# Quantum mechanics, Molecular modeling by MD simulation, Characterization (SEM/EDXS/UV-Visible), Thermodynamic and Electrochemical studies of the inhibitory power of two quinoline derivatives for C38 in aggressive area.

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The present paper aims to validate the power inhibition of the two new organic compounds of the Quinoline family [DEMQ] and [HBMQ] against the dissolution of C38 steel in HCl electrolyte. Gravimetric, ac impedance, potentiodynamic polarization measurements (PDP) and surface morphology analyze by scanning electron microscopy with energy dispersive spectroscopy (SEM/EDS) were coupled to establish inhibition performance. Then, quantum mechanics methods like Density Functional Theory (DFT) and Molecular Dynamic Simulation (MD) were used to demonstrate the adsorption process of inhibitory molecules. Based on EIS results, the investigated derivatives effectively inhibit the degradation of C38 steel over the entire concentration range with a maximum efficiency of 97,9 % and 95,8 % for [DEMQ] and [HBMQ], respectively at 10-3 M. In addition, the PDP studies revealed that [HBMQ] and [CBMQ] compounds acted according to a mixed-type mechanism. Moreover, the adsorption mechanism follows the Langmuir isotherm model. The quantum theoretical study by DFT and MD confirmed the experimental results.

**Keywords:** Corrosion, quantum mechanics, carbone steel, quinoline, EIS, molecular dynamics, PDP, gravimetric, DFT.

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