Towards a Deeper Understanding of the Anticorrosive Properties of Hydrazine Derivatives in Acid Medium: Experimental, DFT and MD Simulation Assessment

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Abstract

The corrosion inhibition properties of two compounds namely, 1,2-dibenzylidenehydrazine (C1) and 1,2-bis(1-phenylethylidene)hydrazine (C2) for mild steel (MS) in 1.0 M HCl were studied by using weight loss, electrochemical techniques, density functional theory (DFT), and molecular dynamic (MD) simulations. Experimental results show that both C1 and C2 behave as mixed-type inhibitors. Both inhibitors showed efficient binding with metal surface. With C1 exhibiting the highest inhibition efficiency, resulting in low double layer capacitance and a high polarization resistance. The mechanism of inhibition action of the studied compounds was discussed in the light of the DFT and MD simulations studies. MD simulation revealed a nearly flat configuration for the C1 molecule on the metal surface, with more negative interaction energy in comparison to C2. Theoretical results are in line with the experimental results.

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Electronic supplementary material

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Notes

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Conflict of interest

The authors declare that they have no conflict of interest.

Supplementary material

11661_2018_4828_MOESM1_ESM.docx (154 kb)
Supplementary material 1 (DOCX 153 kb)

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