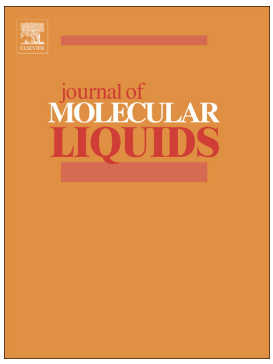


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# Experimental, Density functional theory and molecular dynamics supported adsorption behaviour of environmental benign imidazolium based ionic liquids on mild steel surface in acidic medium

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## Abstract:

This study describes the adsorption behavior of three 1-butyl-3-methyl-imidazolium ionic liquids namely, 1-butyl-3-methylimidazolium chloride ([bmim][Cl]), 1-butyl-3-methylimidazolium acetate ([bmim][Ac]) and 1-butyl-3-methylimidazolium trifluoromethanesulphonate ([bmim][$CF_3SO_3$]) at mild steel/1 M HCl interface using experimental and computational studies. Electrochemical and gravimetric measurements revealed that the inhibition efficiency of the studied ionic liquids increases with increase in concentrations, such that [bmim][Cl], ([bmim][$CF_3SO_3$] and [bmim][Ac] gave the maximum inhibition efficiencies of 93.18%, 96.02% and 97.15%, respectively at a concentration as low as $8.67\times10^{-4}$ molL$^{-1}$. The studied ionic liquids act as interfacial corrosion inhibitors and their adsorption at mild steel/electrolyte interface obeyed the Temkin adsorption isotherm. Polarization study suggested that the ionic liquids are mixed-type corrosion inhibitors. SEM and AFM analyses were undertaken to support the adsorption of the ionic liquid molecules on mild steel surface in 1 M HCl solution. Orientation and adsorption mode of 1-butyl- 3-methyl-imidazolium molecules on mild steel surface was investigated using molecular dynamic (MD) simulations, which revealed that 1-butyl-3-methyl-imidazolium molecules adsorb on mild steel surface in flat orientations. Quantum chemical parameters for the neutral and protonated forms of the ionic liquids as well as the binding energies and radial distribution function indices obtained from molecular dynamic simulations corroborate the experimental results.