Short Communication

A Theoretical Study of Some Schiff Bases as 304 Stainless Steel Inhibitors in HCl Solution

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For four types of molecular Schiff inhibitors, the relationships between their corrosion inhibition efficiencies (*IE*) and some specific molecular property-related parameters, are investigated by using three different theoretical *ab initio* methods: Hartree-Fock (HF), Möller-Plesset perturbation theory on the 2nd order (MP2), and density functional theory (DFT). The parameters calculated include the energy of the highest occupied molecular orbital (E_{HOMO}), the energy of the lowest unoccupied molecular orbital (E_{LUMO}), the energy difference between E_{HOMO} and E_{LUMO} (ΔE), the dipole moment (μ), the electronegativity value (χ), the global hardness (η), the softness (σ), the fraction of transferred electrons between the molecular inhibitor and Fe (ΔN), and Mulliken atomic charges (Q). By using linear regression analysis, the relationships between *IE* and each of these parameters are carefully studied with the purpose to find the most effective parameters for the best inhibition efficiency. As a result, the comparison between the three different theoretical methods shows that the Hartree Fock (HF) method, with the 6-31++G(d, p) basis set, gives the most accurate results. In addition, the corrosion inhibition performances of all four molecular Schiff inhibitors show a linear relationship with the E_{HOMO} , E_{LUMO} , ΔE , μ , χ , η , σ , and ΔN parameters. In conclusion, this work provides a theoretical method by which it is possible to predict the corrosion inhibition performance of molecules with geometrical structures like the Schiff inhibitors.

Keywords: modeling studies; corrosion inhibition; Schiff base

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