

Accepted Manuscript

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PII: S0167-7322(18)30091-6
DOI: doi:[10.1016/j.molliq.2018.03.045](https://doi.org/10.1016/j.molliq.2018.03.045)
Reference: MOLLIQ 8819
To appear in: *Journal of Molecular Liquids*
Received date: 6 January 2018
Revised date: 19 February 2018
Accepted date: 11 March 2018

Please cite this article as: Chandrabhan Verma, H. Lgaz, D.K. Verma, Eno E. Ebenso, I. Bahadur, M.A. Quraishi , Molecular dynamics and Monte Carlo simulations as powerful tools for study of interfacial adsorption behavior of corrosion inhibitors in aqueous phase: A review. The address for the corresponding author was captured as affiliation for all authors. Please check if appropriate. Molliq(2017), doi:[10.1016/j.molliq.2018.03.045](https://doi.org/10.1016/j.molliq.2018.03.045)

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Molecular dynamics and Monte Carlo simulations as powerful tools for study of interfacial adsorption behavior of corrosion inhibitors in aqueous phase: A review

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Abstract

The study of adsorption mechanism of corrosion inhibitors at the metal and electrolyte interfaces is the most important aspect of metallic corrosion inhibition in aqueous media. Recently, computational modeling particularly DFT based quantum chemical calculation, molecular dynamics (MD) and Monte Carlo (MC) simulations have emerged as relatively new and greener pathways to study the adsorption behavior of aqueous phase corrosion inhibitors for the scientists working in the field of corrosion science and engineering. The greenness of these computational techniques is based on the fact that these do not require use or discharge of any environmentally malignant chemicals into the surrounding environment unlike to the experimental techniques. Moreover, MD and MC simulations provide useful information regarding orientation and adsorption behavior of corrosion inhibitor on the metal-electrolyte

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