Communications in Computational Chemistry
*Commun. Comput. Chem., Vol. 7, No. 4,* 361–371
doi: 10.4208/cicc.2025.192.01

**Regular Article**

# Adsorption of Some Pteridine-Based Compounds on Fe (110) Surface and Potential for Corrosion Inhibition: Quantum Computations Molecular Dynamics Simulations

Ekemini Ituen[1,2*], Godstime Chuwkudike[1,2], Ubong Essien[3], Bright Daniel[4], Prince Micheal[5], Adebola Oyeniran[6], Muhammad Oshafu[7], Aduanya David[8] and Udoinyang Inyang[9]

[1]*Computational Materials Science Group, TETFUND Centre of Excellence in Computational Intelligence, University of Uyo, Uyo 52003, Nigeria;*

[2]*Department of Chemistry, Faculty of Physical Sciences, University of Uyo, Uyo, Nigeria;*

[3]*Department of Animal and Environmental Biology, University of Uyo, Uyo, Nigeria;*

[4]*Department of Chemistry, College of Arts and Sciences, University of Tennessee, Knoxville, USA;*

[5]*Department of Pure and Industrial Chemistry, University of Port Harcourt, Nigeria;*

[6]*Department of Chemistry, University of Lagos, Lagos, Nigeria;*

[7]*Department of Physics, Federal University of Lafia, Nasarawa State, Nigeria;*

[8]*Department of Mechanical Engineering, Michael Okpara University of Agriculture, Umudike, Nigeria;*

[9]*Department of Data Science, Faculty of Computing, University of Uyo, Uyo, Nigeria.*

[*] Corresponding authors: ekeminiituen@uniuyo.edu.ng

Received on 11 July 2025; Accepted on 22 August 2025

**Abstract:** The adsorption of organic molecules onto steel surfaces has been a key strategy in the selection of materials for mitigation of corrosion in various aggressive media. Computational chemistry offers valuable insight into the electronic interactions that govern this process. In this study, five pteridine-based compounds, namely, isoxanthopterin, leucopterin, lumazine, pterin and xanthopterin, were assessed for their adsorption behaviour and corrosion inhibition potential on Fe(110) surface using density functional theory (DFT) and molecular dynamics (MD) simulations. Geometry optimization, frontier molecular orbital analysis, and quantum reactivity descriptors were computed using the B3LYP/DNP level of theory via the Dmol³ module in BIOVIA Material Studio. Fukui indices and Mulliken charge distributions were analyzed to predict adsorption sites. Additionally, adsorption energies and molecular configurations on the Fe(110) surface were examined using the Forcite and Adsorption Locator tools. Results showed that all the studied compounds exhibit planar geometries favorable for surface interaction, with isoxanthopterin and xanthopterin demonstrating the strongest adsorption energies. Key adsorption sites were localized around nitrogen and oxygen heteroatoms. The compounds are predicted to form stable interactions with the iron surface through both physisorption and chemisorption, indicating excellent potential for use as green corrosion inhibitors.

**Key words:** adsorption energy, corrosion inhibition, DFT, Fukui function, HOMO and LUMO, molecular dynamics simulation.

## 1. Introduction

The interface between the surface of metallic or alloy materials and organic compounds presents a rich and interesting phenonemon, particularly in corrosion science. This phenomenon is termed adsorption, and it is the central process underlying corrosion inhibition, whereby organic molecules interact with the alloy or metal surface to form a protective film that minimizes degradation [1]. The protective film forms due to either physical (electrostatic) interactions or chemical bonding between electron-rich sites on the inhibitor and the active sites on the surface [2].

Corrosion, especially in steel used across the construction, petrochemical, and marine sectors, contributes to significant economic loss and structural failure globally. Traditional methods for corrosion prevention often involve the use of corrosion inhibitors, which are mainly organic molecules with heteroatoms such as N, O, or S, that can adsorb onto the steel surface and prevent corrosive species from reaching the metal surface [3-5]. Despite the wide array of organic molecules investigated for this purpose, the corrosion inhibition potential of pteridine-based compounds remains relatively underexplored.

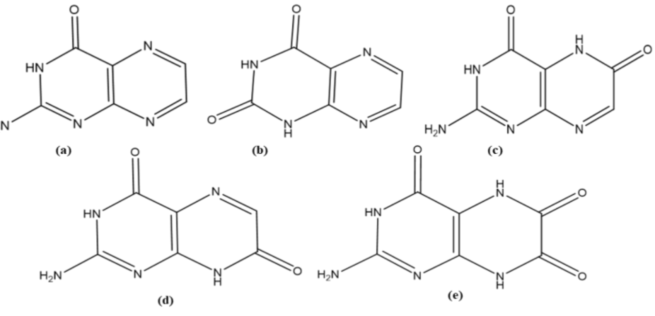

**Figure 1.** Molecular structures of (a) pterin (b) lumazine (c) xanthopterin (d) isoxanthopterin and (e) leucopterin.

Pteridine is a bicyclic nitrogen-containing heterocyclic compound, made specifically up of a fused pyrimidine and pyrazine ring. It is characterized by two nitrogen atoms at positions 1 and 4 in the pyrimidine ring (ring A) and two nitrogen atoms at positions 1 and 3 in the pyrazine ring (ring B). Pteridine and its derivatives are nitrogen-rich heterocycles structurally related to purines and flavins. They are known for their stable planar configurations and multiple functional groups capable of engaging in surface interactions. Compounds such as isoxanthopterin, leucopterin, lumazine, pterin and xanthopterin contain multiple electron-donating sites, making them strong candidates for corrosion inhibition. In addition, a careful look at the chemical structures of the molecules (Figure 1) would clearly reveal some variations in the functionalities attached to the pteridine moeities, which could give rise to interesting comparative and quantitative structure-function behaviour and mechanism of adsorption.

Some studies have reported various nitrogen-containing heterocycles such as imidazoles, triazoles and pyridines as corrosion inhibitors due to their high electron density and ability to coordinate with metal surfaces [6-8]. Despite their unique fused ring structure containing two nitrogen atoms in a diazine configuration, very little or nothing is known about the adsorption behaviour of these compounds, especially on iron based surfaces. The molecular structure, as it appears, may enhance surface adsorption and corrosion inhibition. To the best of our knowledge, few (if any) studies have employed pteridine derivatives specifically for corrosion inhibition on iron surfaces, especially using DFT-based predictive analysis. This study thus pioneers the evaluation of pteridine derivatives as potential eco-friendly inhibitors with promising electronic and adsorption properties.

The mechanism of interaction of organic molecules on surfaces and resultant corrosion inhibition is a complex one [9], hence, experimental studies alone are often insufficient in decoding the molecular-level mechanisms. In addition, experiments and laboratory procedures for cossorion monitoring, tests and assessments are associated with considerable cost, time, energy and safety limitations. Computational chemistry, particularly density functional theory (DFT) and molecular dynamics (MD) simulations, has emerged as a robust predictive tool that complements experimental approaches [10-12]. These methods provide insights