Eclética Química Journal

Editorial

The Eclética Química Journal's team proudly announces the third issue of vol. 47 of 2022nd year desiring to all a continue and fruitful scientific research. The first article focuses on the impact of the sulfur vacancies on the photocatalytic response of the ZnS nanocrystals synthesized by solvothermal method varying the concentration of the precursors zinc acetate and thiourea. The obtained products have hexagonal structure with different degrees of crystallinity and a comparison of experimental results and theoretical calculations revealed the formation of intermediate levels inside the bandgap due to structural polarization. The bandgap engineering has a significant impact on the photocatalytic response of these samples and the mechanism investigation confirmed the formation of the reactive oxygen species, usually responsible for methylene blue dye degradation. Sequentially, an electroanalytical method based on differential pulse voltammetry with glassy carbon electrode is described for analysis of doxorubicin (DOX), an anthracycline antibiotics widely used in the clinical treatment of cancer patients. It was performed the DOX stability after reconstitution and determined the correct time for safe administration to patients in hospitals, allowing application in the drug quality control with low-cost methodology and with similar results to those obtained using high-performance liquid chromatography analysis of pharmaceutical samples containing DOX. Follows an experimental and theoretical study of a pure commercial sample of dichlorodiphenyltrichloroethane (DDT) and its application for molecular docking against human estrogen receptor alpha is presented. The DDT molecule was experimentally characterized by means of FT-IR and GC-MS and the results compared to those obtained from theoretical molecular calculations. According to molecular docking investigation, the only interaction found in the complex after docking was steric interaction and the most reactive sites in the compound and its overall reactivity were identified. Closes this issue a case study of 2101 duplex stainless steel tank applying a portable electrochemical microcell system for *on-site* weld inspection and corrosion monitoring from the manufacturing until 12 months of operation. The double loop electrochemical potentiokinetic reactivation technique was used to evaluate the sensitization degree on the welded regions during the tank manufacturing and a passivation treatment was applied to improve the passivation level, confirmed by on-site cyclic polarization tests. After 12 months of operation the passivation level decreased, new passivation treatment was applied and evaluated. Final, an acceptance criterion to passivation level was proposed.

The Editor and members of Editorial Board of Eclética Química Journal want to thank the great effort developed by the Authors and Reviewers making possible this publication.

Assis Vicente Benedetti Editor-in-Chief of EQJ