**Performance evaluation and assessment of the corrosion inhibition mechanism of carbon steel in HCl medium by a new hydrazone compound: Insights from experimental, DFT and first-principles DFT simulations**

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**I. Density functional theory details**

The Dmol3 program in Material Studio Software was used to optimize the geometry of the hydrazone molecule according to the generalized gradient approximation (GGA) with the Perdew-Burke-Enzerhof (PBE) functional (Weston et al., 2012). The Conductor-like Screening Model (COSMO) was used to simulate the effect of water as a solvent during the calculations (Heidari et al., 2021). Based on the energies of the highest occupied molecular orbital (EHOMO) and the lowest unoccupied molecular orbital (ELUMO), the reactivity and electronic properties of the studied molecule were determined by calculating the quantum chemical parameters using the following equations (Dagdag et al., 2020):

$ΔE=E\_{LUMO}-E\_{HOMO}$ (S1)

$IE=-E\_{HOMO}$ (S2)

$EA=-E\_{LUMO}$ (S3)

$ŋ=\frac{IE-EA}{2}$ (S4)

$σ=\frac{1}{ŋ}$ (S5)

$χ=\frac{IE+EA}{2}$ (S6)

$μ=\frac{-(IE+EA)}{2}$ (S7)

Local reactivity indices were used to examine the reactivity of each atom in HTH molecule. To this end, the Fukui indices were analyzed and calculated using the following equations (Fukui, 1982):

$f\_{k}^{+}=q\_{k}\left(N+1\right)-q\_{k}(N)$ (S8)

$f\_{k}^{-}=q\_{k}\left(N\right)-q\_{k}(N-1)$ (S9)

where, qk (N+1), qk (N), and qk (N-1) are the electron densities on atom k corresponding to N+1, N and N-1 electrons systems, respectively.