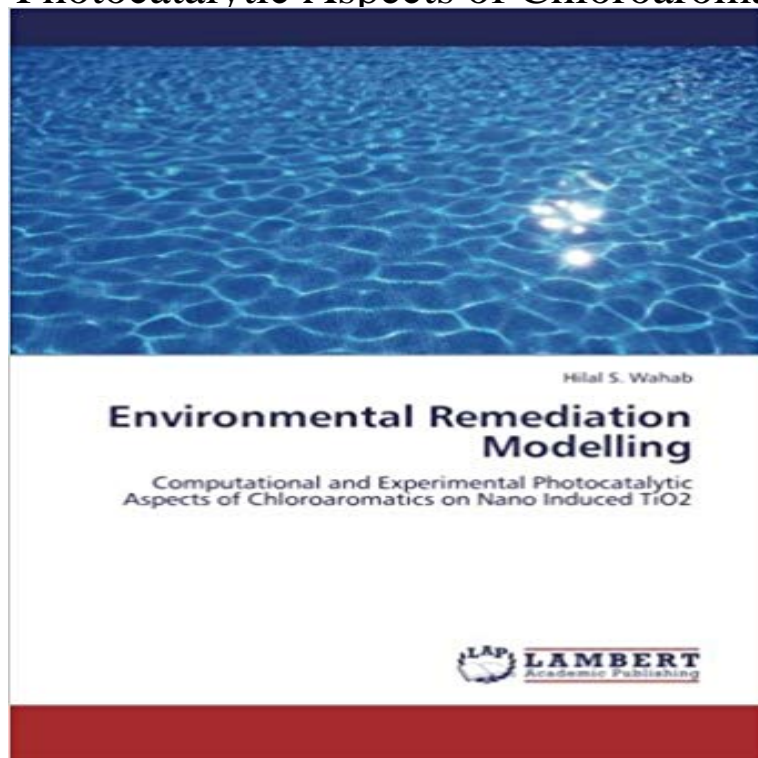


Environmental Remediation Modelling: Computational and Experimental Photocatalytic Aspects of Chloroaromatics on Nano Induced TiO₂



Chloroaromatics are widely distributed organic pollutants in the environment. These compounds are classified as high priority ecotoxicants due to their persistence, carcinogenicity and low biodegradability. It is known that the adsorption of the organic species is an important factor for the highly efficient decomposition process. And due to the clear relationship between the adsorbability of the chloroaromatic moieties and their photocatalytic detoxification, the book herein elucidates the computational and experimental mechanistic pathways for the adsorption and photocleavage of two common recalcitrant contaminants, chlorobenzene and 4-chlorophenol, onto the TiO₂ photocatalyst surface that has become the most attractive and commonly employed semiconductor over the last three decades. The key mechanism ring opening step, employing various oxygen species is still experimentally argumentative. A theoretical approach is therefore, strongly motivated for predicting the non-aromatic and acyclic intermediates. This book, accordingly, provides detailed mechanistic approaches and should be especially useful for theoreticians and applied scholars in environmental chemistry and engineering fields.

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