Electrochemical, DFT and Mont Carlo Simulations Studies to Evaluate the Inhibition Effect of Novel Pyridazine Derivatives on Iron Pitting Corrosion in 3.5 % NaCl

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(6-Phenyl-pyridazin-3-ylsulfanyl)-acetic acid ethyl ester (PPS-A) and 4-(6-Phenyl-pyridazin-3-ylsulfanyl)-butyric acid ethyl ester (PPS-B) are synthesized and characterized as novel *S*-alkylated pyridazine derivatives with different side chain lengths. The effect of *S*-alkylated side chain lengths in PPS-A and PPS-B is investigated for their protective mechanism towards iron pitting corrosion in 3.5 % NaCl and compared to their parent pyridazine (PPS) using electrochemical measurements and theoretical calculations. It is found that, the studied pyridazine derivatives shift both the corrosion potential and the pitting potential of iron to more noble values. Furthermore, the mechanism of the inhibition is correlated to the presence of the *S*-alkylated side chain in PPS-A and PPS-B compared to PPS, as well as to its different lengths between PPS-A and PPS-B. Moreover, the structure of Fe/electrolyte interface in case of PPS-B behaves as more ideal capacitive rather than that in case of PPS-A, due to the adsorption of insulating barrier layers on Fe/electrolyte interface. The best fit adsorption isotherm is found to be Langmuir adsorption isotherm with physical nature. DFT calculations show that, the charge density around the adsorption active sites increase as the *S*-alkylated side chain became more length. The adsorption behaviour of the studied pyridazine derivatives is simulated using Mont Carlo molecular dynamics that agree well with the experimental data.

Keywords: Pyridazine derivatives, Iron, Pitting corrosion, EIS, Mont Carlo simulations

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