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Insight of development of two cured epoxy polymer composite coatings as highly protective efficiency for carbon steel in sodium chloride solution: DFT, RDF, FFV and MD approaches

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ABSTRACT

Cured epoxy polymers namely 3.3′-(phenylazanediyl) bis(1-((6-aminohexyl)amino)propan-2-ol) (EP/AlA) and 3.3′-(phenylazanediyl) bis(1-((4-(4-aminobenzyl)phenyl)amino)propan-2-ol) (EP/ArA) were used as potential protection coatings for carbon steel (CS) in 3.5% NaCl solution. The protection coatings of EP/AlA and EP/ArA on CS were investigated through, electrochemical impedance spectroscopy (EIS), potentiodynamic polarization curves (PC), atomic force microscope (AFM), scaning electron microscopy (SEM), contact angle (CA), natural bond orbitals (NBO), frontier molecular orbitals (FMO), fractional free volume (FFV), radial distribution function (RDF) and molecular dynamics (MD) simulations. PC and EIS data indicated that the two cured epoxy polymers investigated have excellent protective efficiencies. Further, protective efficiencies of EP/ArA (92 and 94.6% for EIS and PC, respectively) are higher than that of EP/AlA (86.3 and 88.7% for EIS and PC, respectively) in 3.5 %NaCl solution. SEM and AFM results displayed the protective layer formed on CS coated through EP/AlA and EP/ArA could be stopped the chloride ions attack. Also, the quantum chemical analyzes of cured epoxy polymers EP/A1A and EP/ArA were employed at DFT/B3LYP/6-31G(d,p) level to appraise the reactivity behaviors and possible regions via using the FMO and NBO methods. The results disclosed that the dominant interactions for both molecules were determined as the resonance ($n \rightarrow \Pi^*$ and $\Pi \rightarrow \Pi^*$) interactions. FFV value of EP/ArA film (20.22%) is lower than compared to EP/AlA (28.02%), due to the most condensed film by the EP/ArA on CS surface. Experimental results combined with theoretical approaches were used to investigate the proction coatings.

1. Introduction

Cured epoxy polymer derivatives containing different functional groups such as carbamide ($(RR'N)_2$-C = O), anhydride (–COOOC-), amide (–$CONH_2$), ester (-CO_2R), cyanide (–CN), sulphur dioxide (SO_2), hydroxy (–OH), nitro (–NO_2), alkoxy (-OR), amino (–NH_2), thiol (-SH),… and possess heteroatoms namely nitrogen, oxygen, sulfur and phosphorus are the most utilized as excellent cured epoxy polymer coatings for carbon steel in varying aggressive solution (HCl, H_2SO_4, HNO_3, H_3PO_4, NaCl) [1–8]. The charge donation of cured epoxy polymer derivatives having double bond of aromatic rings, free pair electrons presents in the functional heteroatoms (N, O, S and P) into the d orbital to the metallic substrates leads to the chemical adsorption of cured epoxy polymer coatings on substrates surface [9–11]. In presence of the strong corrosive solution namely HCl, H_2SO_4, HNO_3, H_3PO_4, NaCl,… the electrostatic interaction between cured epoxy polymers and CS area give the

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