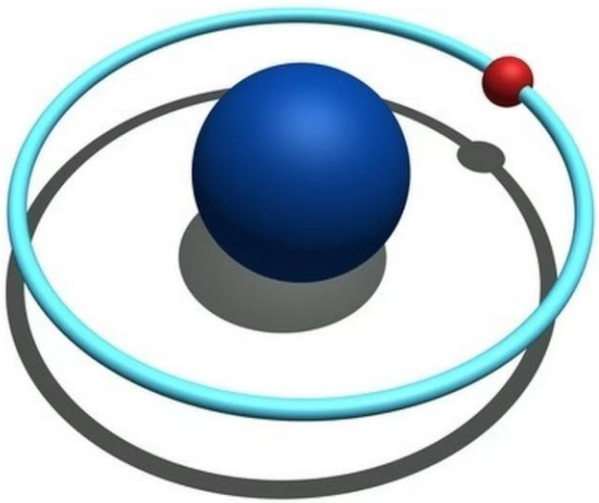
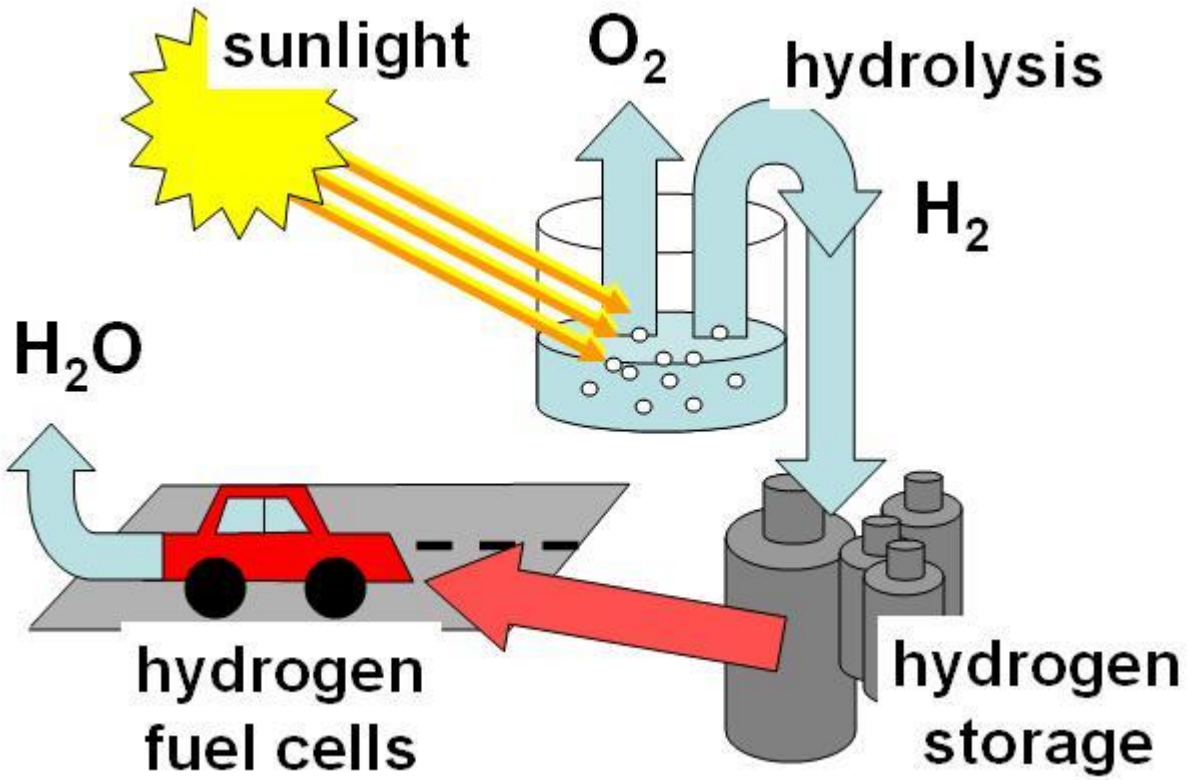
a discussion on

HYDROGEN PRODUCTION: PHOTOELECTROCHEMICAL WATER SPLITTING





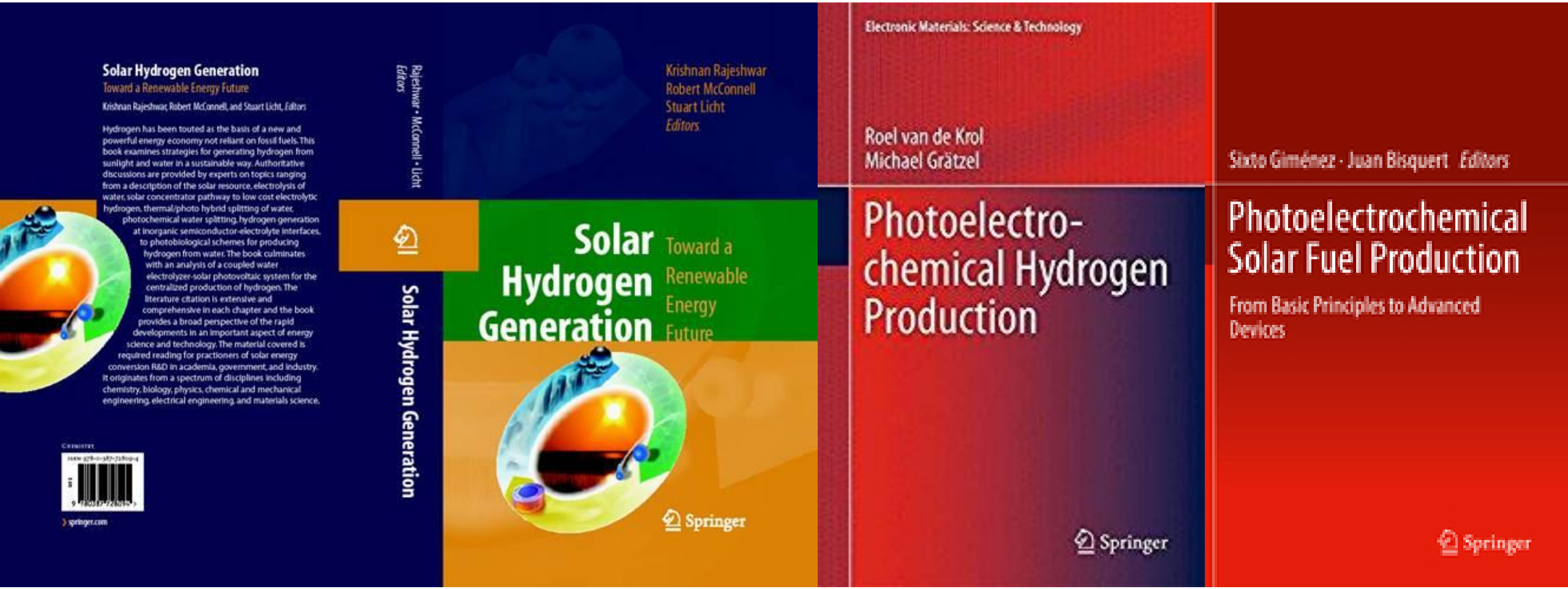
PURPOSE OF THE PRESENTATION

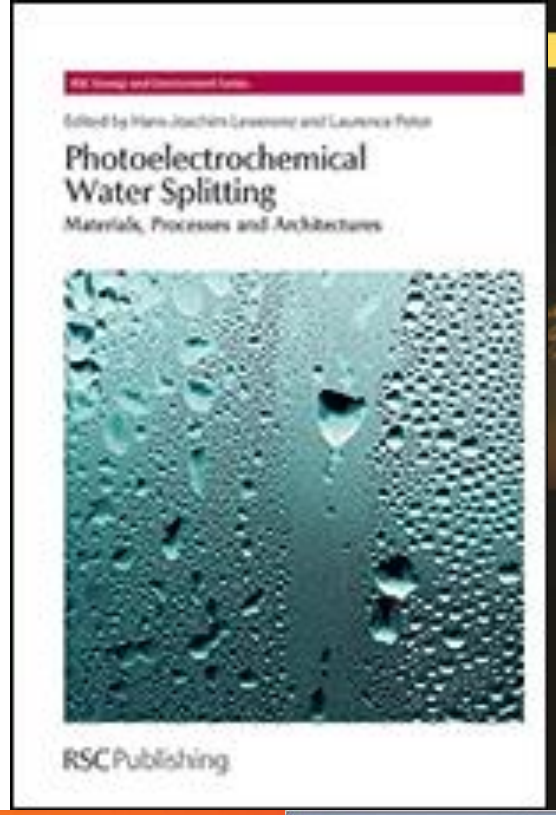
- **Solar Hydrogen Production**, Editors: Francesco Calise, Massimo Dentice d'Accadia, Massimo Santarelli, Andrea Lanzini, Domenico Ferrero, Elsevier 2018.
- Proposed to covers the all aspects of solar hydrogen from lab to business.
- Photoelectrochemical Hydrogen Production
- A discussion on the table of content of the book chapter.
- What new we need to discuss in this chapter apart from the massive literature.

