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Theoretical investigation of heterocyclic compounds on corrosion inhibition behavior of copper in hydrochloric acid medium

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Abstract : Quantum chemical calculations based on DFT method were performed on two schiff bases compounds, used as corrosion inhibitors for copper in HCl media to determine the relationship between the molecular structure of schiff base and inhibition efficiency. Quantum chemical parameters such as the highest occupied molecular orbital energy (EHOMO), the lowest unoccupied molecular orbital energy (ELUMO), energy gap (?E), dipole moment (l), electronegativity (v), electron affinity (A), global ionization potential (I), the fraction of electrons transferred (?N), and the total energy (TE), were calculated. The theoretically obtained results were found to be consistent with the experimental data reported

Keywords : optimization, DFT, Quantum chemical