1. Record Nr. UNINA9910877098203321 Autore Shukla Sudheesh K Titolo Electrocatalytic Materials for Renewable Energy Pubbl/distr/stampa Newark:,: John Wiley & Sons, Incorporated,, 2024 ©2024 **ISBN** 1-119-90131-6 1-119-90130-8 Edizione [1st ed.] Descrizione fisica 1 online resource (419 pages) HussainChaudhery Mustansar Altri autori (Persone) PatraSantanu ChoudharyMeenakshi Soggetti Materials science Renewable energy sources Lingua di pubblicazione Inglese **Formato** Materiale a stampa Livello bibliografico Monografia Cover -- Title Page -- Copyright Page -- Contents -- Preface --Nota di contenuto Chapter 1 An Introduction to the Exploration of the Electronic Structure Properties of Biologically Active Natural Compounds Using Quantum Chemical Methods -- 1.1 Natural Compounds: Past, Present, and Future -- 1.2 Theoretical Framework for Quantum Chemical Calculations --1.2.1 Ab-Initio Methods --1.2.1.1 Hartree–Fock 1.2.1.2 Moller-Plesset (MP) Perturbation Theory --(HF) Theory --1.2.1.3 Configuration Interaction (CI) Method --1.2.1.4 Coupled Cluster Method (CCM) --1.2.2 Semiempirical Methods --Molecular Mechanics --1.2.4 Molecular Dynamics --Density Functional Theory (DFT) -- 1.3 Theoretical Framework for 1.3.1 Quantitative Structure-Activity Biological Activity --Relationship (QSAR) --1.3.2 Quantitative Structure-Property Relationship (QSPR) --1.3.3 Molecular Docking -- 1.4 Future Scope -- References -- Chapter 2 Facile Synthesis of Hybrid Fe3O4/ZnO Nanosphere Composites and Their Potential Applications in Dye-Sensitized Solar Cells -- 2.1 Introduction -- 2.2 Materials and 2.2.2 Photocatalyst Synthesis Methods --2.2.1 Materials --

Methods --

2.2.3 Prepared Sample Characterization -- 2.3 Results

## and Discussion

## Sommario/riassunto

This book, 'Materials for Renewable Energy,' edited by Sudheesh K. Shukla and others, explores advancements in materials science for renewable energy applications. It covers topics like the synthesis and application of nanomaterials, hybrid heat pipes, and metal oxide-based catalysts in renewable energy technologies. The book provides a comprehensive overview of the electronic properties of biologically active compounds using quantum chemical methods, as well as the role of conductive metal-organic frameworks (MOFs) in energy applications. It is intended for researchers and professionals in chemical engineering and environmental sciences, aiming to enhance the development of sustainable energy solutions.