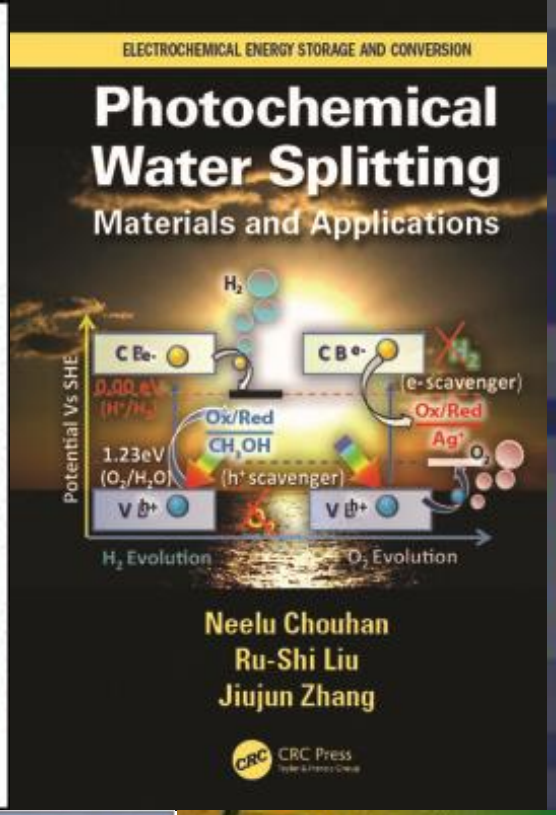
2008

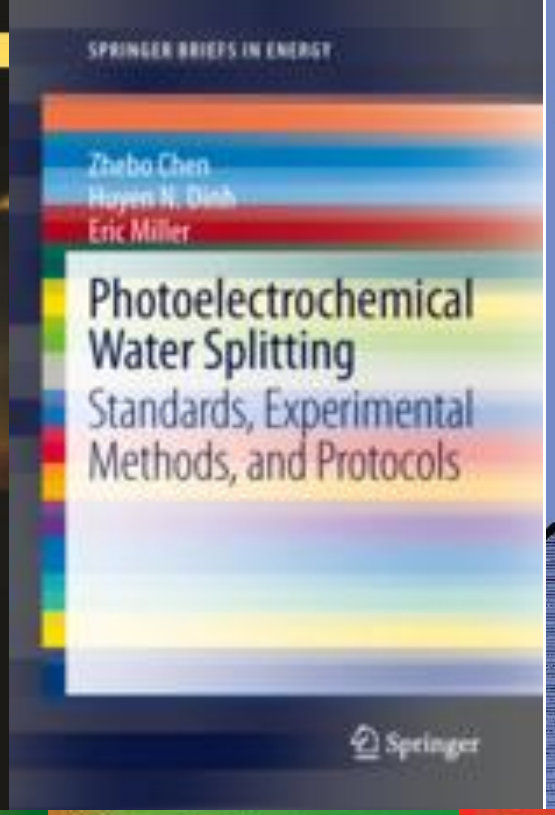
2012

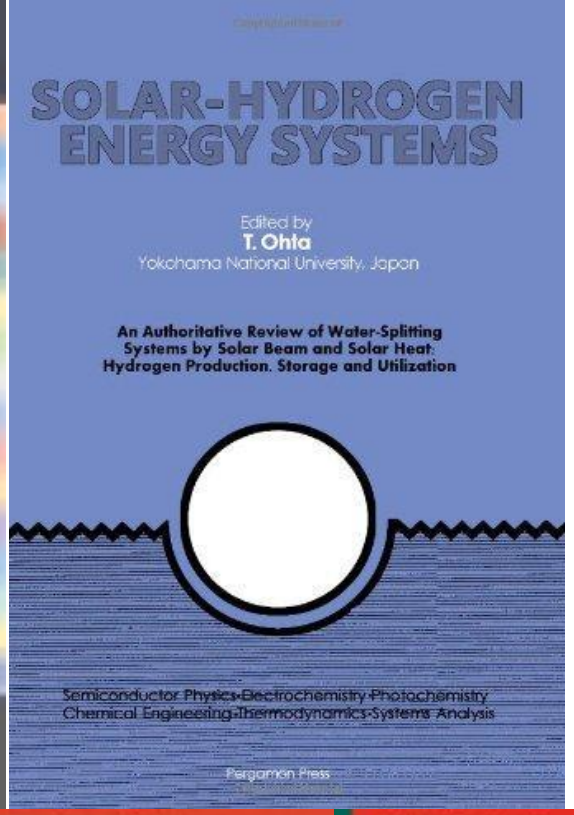
2016

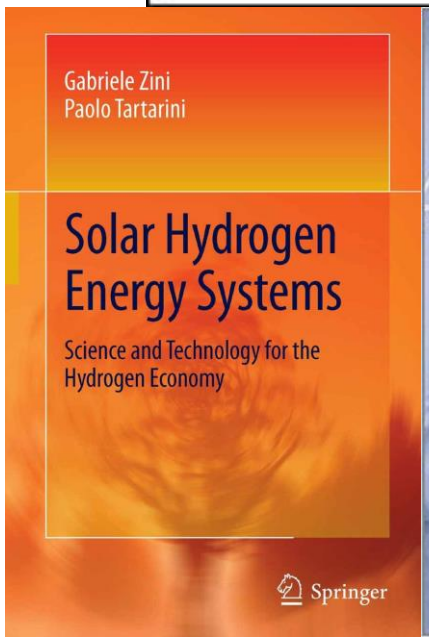


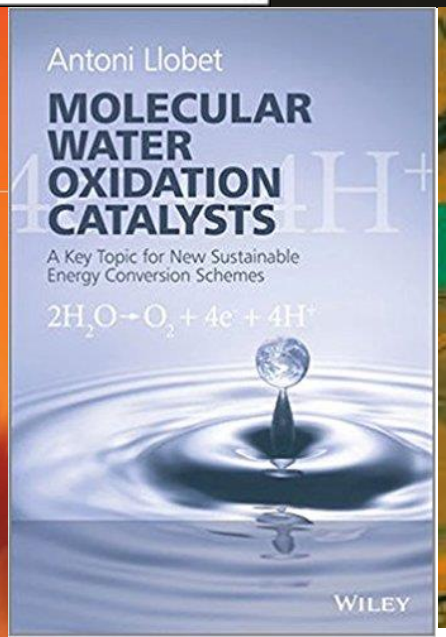

Photoelectrochemical
Water Splitting
Materials, Processes and Architectures
RSC Publishing

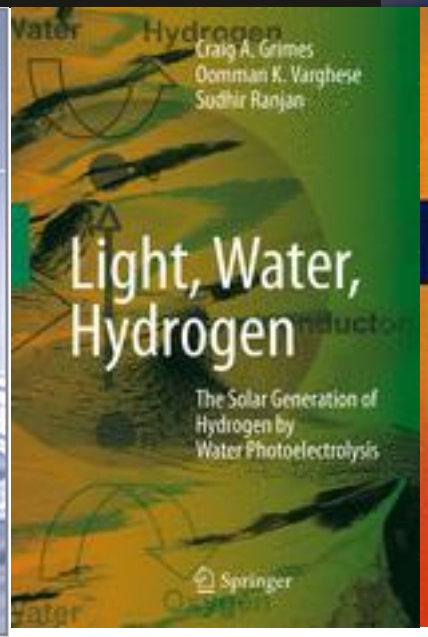

ELECTROCHEMICAL ENERGY STORAGE AND CONVERSION
Photochemical
Water Splitting
Materials and Applications
Neelu Chouhan
Ru-Shi Liu
Jiujun Zhang
CRC Press

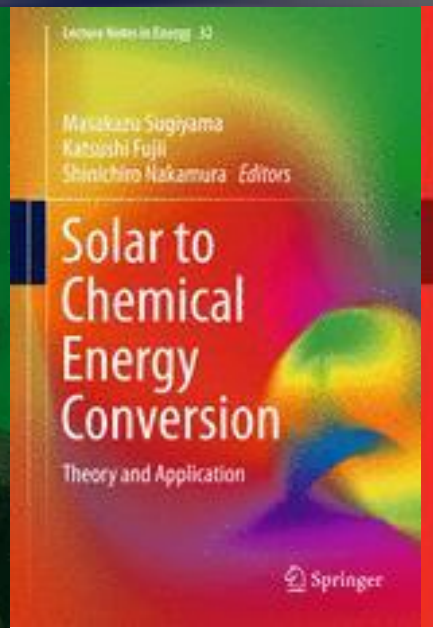

SPRINGER BRIEFS IN ENERGY
Zhebo Chen
Hoyen N. Dinh
Eric Miller
Photoelectrochemical
Water Splitting
Standards, Experimental
Methods, and Protocols
Springer

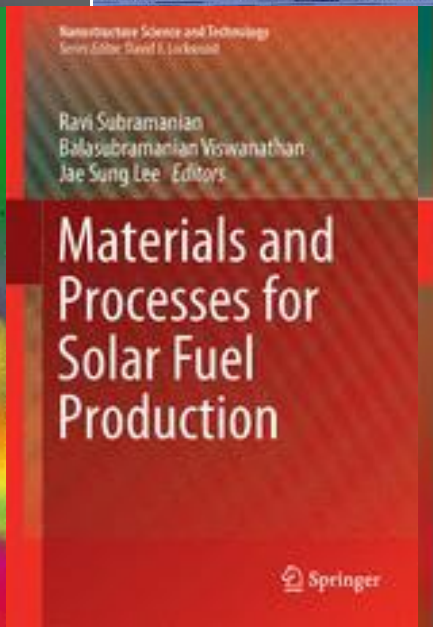

SOLAR-HYDROGEN
ENERGY SYSTEMS
Edited by
T. Ohta
Yokohama National University, Japan
An Authoritative Review of Water-Splitting
Systems by Solar Beam and Solar Heat:
Hydrogen Production, Storage and Utilization
Semiconductor Physics-Electrochemistry-Photochemistry
Chemical Engineering-Thermodynamics-Systems Analysis
Pergamon Press

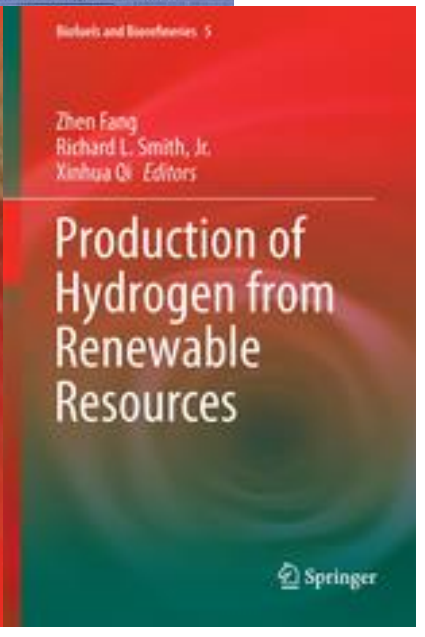

Gabriele Zini
Paolo Tartarini
Solar Hydrogen
Energy Systems
Science and Technology for the
Hydrogen Economy
Springer


Antoni Llobet
MOLECULAR
WATER
OXIDATION
CATALYSTS
A Key Topic for New Sustainable
Energy Conversion Schemes
WILEY


Craig A. Grimes
Oommen K. Varghese
Sudhir Ranjan
Light, Water,
Hydrogen
The Solar Generation of
Hydrogen by
Water Photoelectrolysis
Springer


Masakazu Sugiyama
Katsushi Fujii
Shinichiro Nakamura Editors
Solar to
Chemical
Energy
Conversion
Theory and Application
Springer


Ravi Subramanian
Balasubramanian Viswanathan
Jae Sung Lee Editors
Materials and
Processes for
Solar Fuel
Production
Springer


Zhen Fang
Richard L. Smith, Jr.
Xinhua Qi Editors
Production of
Hydrogen from
Renewable
Resources
Springer

