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Design of novel imidazole-based corrosion inhibitors - molecular dynamics simulations and electrochemical studies

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Obtaining a detailed insight into the mechanism of the protective action of various organic corrosion inhibitors on mild steel corrosion has remained an active area of research over the years. The use of computational chemistry as a tool in this aspect have greatly enhanced the prediction of the inhibition efficiencies of these inhibitors based on their electronic and molecular properties and reactivity indices, which are subsequently validated by experimental measurements. In the present study, we investigated the corrosion inhibition efficiency of mild steel in 1.0 M HCl of the following compounds; imidazole (Imz), 2-bromo-1H-imidazole (2-Br-Imz), 2-chloro-1H-imidazole (2-Cl-Imz), 2-iodo-1H-imidazole (2-I-Imz) and 4-phenyl imidazole (4-Ph-Imz). Density functional theory (DFT) calculations showed that the inhibitor molecules dissociate to form a network of protective film on the iron surface. The equilibrium adsorption energies obtained from DFT calculations decreases in the order 2-I-Imz>4-Ph-Imz>2-Br-Imz>Imz>2-Cl-Imz. Electrochemical studies of the two extreme cases showed that 2-I-Imz exhibited the best inhibition efficiency of 82.95% at 10 mM concentration acting as anodic-type inhibitor while 2-Cl-Imz exhibited an efficiency of 50.70% at the same concentration acting as cathodic-type inhibitor. Both inhibitors were found to fit the Langmuir adsorption isotherm with Gibbs free energy of adsorptions -27.34 KJ/mol and -25.24 KJ/mol at 25°C for 2-I-Imz and 2-Cl-Imz respectively. SEM of the steel samples after immersion in the inhibitors for 24 h revealed a significant formation of pits on the 2-Cl-Imz sample possibly due to chloride attack, and the absence of such in the 2-I-Imz sample indicating its ability to form a protective film. XPS analysis confirmed the adsorption of the inhibitor molecules on the metal surface from the functional group analysis of the peaks obtained. AFM analysis showed a decrease in surface roughness of the 2-I-Imz sample as compared to the 2-Cl-Imz, indicative of a better adsorption and consequent inhibition efficiency observed of both inhibitor molecules.

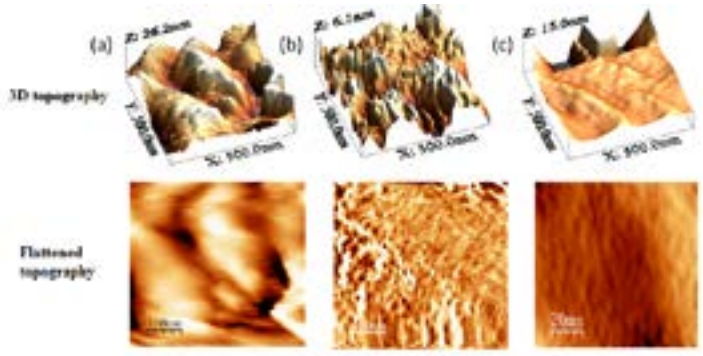

Figure 1: AFM images of (a) bare steel and after treatment with (b) 2-Cl-Imz and (c) 2-I-Imz.

Biography

Richard M W Wong received his PhD. degree from Australian National University (1989). Subsequently, he held Post-doctoral position at IBM Kingston and Yale University. In 1992, he took up an Australian Research Fellowship, hosted in University of Queensland. He joined the National University of Singapore in 1997 and is currently a Full Professor and Head of Department. He was the recipient of Fukui Award recently for his outstanding work in theoretical and computational chemistry. He has published about 200 scientific publications, which received over 9000 citations and H-index of 42. His research interests include application of computational quantum chemistry to a range of chemical problems, reactive intermediates, catalysis, materials design, chemical sensors, weak intermolecular interactions and drug design.

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