

عنوان مقاله:

Removal of Methylene Blue from Aqueous Solution using Nano Metal Oxide Prepared from Local Nigerian Hen Egg Shell: DFT And Experimental Study

محل انتشار:

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خلاصه مقاله:

Adsorption capacity of nano metal oxide synthesized from waste hen egg shell for the removal of methylene blue dye from aqueous solution was investigated using batch and density function theory (DFT) process. The prepared egg shell nano particle (PESNP) were characterized using proximate X-ray fluorescence, Scanning electron microscopy, (SEM) and Thermogravimetric analysis. The results obtained indicated that PESNP is a good adsorbent for methylene blue. Their adsorption capacity was found to be influenced by initial dye concentration, adsorbent dose, pH, temperature and by the period of contact. The adsorption of the dye onto PESNG was found to be physical, spontaneous and best described by Freundlich and Temkin adsorption models. Adsorption kinetic study indicated that a pseudo second order kinetics is favoured. Result from the quantum chemical study indicated that the adsorption of .methylene blue onto PESNP will preferentially occur through the sulphonium sulphur, nitrogen and benzene ring

کلمات کلیدی:

Adsorption kinetics, DFT, Dye, Egg shell nanoparticles, Mechanism :

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