THE ENERGY CHALLENGE

- World Population 7.6 Billion
- Energy Requirements ~17TW
- 9 Billion in 2050, 30TW
- Fossil Fuel Based Energy Resources. Coal (400 years), Oil (100 years) and Natural Gas (160 years)
- Carbon Dioxide Emission and Consequences

4° Turn Down the Heat

Why a 4°C Warmer World Must be Avoided

November 2012

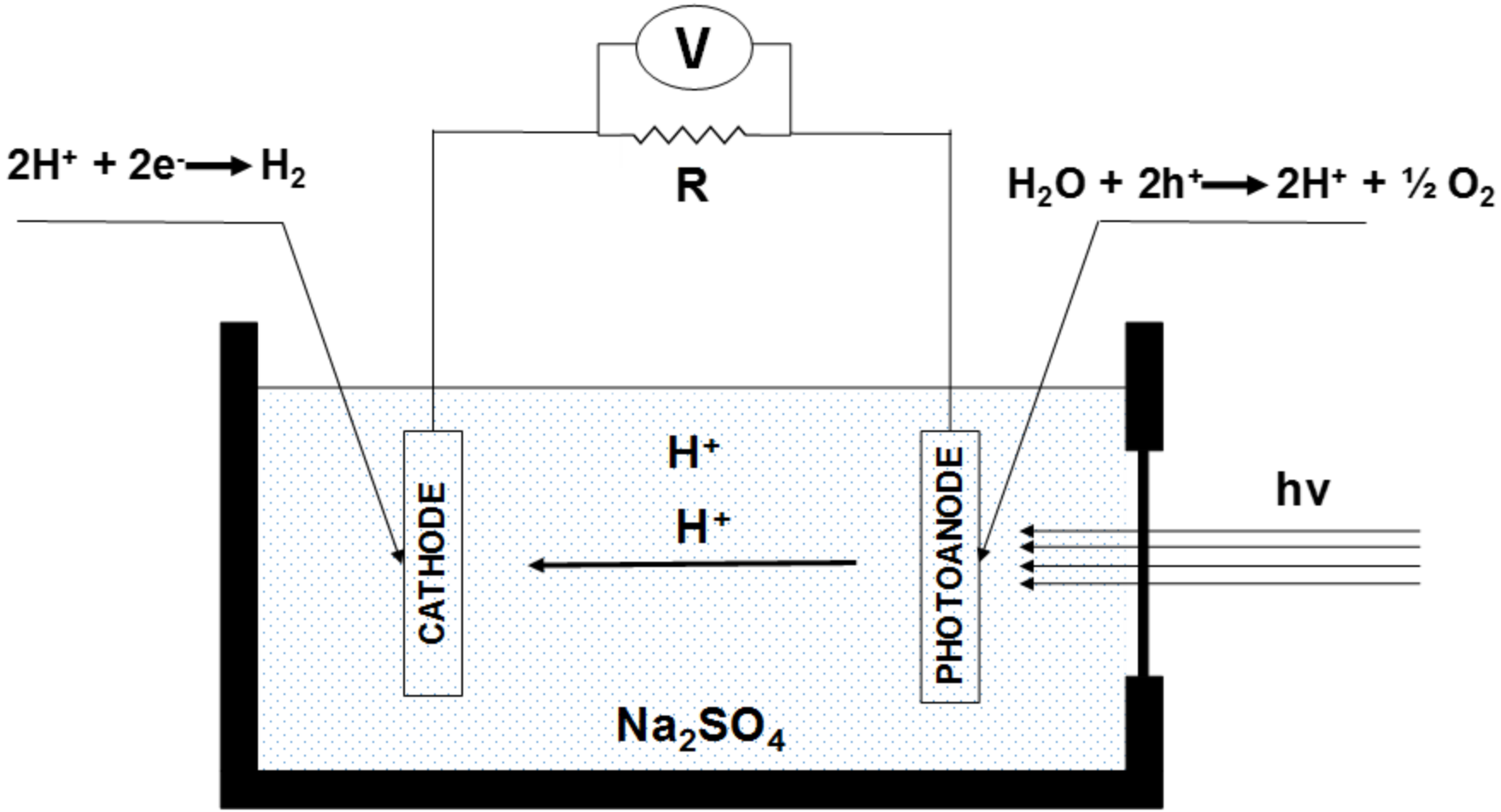
A Report for the World Bank
by the Potsdam Institute for
Climate Impact Research and
Climate Analytics

- We Must Re-invent Our Entire Energy Economy in the Next Few Decades if We are to Make This Transition
- We Likely Will Need Every Possible Energy Source at Significant (10% or more) Scale Just to Stabilize Carbon Emissions
- Longer Term: Require Fundamental Research Breakthroughs & Innovation

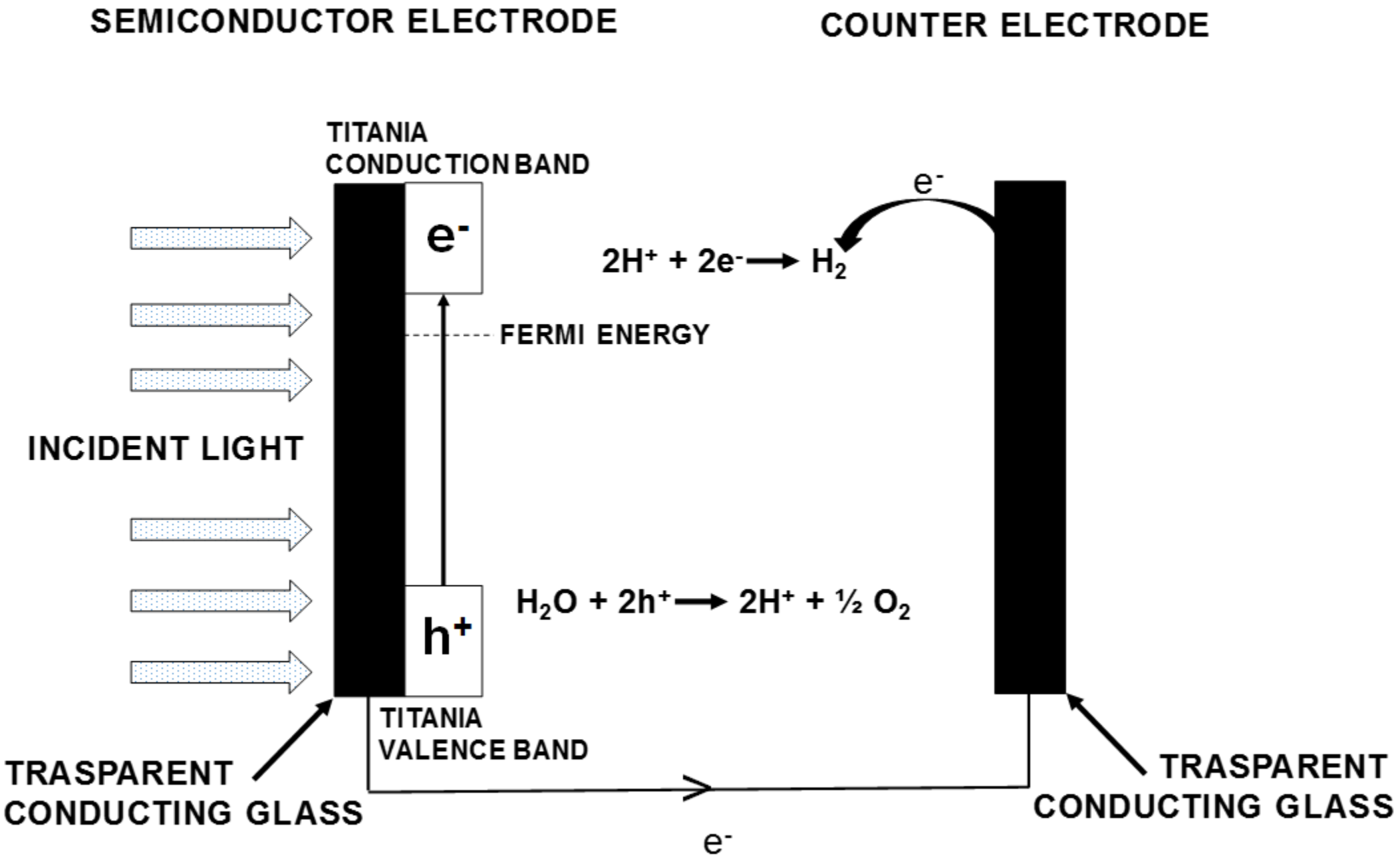
Why Photoelectrochemical Hydrogen Production?

- Hydrogen and oxygen are produced at separate electrodes. This avoids serious safety concerns and allows easy separation of these gases without having to pay a heavy energy penalty for post separation.
- It can be carried out at room temperature, i.e., there is no need for large-scale solar concentrators that would limit its application to large central facilities in sunny regions of the world.
- Photoelectrochemical water splitting device can be constructed entirely from inorganic materials. This offers a degree of chemical robustness and durability that is difficult to achieve for organic or biological systems.

