عنوان مقاله:

A Comparative Computational Stimulation Studies on Corrosion Inhibition and Adsorptive Qualities of Coumarin Derivative on Iron, Zinc, Copper and Aluminium

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خلاصه مقاله:

Metals, such as Iron, zinc, zluminium, and copper are vital in various industries and construction. However, these metals are susceptible to corrosion upon exposure to corrosive elements. Metals used at homes and part of our car bodies under goes corrosion at a little contact of the corrosion factors. In this research, a coumarin derivative was theoretically studied using quantum parameters such as Electronegativity (χ), Global hardness (η), Electron donating power(ω-), Electron accepting power (ω+), Global softness (σ), Global hardness (η), and fraction of electron transfer (ΔN) couple with the simulation process to ascertain and compare the corrosion inhibition of metals such Zn, Al, Cu, and Fe. Based on the results, low magnitude of ELUMO combined with the high magnitude of EHOMO reveals that Coumarin-۶-ol, ۳,۴-dihydro-۴,۴-dimethyl-۷-nitro- (CML) molecule was reactive by serving as a donor, hence confirming the predicted inhibition of the simulated parameters. The electronegativity atoms have a significant effect on the corrosion inhibition efficiency of CML inhibitor molecule, and the atom with a negative charge depicts the potential of a HOMO center. The binding energy of the inhibitor (CML) on the metals were in order of CML-Fe (۱۱۱)> CML-Cu (۱۱۰)> CML-Al (۱۱۰)> CML-Zn (۱۱۰) for -۹۰.۷۶۸۸۳۴kcal/mol, -۴۸.۶۴۳۵۴۴ kcal/mol, -۴۵.۷۳۴۴۸۵ kcal/mol, and -۲۶.۹۰۹۹۵۲ kcal/mol, respectively. According to the results, CML inhibitor molecule shows high significant corrosion protection properties and is shown to be highly effective on CML-Fe (۱۱۱) compare to the other metals studied. All CML-metal .contact in the study depicts a physical adsorption based on the values of binding and obtained adsorption energy

کلمات کلیدی:

Coumarin, Simulation, Binding energy, Quantum-Parameters