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A Density Functional Theory Computational Study on the Inhibiting Action of Some Derivatives of 1,8-Bis(Benzylideneamino)Naphthalene against Aluminum Corrosion

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Abstract : The inhibiting action against aluminum corrosion by three derivatives of 1,8-bis (benzylideneamino) naphthalene (BN) Schiff base has been investigated by means of DFT quantum chemical calculations at the B3LYP/6-31G(d) level of theory. The derivatives (CBN, NBN and MBN) were prepared from the condensation reaction of 1,8-diaminonaphthalene with substituted benzaldehyde (4-CN, 3-NO_2 and 3,4-$(OMe)_2$, respectively). Calculations were conducted to study the adsorption of each Schiff base on aluminum surface to evaluate its potential as a corrosion inhibitor. The computational structural features and electronic properties of each derivative such as relative energies and energies of the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) have been reported. Thermodynamic functions and quantum chemical parameters such as the hardness of the inhibitor, the softness and the electrophilicity index were calculated to determine the derivative of the highest inhibition efficiency.

Keywords : corrosion, aluminum, DFT calculation, 1,8-diaminonaphthalene, benzaldehyde
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