SCHEMATIC SHOWING THE STRUCTURE OF A SIMPLE PEC CELL

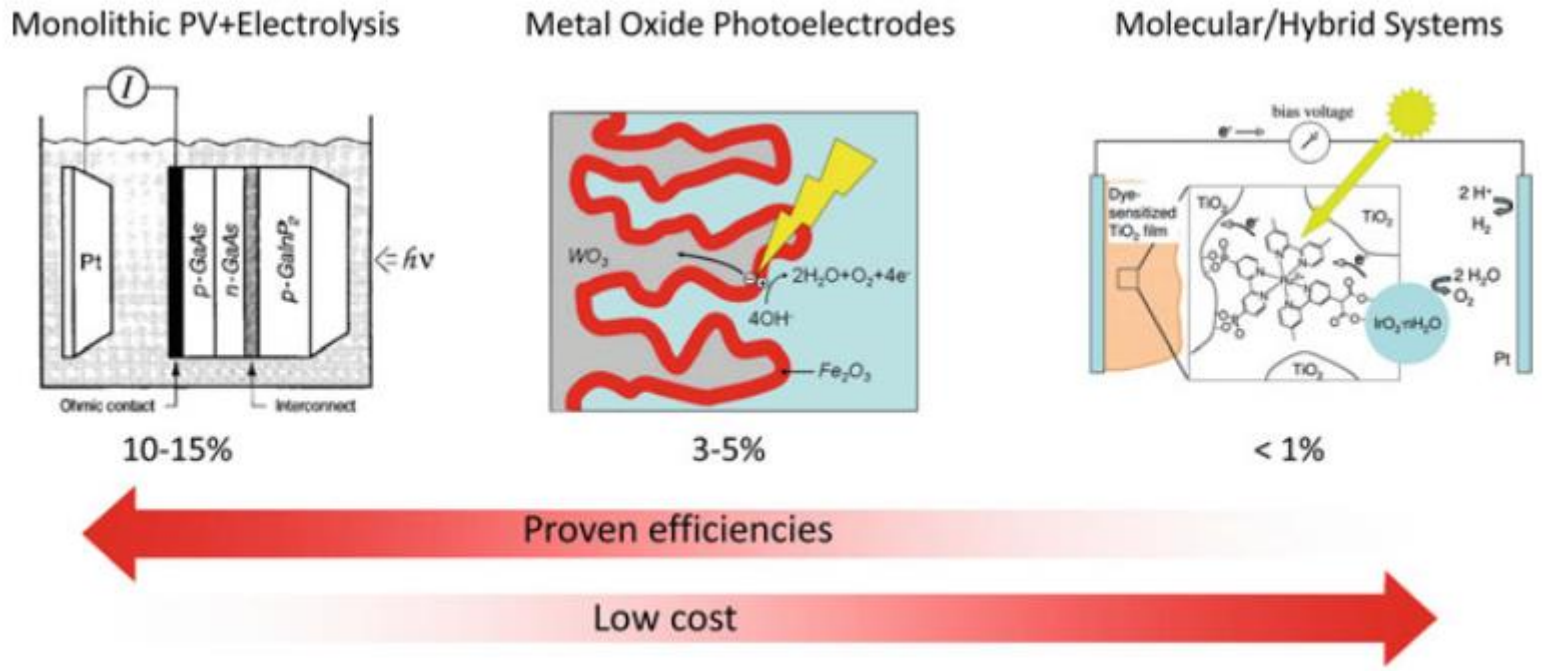


OPERATING PRINCIPLE OF A PHOTOELECTROCHEMICAL CELL



Materials for PEC Devices

- Light absorption, charge separation, charge transport, and H_2 or O_2 evolution at its surface.
- It needs to be stable in an aqueous solution, and have the potential to be made at low cost.
- No semiconducting material has yet been found that comes even close to meeting these contradictory demands.



- **Solutions for these and other challenges have been proposed in the form of mesoporous materials, guest–host nanostructures, tandem junctions, plasmonics, and combinatorial search methods for new metal oxide semiconductors.**

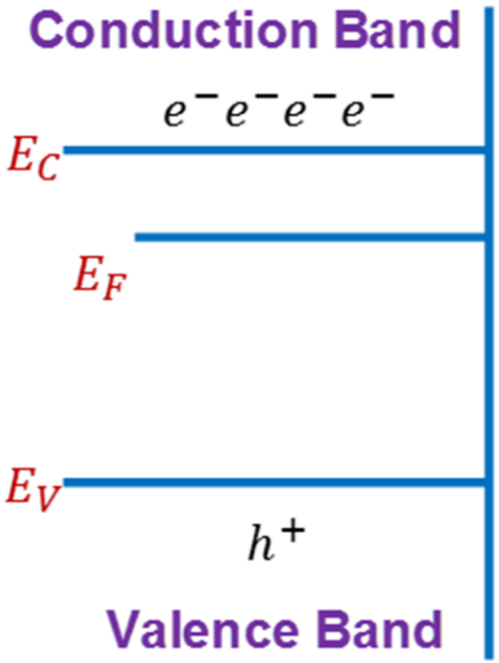
PEC vs PV + ELECTROLYSIS

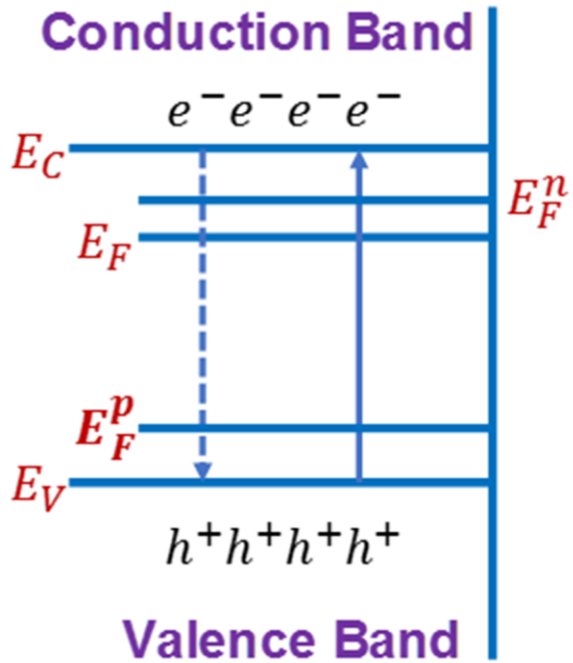
- Commercial electrolyzers require cell voltages of ~1.9 V in order to reach their optimal operating current densities of ~1 A/cm^2. Since the thermodynamically required potential for water splitting is 1.23 V, this places an upper limit of 65% (1.23/1.9) on the overall energy conversion efficiency.
- The current density at a semiconductor photoelectrode immersed in water is much smaller (10–20 mA/cm^2 at most) and the required overpotential is therefore substantially lower.
- PEC system can be constructed as a single, monolithic device.

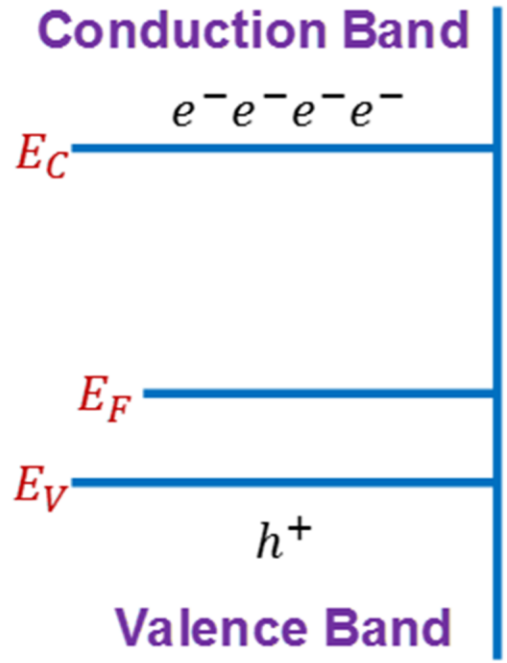
THEORY OF SEMICONDUCTOR PHOTOELECTRODES

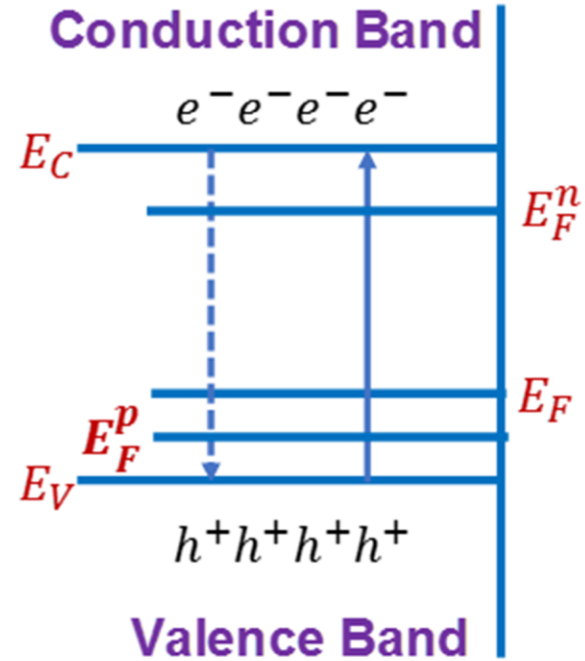
- Concept of Quasi Fermi Levels and Photopotential
- Excited State Photoelectrode Dynamics
  - Photocurrent
  - Range of Photoelectrode Reactions
  - Concept of Flat Band Potential
- Rate of Photoelectrode Reactions (Overvoltage Concepts)
- Photoelectrochemical Cells
- Photoelectrolytic Cells
- Photovoltaics Cells

