage: (left) imidazole tetramer and (right) imidazoline dimer.

CONCLUSIONS

In this work, a model is proposed to explain the inhibition performance of two organic heterocyclic compounds. Preliminary results show that the inhibition performance of imidazole and imidazoline molecules can be explained by the formation of a film. The formation of the films is due to a cooperative effect on the adsorption, caused by the breaking of double bonds on the rings and the formation of C–C sigma bonds between the molecules on the surface.

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