## **Evaluation of Chitin Filled Epoxy Coating for Corrosion Protection of Q235** Steel in Saline Environment

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Abstract : Interest in the development of eco-friendly anti-corrosion coatings using bio-based renewable materials is gaining momentum recently. To this effect, chitin biopolymer, which is non-toxic, biodegradable, and inherently possesses antimicrobial property, was successfully synthesized from snail shells and used as a filler in the preparation of epoxy coating. The chitin particles were characterized with contact angle goniometer, scanning electron microscope (SEM), Fourier transform infrared (FTIR) spectrophotometer, and X-ray diffractometer (XRD). The performance of the coatings was evaluated by immersion and electrochemical impedance spectroscopy (EIS) tests. Electronic structure properties of the coating ingredients and molecular level interaction of the corrodent and coated Q235 steel were appraised by quantum chemical computations (QCC) and molecular dynamics (MD) simulation techniques, respectively. The water contact angle (WCA) measurement of chitin particles was found to be 129.30 while that of chitin particles modified with amino trimethoxy silane (ATMS) was 149.60, suggesting it is highly hydrophobic. Immersion and EIS analyses revealed that epoxy coating containing silane-modified chitin exhibited lowest water absorption and highest barrier as well as anti-corrosion performances. The QCC showed that quantum parameters for the coating containing silane-modified chitin are optimum and therefore corresponds to high corrosion protection. The high negative value of adsorption energies (Eads) for the coating containing silane-modified chitin indicates the coating molecules interacted and adsorbed strongly on the steel surface. The observed results have shown that silane-modified epoxy-chitin coating would perform satisfactorily for surface protection of metal structures in saline environment. Keywords: chitin, EIS, epoxy coating, hydrophobic, molecular dynamics simulation, quantum chemical computation

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