Quasi Fermi Level Concept



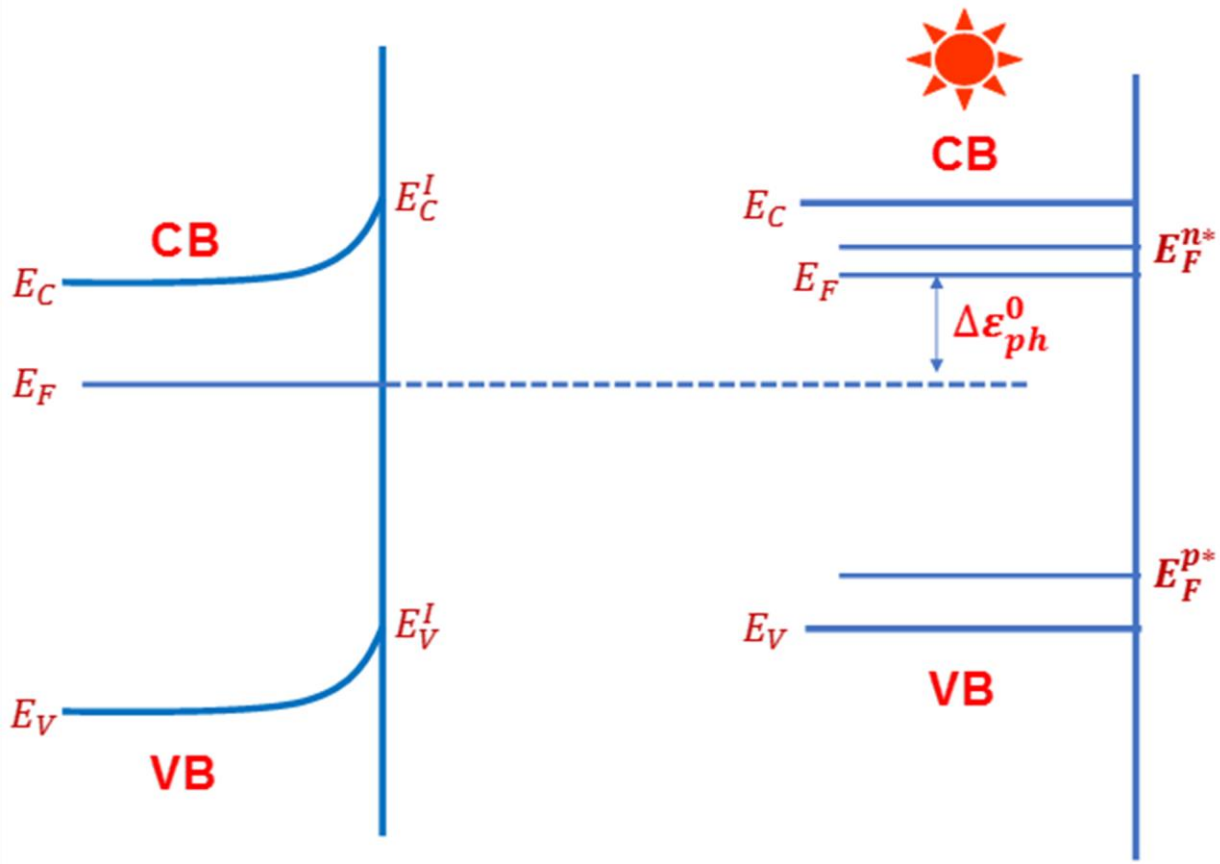




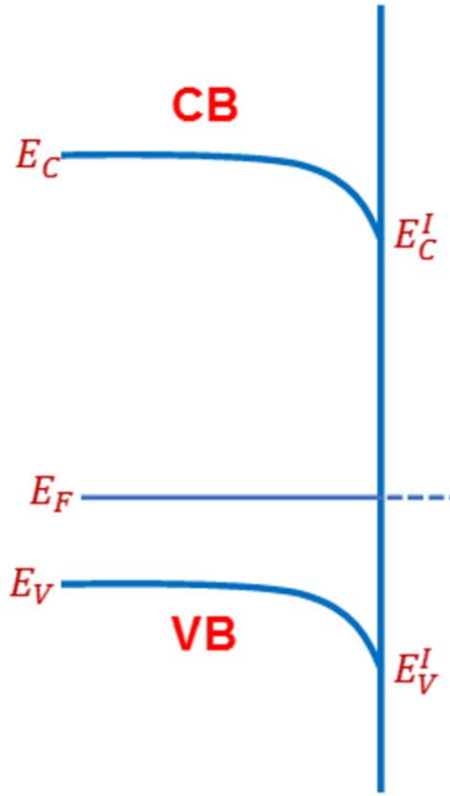


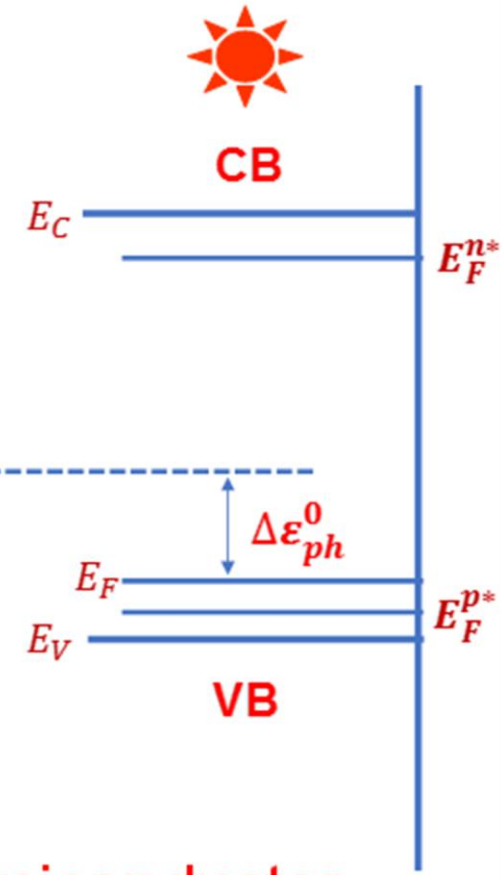
n-type semiconductor

p-type semiconductor

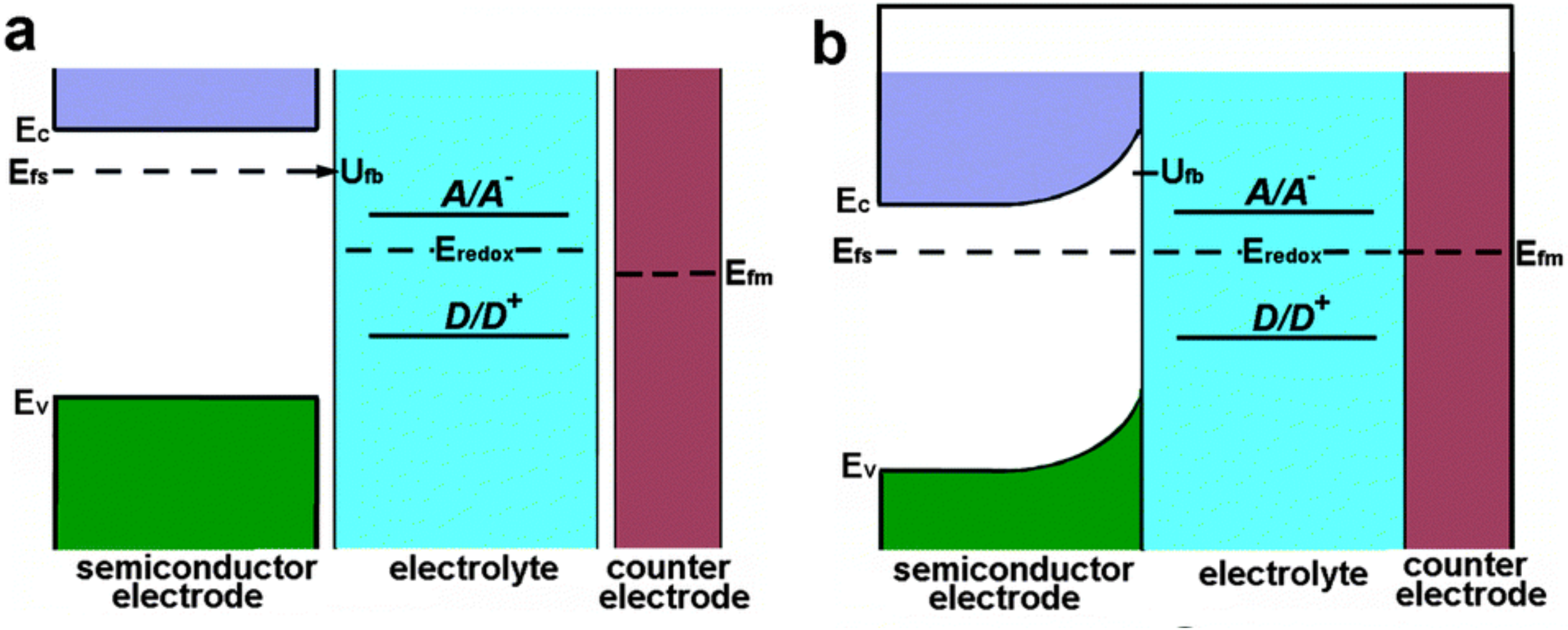


n-type semiconductor

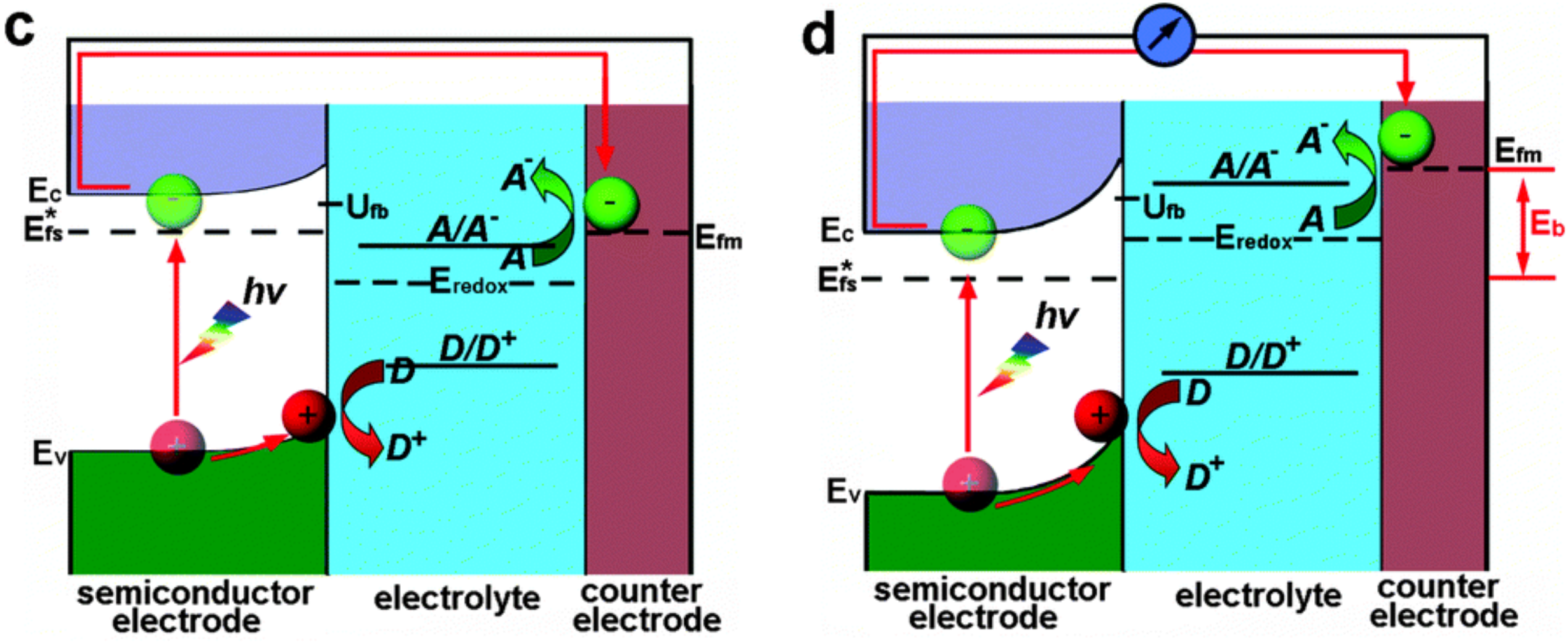




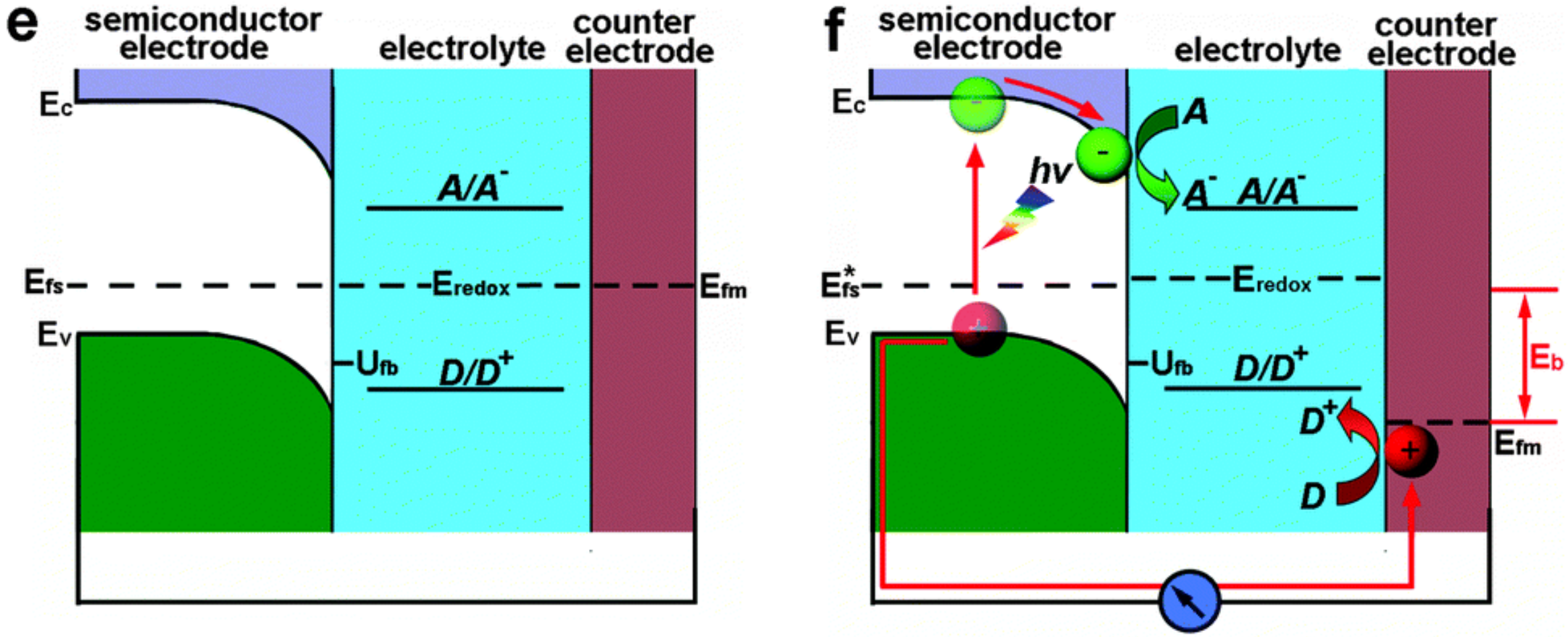
p-type semiconductor



Schematic band diagrams illustrating PEC processes: (a) before contact for an n-type semiconductor; (b) after contact for an n-type semiconductor in the dark;



Schematic band diagrams illustrating PEC processes: (c) n-type semiconductor under light irradiation without external bias; (d) n-type semiconductor under light irradiation with external bias

