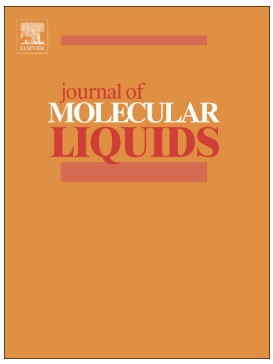

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Computational study of some thiophene derivatives as aluminium corrosion inhibitors

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Abstract

Quantum chemical calculations and molecular dynamics simulations studies of a series of thiophene-based compounds have been performed using the density functional theory (DFT) method to elucidate the relationship between inhibition efficiency and their molecular structures. The global and local quantities such as highest occupied molecular orbital energy (HOMO), lowest unoccupied molecular orbital energy (LUMO), energy gap (ΔE), dipole moment (μ), total energy (TE), ionization potential (I), electron affinity(A), electronegativity (χ), chemical potential (π), global hardness (η), global softness (σ), global electrophilicity (ω), polarizabilities $< \alpha >$, fraction of electrons transferred (ΔN), Fukui indices, local electrophilicity and local softness were calculated in vacuo and in water solution. The calculated values of inhibition efficiency show overall a good agreement with the experimental order. Finally, the interaction energies between the inhibitor molecules and the aluminium Al(111) surface were calculated and rationalized using molecular dynamics simulation technique.

Keywords: Thiophene derivatives, DFT, corrosion inhibitors, reactivity parameters, molecular structure, molecular dynamics simulations.

1. Introduction

Aluminium and its alloys are commonly used in many industries, including transportation, building materials, and aerospace, particularly because of their light weight and corrosion resistance [1,2], which is attributed to the formation of a protective surface oxide film [3].