Understanding Corrosion Protection Behavior of Polyaniline Graphene Nanocomposite Coatings Using Quantum Chemical Calculations

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Theoretical calculations based on density functional theory (DFT) have been carried out to correlate the experimentally observed anticorrosion properties of polyaniline-graphene nanocomposite coating. The nanocomposites were synthesized via in-situ polymerization of aniline monomers on graphene nanoflakes suspended in 1N HCl solution. During corrosion, the polyaniline undergoes various degrees of redox reactions and its conformation changes. Graphene being impermeable to hydronium ions prohibits reduction of polymer chains. To investigate the behavior of the nanocomposite coatings, frontier molecular orbital energy EHOMO (Energy of highest occupied molecular energy), ELUMO (Energy of lowest unoccupied molecular energy), the energy gap, (ΔE) and mutual orbital 'interaction between additive molecules and metal surface ($\Delta E1$ and $\Delta E2$) have been calculated and correlated with the experimental results. Quantum chemical calculations show that graphene addition to polyaniline polymer chain form a network like structure that protects the surface in acidic environment and are in good agreement with the experimental results.