Ab Initio investigation of chemically modified Carbon Nanocones via aryldiazonium salts as a promising mild steel corrosion inhibitors

Avni Berisha
Fetah Podvorica
Arianit Reka
Makfire Sadiku
Kledi Xhaxhiu
Ramë Vataj
University of Prishtina "Hasan Prishtina", Prishtinë, Kosovë
avni.berisha@uni-pr.edu

Corrosion products are produced when industrial metals, such as iron, interact with an aggressive environment containing corrosive species such as chloride ions and oxygen, hence lowering the lifespan of the materials. Diverse vital industries [automotive, structural engineering, aerospace, oil and gas (energy), etc.] sustain significant corrosion-related losses. Corrosion inhibitors continue to be the simplest and most effective method for controlling the scale of this process [1-3].

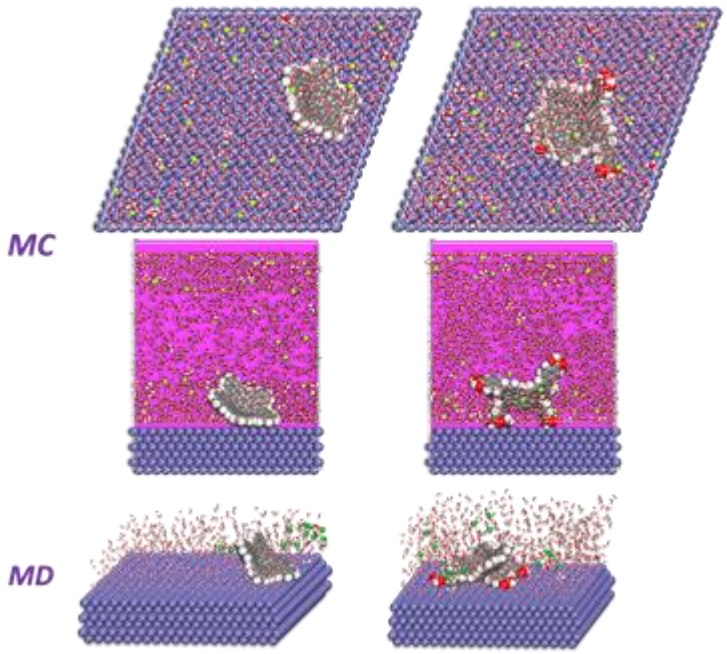

Figure 1: MC and MD poses of the lowest adsorption configurations for the Carbon Nanocones (CNCs) inhibitors in the simulated corrosion media on the iron surface under Periodic Boundary Condition (PBC) model.

Carbon Nanocones (bare and grafted by caboxyphenyl groups) were examined as corrosion inhibitors for mild steel in hydrochloric acid-containing aqueous corrosion medium in an effort to uncover new untapped potential inhibitors. The adsorption of Carbon Nanocones onto the Fe (1 1 0) surface was examined using Density Functional Theory (DFT), Monte Carlo simulation (MC), and Molecular Dynamics simulation (MD). On a molecular level, the obtained results revealed the adsorption capacity, geometry, and adsorption energies of Nanocones on the Fe(1 1 0) interface.

References

[1] A. Berisha. Computational and Theoretical Chemistry, 1201, 113258, (2021)
[2] V. Mehmeti, A. Berisha. Frontiers in Chemistry, 5, 61, (2017)
[3] A. Berisha. Electrochem, 3, 28-41, (2022)