Density functional theory and molecular dynamics simulation studies of bio-based fatty hydrazide-corrosion inhibitors on Fe (1 1 0) in acidic media

ABSTRACT

Corrosion of metal pipelines is a huge industrial concern, with potential environmental pollution and economic loss. The implementation of a cost-effective technology in using waste palm oil as biobased corrosion inhibitors (CIs) has risen. However, the inhibition mechanism of CIs remains unclear due to the lack of comprehensive review and a small number of existing experimental data. Density functional theory (DFT) and molecular dynamics (MD) simulation provided significant insights into the adsorption mechanism. The influence of fatty hydrazide derivatives as effective CIs on ferrous (1 1 0) metal surface in 1.0 M HCl medium at a temperature ranging from 298 to 383 K was studied. DFT predicted inhibition efficacies of these CIs based on electronic/molecular properties and reactivity induced through the band gap energy between the HOMO and LUMO in the range of 7.290 to 7.480 eV. Results from MD simulation showed that the inhibition efficiency increased at low concentration of CIs (0.04 M) and increasing temperature, which was suggestive of chemical adsorption mechanism with the adsorption energy from −200 to −400 kJ/mol. . The result further suggested that thermal stability of CIs at high temperature increased due to adsorption energy of CI-metal interaction from heat supplied. All the findings were consistent with the experimental data reported earlier. Understanding the adsorption mechanism of fatty hydrazide derivatives on the metal surface could be used as a basis for future development of specific biobased CIs for cost-effective corrosion control technology.

Keyword: Corrosion inhibitor; Molecular dynamics; Adsorption; Inhibition efficiency; Fatty hydrazide