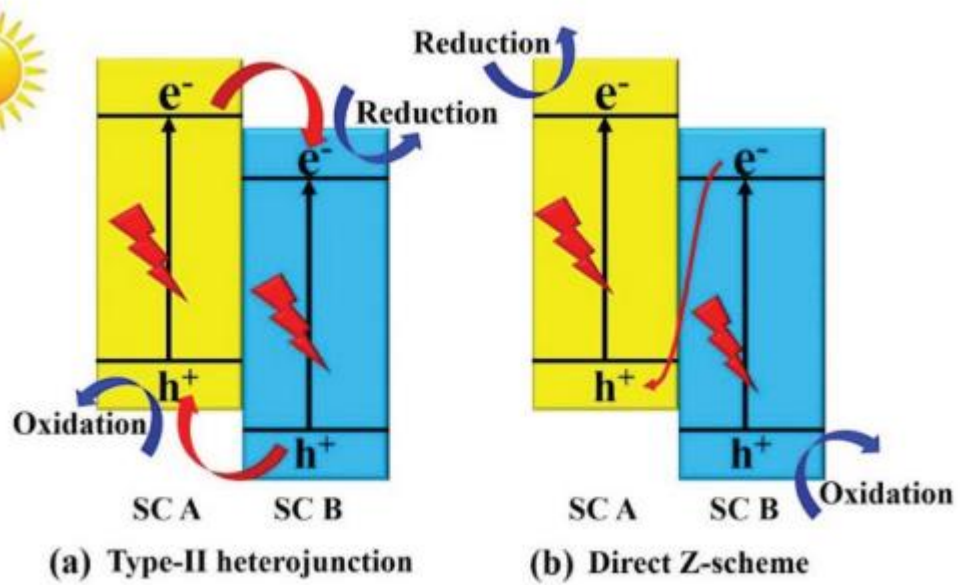


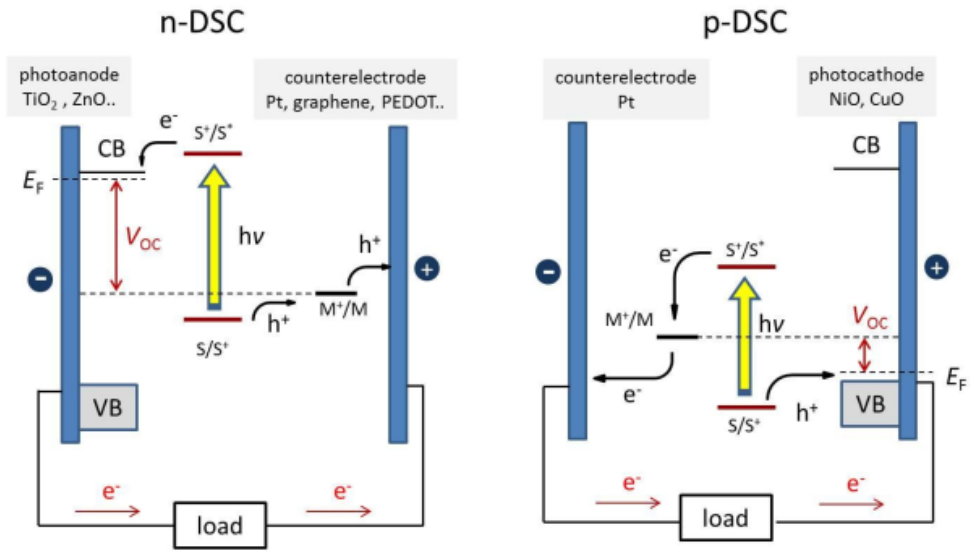
Schematic band diagrams illustrating PEC processes: (e) after contact for a p-type semiconductor in the dark; and (f) p-type semiconductor under light irradiation with external bias.

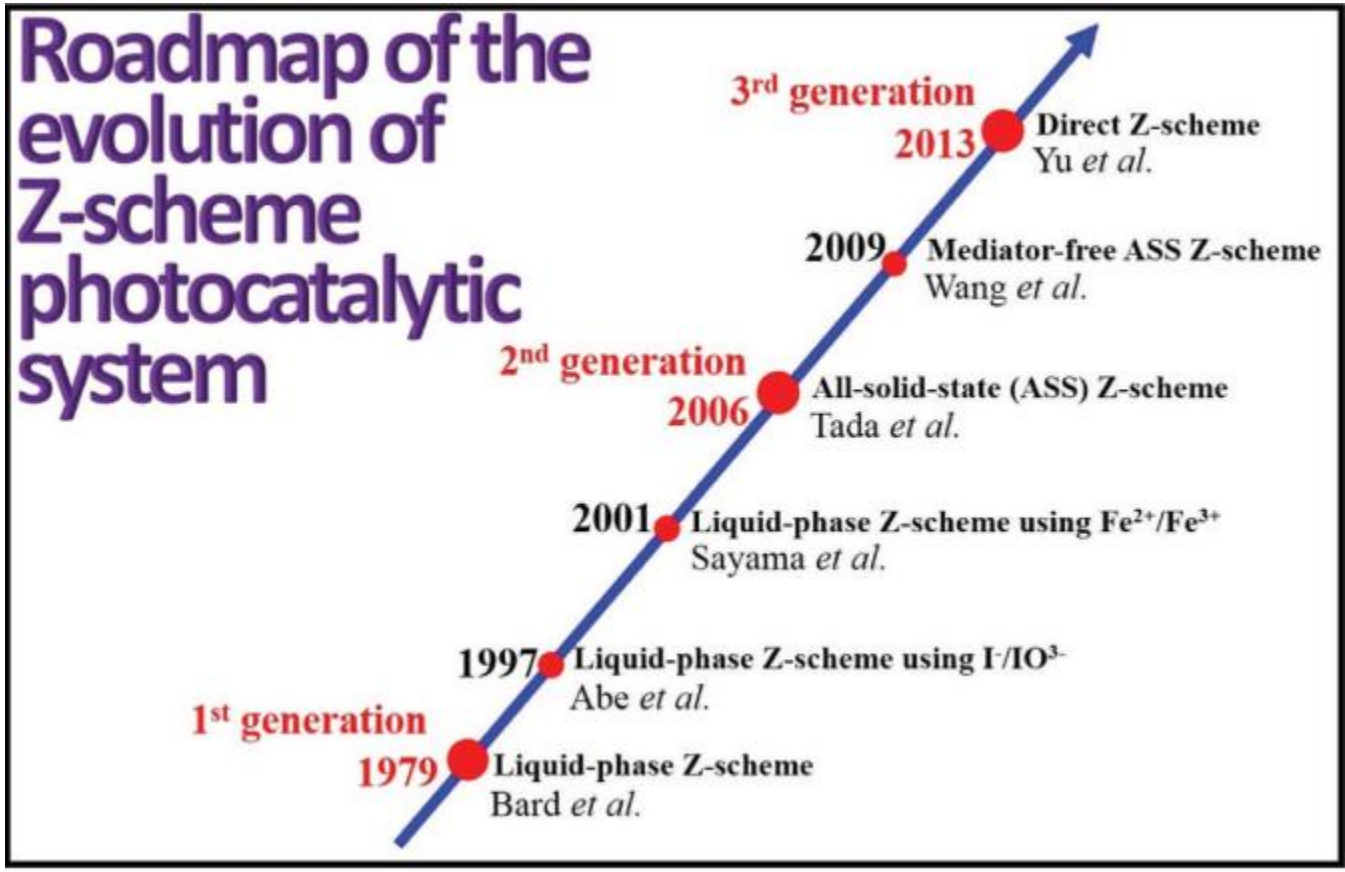
PROSPECTIVE SEMICONDUCTOR PHOTOELECTRODES

- Metal Oxide Photoelectrodes
- Non-Oxide Materials (Nitrides, Chalcogenides and Arsenide’s)
- Computational Screening Approach for Solar Fuels Photoelectrocatalysis
- Nanostructured Materials
- Advance Device Architectures
- Dye- Sensitized Photoelectrosynthesis Cells
- New Generation Materials: Hybrid Organic Inorganic Perovskites

