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Title: **Theoretical investigation of the inhibition of corrosion by some triazole Schiff bases**

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Published in: Materials and Corrosion

Impact Factor: 1.4

Abstract:

An examination of quantum chemical and corrosion inhibition studies is carried out to investigate whether any clear links exist between the results of quantum chemical calculations and the experimental inhibition efficiencies.The influence of the investigated triazole Schiff bases, (benzylidine amino) triazole (a), 4-hydroxy 3-(benzylidine amino) triazole (b), 2-hydroxy 3-(benzylidine amino) triazole (c), and 2- hydroxy 3-(naphthylidine amino) triazole (d) on the inhibition of corrosion of the metal surfaces are studied by density functional theory at the B3LYP/6-31G level. The calculated quantum chemical parameters correlated to the inhibition efficiency are, the highest occupied molecular orbital (HOMO), the lowest unoccupied molecular orbital (LUMO), the separation energy (DE), the dipole moment (m), the softness (s), the total negative charge on the whole molecule (TNC), the total charge on the azo-methine moiety, the molecular volume (Vi), and the total energy (TE). A good correlation between the quantum chemical parameters and the experimental inhibition efficiency is found. High inhibition efficiency for corrosion inhibitors can be achieved by controlling their electronic and structural properties.