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Computational Adsorption and Dft Studies On the Corrosion Inhibition Potentials of Some Phenyl-Urea Derivatives

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ABSTRACT/RESUME

Abstract: *The inhibition performance of [(4-Hydroxy-6-methyl-2-oxo-2H-pyran-3-yl)-phenyl-methyl]-urea and [(4-Hydroxy-6-methyl-2-oxo-2H-pyran-3-yl)-(4-methoxy-phenyl)-methyl]-urea were investigated as corrosion inhibitors using density functional theory (DFT) at the B3LYP/6-31+ G(d,p) level of theory. The calculated quantum chemical parameters correlated to the inhibition of efficiency. The molecular descriptors have been analysed through the Fukui function and local softness indices in order to compare the possible sites for nucleophilic and electrophilic attacks. The success of DFT calculation in predicting the inhibition efficiency was assessed and the result reveals that HPU2 with the adsorption energy of -91.38 kJ/mol is higher than that of HPU1 which is -394.42 kJ/mol.*