10th INTERNATIONAL CONFERENCE ON COMPUTATIONAL AND EXPERIMENTAL SCIENCE AND ENGINEERING (ICCESEN-2023)

2023

Experimental and theoretical studies on the anticorrosion performance of co-polymeric coatings on X70 steel in 3.5% NaCl

Mustapha DJAMA, Lynda BENHADDAD, Brahim IDIR, Imene LADRAA, Chahinez BOUZID

Abstract : Polymeric coatings are used to protect metallic surfaces from corrosion in a marine environment. The novelty of this research lies in the combination of two conductive polymers, namely Polypyrrole (PPy) and Ortho-toluidine (OT), which were tested for their corrosion resistance on steel in a chloride medium. The polymers were synthesized electrochemically using the galvanostatic mode. The corrosion properties were studied using electrochemical methods such as the evolution of open-circuit potential over time and polarization curves. The purpose of this research is to enhance the protective capabilities of polymeric coatings by combining these two polymers. Initially, layers of PPy and OT were deposited on X70 carbon steel. The focus was on optimizing single layers of PPy alone before enhancing the coatings with PPy/OT bilayers. The results indicate that the application of PPy and OT copolymerization could significantly improve the corrosion resistance of tool steel structures. To understand the mechanism involved in electrodeposition, it was deemed useful to use quantum calculations based primarily on the density functional theory (DFT). This study highlights the relationship between the structural arrangement, electronic structure, and inhibitory activity of different compounds through a number of quantum descriptors such as the highest occupied molecular orbital/lowest unoccupied molecular orbital (HOMO/LUMO) energy, the ?E gap, and the dipole moment ? of the surface coating. The results of the DFT calculations obtained are in fairly good agreement with experimental data.

Keywords : Copolymer coating, corrosion resistance, X70 steel, DFT