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Fundamental Process Steps; 1.6 Photoelectrode Implementations; 1.6.1 Single-Junction Performance Limits; 1.6.2 Multijunction Performance Limits; 1.6.3 A Shining Example; 1.7 The PEC Challenge; 1.7.1 What's Needed, Really?; 1.7.2 Tradeoffs and Compromises 1.7.3 The Race with PV-Electrolysis 1.8 Facing the Challenge: Current PEC Materials Research; Acknowledgments; References; 2 Modeling and Simulation of Photocatalytic Reactions at TiO₂ Surfaces; 2.1 Importance of Theoretical Studies on TiO₂ Systems; 2.2 Doped TiO₂ Systems: Carbon and Niobium Doping; 2.2.1 First-Principle Calculations on TiO₂; 2.2.2 C-Doped TiO₂; 2.2.3 Nb-Doped TiO₂; 2.3 Surface Hydroxyl Groups and the Photoinduced Hydrophilicity of TiO₂; 2.3.1 Speculated Active Species on TiO₂ - Superoxide Anion (O₂⁻) and the Hydroxyl Radical (OH[•]) 2.3.2 Theoretical Calculations of TiO₂ Surfaces and Adsorbents 2.3.3 Surface Hydroxyl Groups and Photoinduced Hydrophilic Conversion; 2.4 Dye-Sensitized Solar Cells; 2.4.1 Conventional Sensitizers: Ruthenium Compounds and Organic Dyes; 2.4.2 Multiexciton Generation in Quantum Dots: A Novel Sensitizer for a DSSC; 2.4.3 Theoretical Estimation of the Decoherence Time between the Electronic States in PbSe QDs; 2.5 Future Directions: Ab Initio Simulations and the Local Excited States on TiO₂; 2.5.1 Improvement of the DFT Functional; 2.5.2 Molecular Mechanics and Ab Initio Molecular Dynamics 2.5.3 Description of Local Excited States 2.5.4 Nonadiabatic Behavior of a System and Interfacial Electron Transfer; Acknowledgments; References; 3 Photocatalytic Reactions on Model Single Crystal TiO₂ Surfaces; 3.1 TiO₂ Single-Crystal Surfaces; 3.2 Photoreactions Over Semiconductor Surfaces; 3.3 Ethanol Reactions Over TiO₂(110) Surface; 3.4 Photocatalysis and Structure Sensitivity; 3.5 Hydrogen Production from Ethanol Over Au/TiO₂ Catalysts; 3.6 Conclusions; References; 4 Fundamental Reactions on Rutile TiO₂(110) Model Photocatalysts Studied by High-Resolution Scanning Tunneling Microscopy 4.1 Introduction

Sommario/riassunto

More energy from the sun strikes Earth in an hour than is consumed by humans in an entire year. Efficiently harnessing solar power for sustainable generation of hydrogen requires low-cost, purpose-built, functional materials combined with inexpensive large-scale manufacturing methods. These issues are comprehensively addressed in *On Solar Hydrogen & Nanotechnology* - an authoritative, interdisciplinary source of fundamental and applied knowledge in all areas related to solar hydrogen. Written by leading experts, the book emphasizes state-of-the-art materials and characterization techniques.