• PHOTOELECTRODE MODIFICATIONS







- **BONDING CHARACTERISTICS AND ITS ROLE**

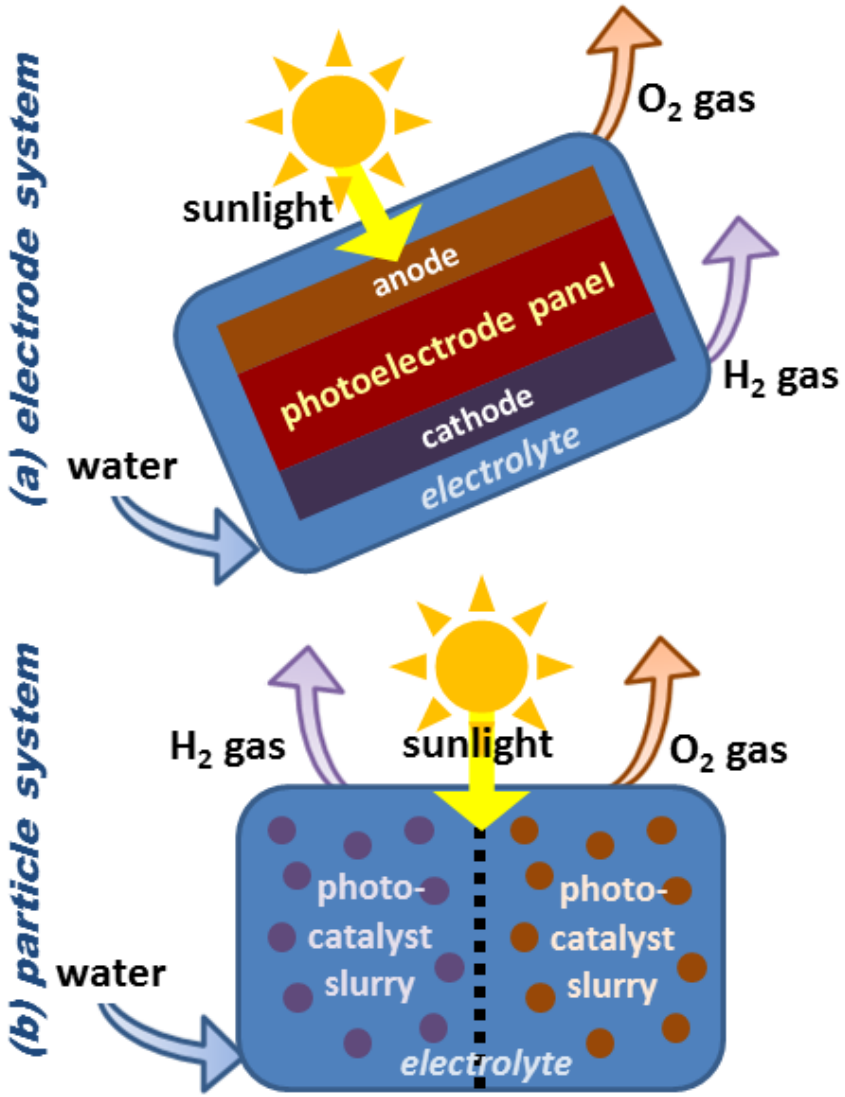
A High-Throughput Computational Screening Approach for Solar Fuels Photoelectrocatalysis

Montoya, J. H., Lawre
Persson, K., Lawrence Berkeley Lab

- In recent years, theoretical overpotential has become increasingly popular as a metric for characterizing the suitability of oxygen evolution electrocatalysts using density functional theory (DFT). In addition, DFT has become an invaluable tool for characterizing photoabsorbing materials in a number of high-throughput screening studies aimed at designing materials for solar fuels production from stability and bandstructure criteria. In this work, we present an approach which integrates calculations of theoretical overpotential with those of band-gap and band-edge positions on mixed metal oxides. Given that the prospect of discovering lone materials fulfilling the criteria of stability, catalytic activity, and photoabsorption efficiency, we also report on how materials with suitable surface chemistry may be more effectively paired with suitable photoabsorbing substrates using interfacial matching. Lastly, we benchmark our approach comparing potential combined metrics with experimentally measured photoelectrocatalytic activity.

• PEC REACTOR APPROACHES

Figure 1. Two different approaches to PEC solar hydrogen production reactors: (a) electrode systems similar to flat-plate photovoltaic panels; and (b) particle systems comprised of slurries of PEC semiconductor particles.



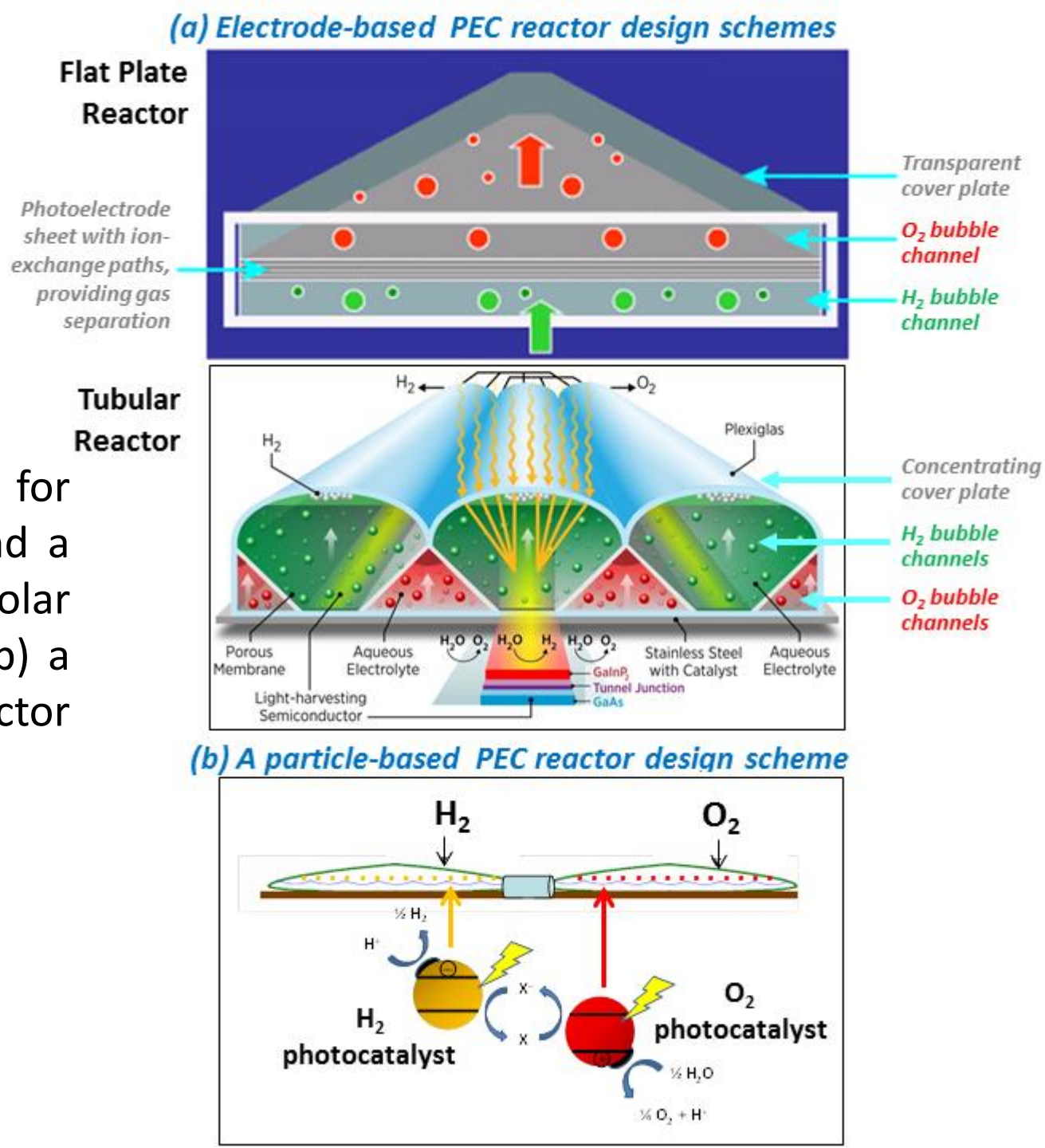


Figure 2. Possible PEC reactor design schemes for (a) electrode systems, including a flat plate and a tubular reactor (providing moderate solar concentration onto one electrode strip); and (b) a plastic "baggie" covered dual bed particle reactor with wide-by-side photocatalyst slurries.

Technoeconomic Boundary Analysis of Photoelectrochemical (PEC) Hydrogen Producing Systems

Photoelectrode Systems

Technical Targets: Photoelectrochemical Hydrogen Production: Photoelectrode System with Solar Concentration[a]

Characteristics	Units	2011 Status	2015 Target	2020 Target	Ultimate Target
Photoelectrochemical hydrogen cost[b]	$/kg	NA	17.30	5.70	2.10
Capital cost of concentrator and PEC receiver (non-installed, no electrode)[c]	$/m^2	NA	200	124	63
Annual electrode cost per TPD H_2[d]	$/yr-TPD H_2	NA	2.0M	255K	14K
Solar to hydrogen (STH) energy conversion ratio[e,f]	%	4 to 12	15	20	25
1-sun hydrogen production rate[g]	kg/s per m^2	3.3E-7	1.2E-6	1.6E-6	2.0E-6

- PROSPECTS PEC OF WATER DECOMPOSITION
- POSTULATES AND FUTURE DIRECTIONS

Photo-Electrochemistry of the decomposition of Water and reduction of carbon dioxide

1. Basic postulates of decomposition of water and their consequences
2. Outline and summary of attempts so far
3. Prospective semiconductor systems

