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Mohammad Ramezanzadeh, Zahra Sanaei, Ghasem Bahlakeh, Bahram Ramezanzadeh



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Highly effective inhibition of mild steel corrosion in 3.5% NaCl solution by green Nettle leaves extract and synergistic effect of eco-friendly cerium nitrate additive: Experimental, MD simulation and QM investigations

Mohammad Ramezanzadeh^a, Zahra Sanaei^a, Ghasem Bahlakeh^{b*1}, Bahram Ramezanzadeh^{a**2}

^a Department of Surface Coatings and Corrosion, Institute for Color Science and Technology, P.O. Box 16765-654, Tehran, Iran

^b Department of Engineering and Technology, Golestan University, Aliabad Katool, Iran

Abstract: The synergistic effects of eco-friendly cerium nitrate additive on the corrosion inhibition performance of green Nettle leaves extract were investigated on mild steel in 3.5% NaCl solution by electrochemical, surface characterization and theoretical molecular dynamics (MD) simulations and quantum mechanics (QM) methods. The effect of Nettle leaves extract: cerium nitrate ratio on the mild steel corrosion inhibition was studied. The electrochemical impedance spectroscopy (EIS) and polarization tests were applied to examine the corrosion inhibition properties. In addition, the adsorption process and the synergistic effects between Nettle leaves extract and cerium cations were theoretically evaluated by using MD simulations and QM computations based on density functional theory (DFT) approach. Surface characterization techniques namely field-emission scanning electron microscopy (FE-SEM),

To whom correspondence should be addressed:

^{1*}Dr. Ghasem Bahlakeh: Tel.: +981734266235; Fax, +981734266235; e-mail, Gh.Bahlakeh@gu.ac.ir, Ghasem.bahlakeh@gmail.com

^{2**}Dr. Bahram Ramezanzadeh: Tel.: 2122969771, e-mail, ramezanzadeh-bh@icrc.ac.ir, ramezanzadeh@aut.ac.ir.

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