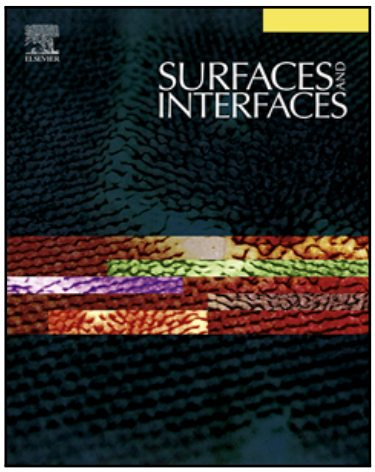

Molecular level insights for the corrosion inhibition effectiveness of three amine derivatives on the carbon steel surface in the adverse medium: A combined density functional theory and molecular dynamics simulation study

Sourav Kr Saha , Manilal Murmu , Naresh Chandra Murmu , I.B. Obot , Priyabrata Banerjee

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Molecular level insights for the corrosion inhibition effectiveness of three amine derivatives on the carbon steel surface in the adverse medium: A combined density functional theory and molecular dynamics simulation study

Sourav Kr. Saha [a,b], Manilal Murmu [a,b], Naresh Chandra Murmu [a,b], I. B. Obot [c] and Priyabrata Banerjee [a,b]*

[a]Surface Engineering & Tribology Group, CSIR-Central Mechanical Engineering Research Institute, Mahatma Gandhi Avenue, Durgapur 713209, West Bengal, India.
E-mail: pr_banerjee@cmeri.res.in; Fax: +91-343-2546 745; Tel: +91-343-6452220

[b]Academy of Scientific and Innovative Research (AcSIR), CSIR-CMERI Campus, Durgapur 713209, West Bengal, India.

[c]Centre of Research Excellence in Corrosion, Research Institute, King Fahd University of Petroleum and Minerals, Dhahran 31261, Kingdom of Saudi Arabia.

Abstract

The adsorption behaviour and mechanism of corrosion inhibition for three amine derivatives, *viz,* N^1-(2-aminoethyl)ethane-1,2-diamine (DETA), N^1-(2-(2-aminoethylamino)ethyl)ethane-1,2-diamine (TETA) and N^1-(2-(2-(2-(2-aminoethylamino)ethylamino)ethylamino)ethyl)ethane-1,2-diamine (PEHA) on the steel surface have been explored by density functional theory (DFT) and molecular dynamics (MD) simulations. Quantum chemical parameters *like* E_{HOMO}, E_{LUMO}, energy gap (ΔE), electron affinity (A), electronegativity (χ), global hardness (η), softness (σ) and the fraction of electron transferred (ΔN) from the inhibitor molecule to the metal surface have been calculated and discussed. Fukui indices analysis has also been carried out for investigating the active sites present in these molecules. Additionally, MD simulations have been executed to explore the configurationally adsorption behaviour of these amine derivatives on Fe (1 1 0) surface. The obtained binding energy of these three inhibitors follows the order PEHA > TETA > DETA, is also similar to a trend obtained from experimental analysis.

Keywords: Steel, Acid inhibition, DFT study, Fukui indices analysis, MD Simulation

1. Introduction