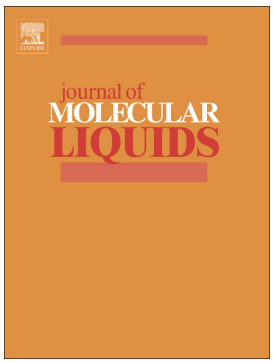

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Molecular dynamics and Monte Carlo simulations as powerful tools for study of interfacial adsorption behavior of corrosion inhibitors in aqueous phase: A review

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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 immerged 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