A Combined Density-Functional Theory and Molecular Dynamics Study on the Adsorption Behavior of Corrosion Inhibitors at the Iron-Water Interface

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Corrosion inhibitors (CIs) well-rooted their presence in the industry to combat internal metal deterioration, but in some cases fundamental understanding on their performance is lacking. Quantum mechanical calculations and molecular simulations can be used to tailor organic molecules, providing relationship between their molecular structure and protectiveness ability in different aqueous environments. In this contribution, we will present results concerning all-atom molecular dynamics (MD) simulations and chemical quantum calculations (DFT) in order to understand and quantify the effect of the environment on the surface adsorption of CI molecules. Three CIs abbreviated: TEPA, iTEPA and HC-iTEPA were selected for this work in order to systematically investigate the influence of the alkyl tail, N-pendant group, imidazoline and benzene rings, on their adsorption behaviour in different environments. DFT results reveal the electron distribution in inhibitors structures, indicating their ability to accept/donate charges from the Fe atoms in vacuum and in water solvation. MD simulations show nearly 53%, 39%, 59% reduction in adsorption energies shifting from pure water to CO_2-saline media, for single inhibitor molecule of TEPA, iTEPA, and HC-iTEPA, respectively. The formation of a water double adsorption layer contributes to decreasing the CIs adsorption energies by the larger surface separation distances spotted in the density profiles. Nevertheless, the multi-inhibitors study reveals strong adsorption of TEPA and iTEPA on the iron surface, while HC-iTEPA neglects cooperative adsorption and aggregates as a spherical-like micelle with lower surface coverage propensity. Furthermore, results concerning the effect of the surface roughness on their adsorption behaviour in aqueous environments, mimicking a partially corroded surface will also be presented.

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