Theoretical modeling and molecular level insights into the corrosion inhibition activity of 2-amino-1,3,4-thiadiazole and its 5-alkyl derivatives

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Abstract

Density functional theory (DFT) with two functionals, namely B3LYP and CAM-B3LYP with the 6-311 + +G(d,p) basis set was performed on six 2-amino-5-alkyl-1,3,4-thiadiazole derivatives (IC-2 to IC-13) used as corrosion inhibitors for steel in 1.0 M H2SO4 solution, along with the calculations on the parent compound 2-amino-1,3,4-thiadiazole (IC). The computations were carried out in non-protonated and protonated forms. The results obtained found a relationship between the molecular structures of the studied IC inhibitors and their experimental inhibition efficiencies. The order of the experimental inhibition efficiencies was matched with the order of a good number of the calculated global and local reactivity descriptors but with varying degrees of correlation. Supported by the Mulliken population analysis and natural population analysis, molecular electrostatic potential plots, and natural bond orbital analysis, the active sites in the inhibitors responsible for their adsorption on a steel surface have been predicted. Molecular dynamic simulations were further carried out on the protonated forms of IC-2 to IC-13 with an Fe (110) surface. Results obtained were in reasonable agreement with experimental data.
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