

## A2-2

# Development of computational design & synthesis methods for highly efficient H<sub>2</sub> production photoelectrode materials

In the present research project, new highly efficient visible light photocatalysts materials for PEC photoelectrodes are pursued, especially in the field of composite metal oxide catalysts. For this purpose, two methodologies using a quantum mechanical material design and the microscopic surface analysis on a nanometer scale are adopted. The catalysts are synthesized by our proprietary soft chemical approaches. Also, a PEC photoelectrodes for the effective solar-hydrogen production will be prepared.

## Goal

### Design and preparation of photoelectrode materials for PEC solar hydrogen production system: The photoelectrode efficiency(STH) : 5%

- Design of the photocatalyst materials for photoelectrode and development of element technology for photoelectrode preparation
- Development of core preparation technology for highly efficient PEC photoelectrode
- Development of preparation method for large size PEC photoelectrode

## Objective

- 1st year
  - Design of new photocatalyst materials for photoelectrode
  - Computational calculation of structure-activity relationship between elements of photocatalyst materials for photoelectrode
  - Preparation of photoelectrode with new photocatalyst materials
- 2nd year
  - Development of basic interfacial model of photocatalyst-photoelectrode for evaluation of physical property
  - Development of photocatalyst preparation method for highly efficient photoelectrode
  - Preparation of thin film type photoelectrode
- 3rd year
  - Development of basic defect model of photocatalyst-photoelectrode for computational calculation of structure-activity relationship
  - Development of efficient coating method for preparation of photoelectrode
- 4th year
  - Preparation of highly efficient photoelectrode with selected active photocatalyst materials
  - Development of preparation method for large size PEC photoelectrode(12.5cm x 12.5cm)



### Jin-Ook Baeg

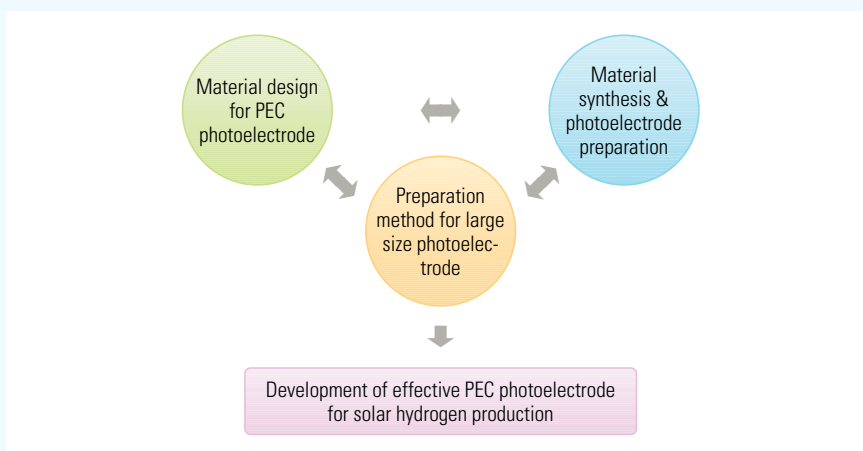
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Researchers : 15 persons (National Institute 10, Univ. 5)

## Strategy



## Outcomes & benefits

- Establishment of the core technology for photocatalyst design & synthesis on a molecular to nanometer scale
- Eco-friendly designed PEC solar-hydrogen production system
- Development of new photochemical or photoelectrochemical reaction systems such as CO<sub>2</sub> or other hydrocarbon conversion process

## Publications (2nd stage)

Patent		Theses							Proceedings		
		domestic			foreign			total sum	domestic	foreign	sum
domestic	foreign	SCI	Non SCI	sum	SCI	Non SCI	sum				
3/4		4	2	6	19		19	25	57	41	98

### ■ Publications

1. Jin-Ook Baeg, Sang Mi Lee, Sang-Jin Moon, Ki-jeong Kong, "Visible Light active pristine and Fe<sub>3</sub><sup>+</sup> doped CuGa<sub>2</sub>O<sub>4</sub> spinel photocatalysts for solar hydrogen production", INT J HYDROGEN ENERG, 2008, 33, 2646.
2. Jin-Ook Baeg, K.Gurunathan, Sang Mi Lee, Sang-Jin Moon, Ki-jeong Kong, E.Subram, "Visible light assisted highly efficient hydrogen production from H<sub>2</sub>S decomposition by CuGaO<sub>2</sub> and CuGa<sub>1-x</sub>InxO<sub>2</sub> delafossite oxides bearing nanostructured co-catalysts", CATAL COMMUN, 2008, 9, 395.