

4th International Webinar on Materials Chemistry

October 21, 2021 | Webinar

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

Hicham Fakhry

Ibn Tofail University, Morocco

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 Hydrochloric Acid (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 Discrete Fourier Transform (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 potentiodynamic polarization (PDP) studies revealed that [DEMQ] and [CBMQ] compounds acted according to a mixed-type mechanism. Moreover, the adsorption mechanism follows the Langmuir isotherm model. The quantum theoretical study confirmed the experimental results.

Biography

Hicham Fakhry is a PhD candidate at Ibn Tofail University in Laboratory of Separation Processes, and Laboratory of Materials, Nanotechnology and Environment, Faculty of Sciences, Mohammed V University (Rabat Agdal).

fakhryh34@gmail.com