**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**

M. En-Nylly1, S. Skal2, Y. El aoufir3, H. Lgaz4,\*, Raihana J. Adnin5, Awad A. Alrashdi6, A. Bellaouchou2, M. R. Al-Hadeethi7, O. Benali1, T. Guedira1, H-S. Lee8,\*, S. Kaya9, S. M. Ibrahim10

1 Laboratory of Organic Chemistry, Inorganic, Electrochemistry, and Environment, Faculty of Science, University Ibn Tofail, B.P 133, 1400 Kenitra, Morocco;

2 Laboratoire des Matériaux Nanotechnologie et Environnement, Université Mohamed V Agdal. Faculté des Sciences. Av. Ibn Battouta. BP 1014, Rabat. Morocco;

3 Laboratory of Organic Chemistry, Inorganic, Electrochemistry, and Environment, Faculty of Science, University Ibn Tofail, B.P 133, 1400 Kenitra, Morocco;

4 Innovative Durable Building and Infrastructure Research Center, Center for Creative Convergence Education, Hanyang University ERICA, 55 Hanyangdaehak-ro, Sangnok-gu, Ansan-si, Gyeonggi-do, 15588, Korea;

5Department of Smart City Engineering, Hanyang University-ERICA, 55 Hanyangdaehak-ro, Sangnok-gu, Ansan-si, Gyeonggi-do 15588, Republic of Korea;

6Chemistry Department, Umm Al-Qura University, Al-Qunfudah University College, Saudi Arabia

7Department of Chemistry, College of Education, University of Kirkuk, Kirkuk 36001, Iraq;

8Department of Architectural Engineering, Hanyang University-ERICA, 55 Hanyangdaehak-ro, Sangnok-gu, Ansan-si, Gyeonggi-do 15588, Republic of Korea;

9Sivas Cumhuriyet University, Health Services Vocational School, Department of Pharmacy, 58140, Sivas, Turkey

10Department of Biochemistry, College of Science, King Saud University, P.O. Box 2455, Riyadh 11451, Saudi Arabia

\*Correspondence: [hlgaz@hanyang.ac.kr](mailto:hlgaz@hanyang.ac.kr) (H.L.) [ercleehs@hanyang.ac.kr](mailto:ercleehs@hanyang.ac.kr) (H-S. L.)

**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):

(S1)

(S2)

(S3)

(S4)

(S5)

(S6)

(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):

(S8)

(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.