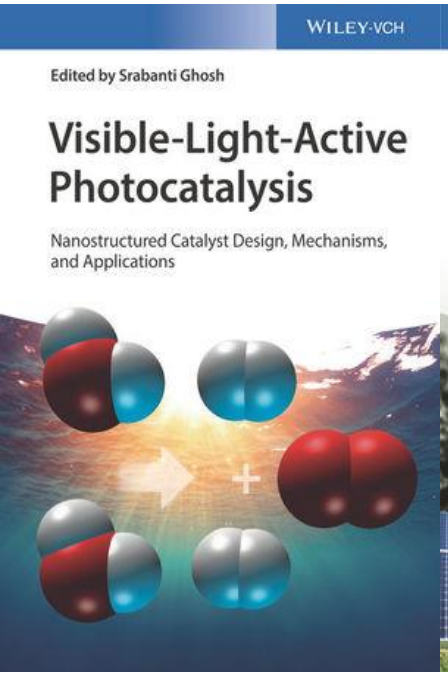
Metal Oxide Photoelectrodes, Non-Oxide Materials (Nitrides, Chalcogenides and *Arsenide's), Computational Screening Approach for Solar Fuels* Photoelectrocatalysis, Nanostructured Materials, Advance Device Architectures, Dye- Sensitized Photoelectrosynthesis Cells, New Generation Materials: Hybrid Organic Inorganic Perovskites, Mesoporous Materials

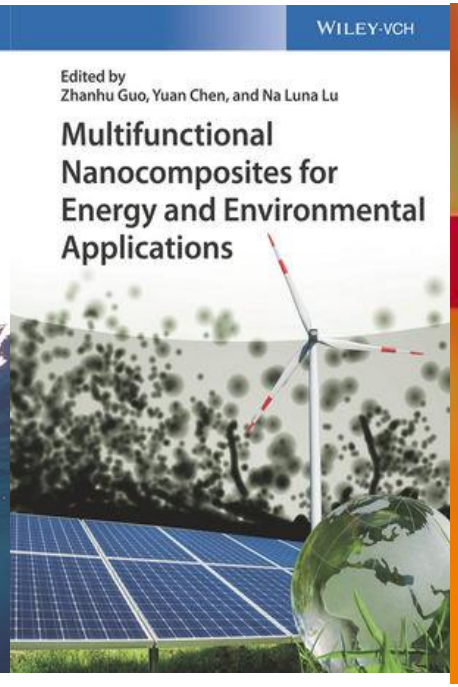
4. Band gap engineering and the consequences

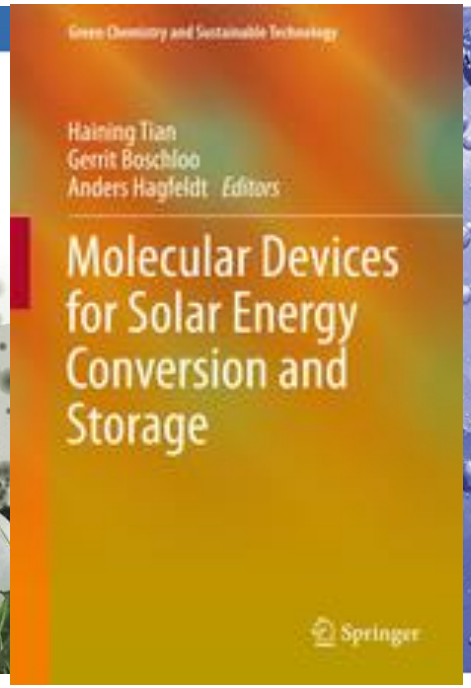
Coupled semiconductors (heterojunctions and Z Scheme) , Sensitization and DSSC as model systems, mesoporous materials, guest–host nanostructures, tandem junctions, plasmonics, and combinatorial search methods for new metal oxide semiconductors.

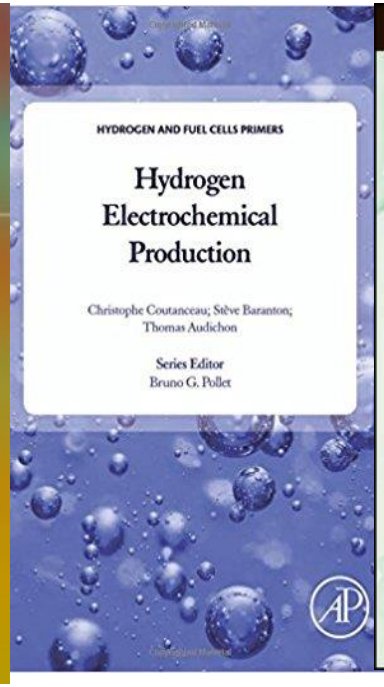
5.Bonding characteristics in semiconductors and their role
6. Reactor Designs and Technoeconomic Boundary Analysis (LCA)
7. Prospects PEC of water decomposition in the near future (Hydrogen Storage, Fuel Cells and Carbon Dioxide Reduction)
9. Postulates and future, directions

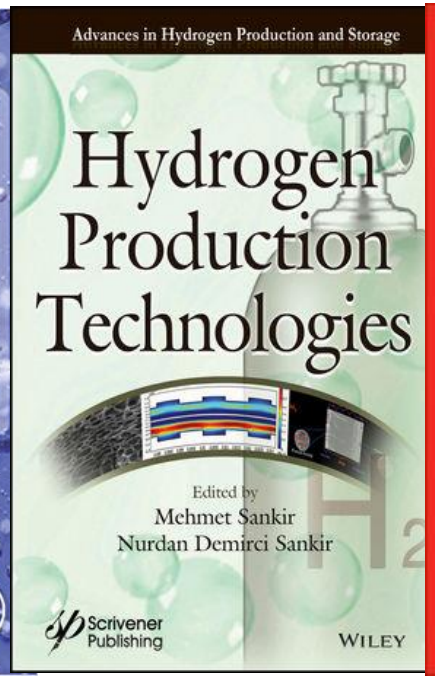
- LITERATURE IS VAST
- NEARLY 140 REVIEWS RELATED TO WATER SPLITTING IN THIS YEAR SO FAR

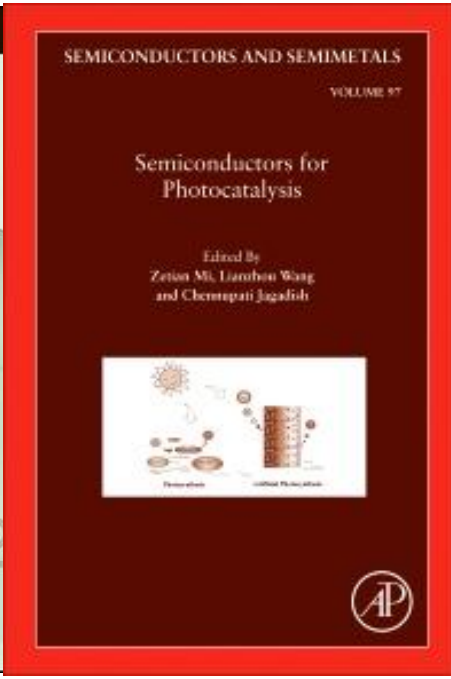













suggestions

New efficiency record for QDSC

SCIENCE ADVANCES | RESEARCH ARTICLE

SURFACE CHEMISTRY

Enhanced mobility $CsPbI_3$ quantum dot arrays for record-efficiency, high-voltage photovoltaic cells

Erin M. Sanehira,[1,2] Ashley R. Marshall,[1,3] Jeffrey A. Christians,[1] Steven P. Harvey,[1] Peter N. Ciesielski,[1] Lance M. Wheeler,[1] Philip Schulz,[1] Lih Y. Lin,[2] Matthew C. Beard,[1] Joseph M. Luther[1]*

We developed lead halide perovskite quantum dot (QD) films with tuned surface chemistry based on A-site cation halide salt (AX) treatments. QD perovskites offer colloidal synthesis and processing using industrially friendly solvents, which decouples grain growth from film deposition, and at present produce larger open-circuit voltages (V_{OC}'s) than thin-film perovskites. $CsPbI_3$ QDs, with a tunable bandgap between 1.75 and 2.13 eV, are an ideal top cell candidate for all-perovskite multijunction solar cells because of their demonstrated small V_{OC} deficit. We show that charge carrier mobility within perovskite QD films is dictated by the chemical conditions at the QD-QD junctions. The AX treatments provide a method for tuning the coupling between perovskite QDs, which is exploited for improved charge transport for fabricating high-quality QD films and devices. The AX treatments presented here double the film mobility, enabling increased photocurrent, and lead to a record certified QD solar cell efficiency of 13.43%.

There is currently a debate on whether Tesla can build semi trucks driven by storage batteries. Venkat Viswanathan at Carnegie Mellon University discusses new approach to overcome the barriers. Original paper appears in ACS Energy Letters

ACS Energy LETTERS

Cite This: ACS Energy Lett. 2017, 2, 2642-2645 http://pubs.acs.org/journal/aelccp

VIEWPOINT

Evaluating the Potential of Platooning in Lowering the Required Performance Metrics of Li-Ion Batteries to Enable Practical Electric Semi-Trucks

There is an explosion of interest in the potential of developing a long-haul electric semi-truck, and this interest has been amplified by Elon Musk outlining potential plans for long-haul electric semi-trucks.[1] In an earlier Viewpoint, we delineated the performance requirements of the batteries to enable long-range electric semi-trucks.[2] We identified that a fully electric semi-truck would require estimated battery pack sizes of roughly 1000, 2000, and 3100 kWh for driving ranges of 300, 600, and 900 miles, respectively, in a realistic driving scenario. Due to the specific energy limitations of current Li-ion batteries, an average of 240−280 Wh/kg at the cell level, the battery packs would weigh an enormous 8, 18, and 27 US tons for the three values of driving ranges considered. The large battery packs and the consequent pack weight restrict the payload capacity of electric semi-trucks due to the on-road gross vehicle weight (GVW) limit imposed on Class 8 vehicles.[2,3] In terms of payload capacity, we found

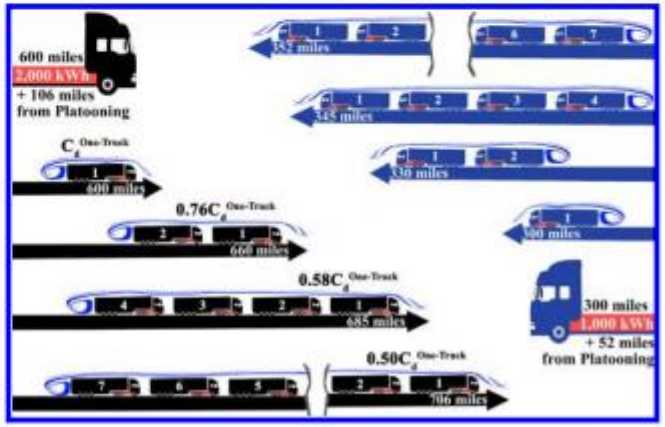


Figure 1. Comparison between the performance of a single truck and a platoon of trucks.