Ab Initio Interpretation of the Experimentally Obsereved Corrosion Inhibition Mechanism

A Thesis

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Abstract

Ab initio and DFT calculations were carried out to investigate the relation between the electronic structure studied by quantum chemical calculations and experimental efficiencies of urea (U), guanidine (GU), thiourea (TU) and selenourea (SeU) as inhibitors for the corrosion of low carbon steel in sulphuric acid medium. Quantum chemical calculations were performed at different levels of theory; *ab initio* molecular orbital and DFT methods were applied. In this work, the quantum chemical investigation was extended to excited electronic states, cationic states, anionic states and protonated species of the inhibitors.

Obvious correlations were found between corrosion inhibition efficiency and some quantum chemical parameters such as the highest occupied molecular orbital energy (E_{HOMO}), lowest unoccupied molecular orbital energy (E_{LUMO}), the energy gap between E_{HOMO} and E_{LUMO} (ΔE) ionization energy (I.E.) and electronic density. Correlation between the quantum chemical calculations and the electrochemical results suggests that the ground electronic state of the inhibitor molecules is responsible for their anticorrosion behavior. The experimental work can thus be verified by theoretical calculations. This study resulted in identifying the $E_{HOMO,}$ ΔE, I.E. and electronic density as reliable indices to predict the anticorrosive behavior of these inhibitors.