New semiconductor materials for photocatalytic hydrogen generation : mechanism formation in the presence of ionic liquids

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1. Research project objectives

The aim of this project is: (1) to develop **novel photocatalysts (ILs assisted $AgTaO_3$, $AgNbO_3$, $SrSnO_3$, $SrTiO_3$, $GaFeO_3$ and $FeVO_4$) for hydrogen generation** obtained during the hydrothermal process in the presence of ionic liquids, (2) describe a relationship between surface properties of new nanocomposites with efficiency of hydrogen generation and (3) to develop of **theoretical model to describe the relationship between properties of new photocatalysts with efficiency of hydrogen generation**.

2. Significance

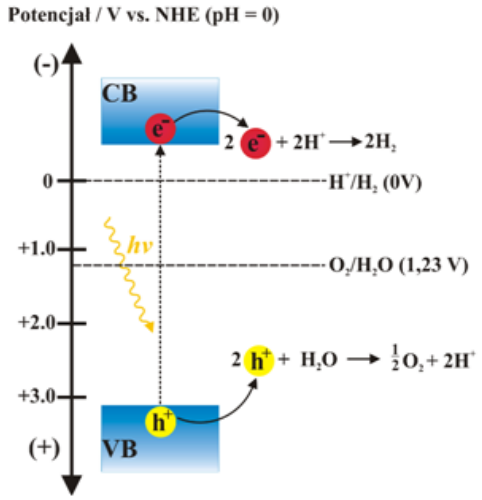

Fig. 1 Schematic illustration of photocatalytic water splitting

Heterogeneous photocatalysis in the presence of semiconductor nanoparticles has been proposed as a green technology applied to degradation of pollutants and inactivation of microorganisms in water and air stream. Recently, great interest is focused on obtain hydrogen is photocatalysis in the presence of semiconductors nanoparticles and UV-Vis or solar irradiation (Fig. 1). The basic requirements for developing and optimum photocatalysts for overall water splitting are (*i*) CB and VB edge potentials suitable for overall water splitting (*ii*) band-gap energy lower than 3 eV for visible-light harvesting (*iii*) physicochemical stability during photocatalytic reaction. Additionally, the bottom of the conduction band must be more negative than the reduction potential of H^+ to H_2 (−0.41 V *vs* NHE at pH 7) and the top of the valence band must be more positive than the oxidation potential of H_2O to O_2 (0.82 V *vs* NHE at pH 7).

Ionic liquids (ILs) are a group of salts which by definition are liquid below 100^{o}C. Ionic liquids have generated interest since many of them have negligible volatility, thermal stability, favorable interacting properties, and thereby presenting new solvating and structural directing media. The real strength of the ionic liquids is related with the possibility to modify the cation and anion structure (ILs are frequently termed “designer solvents”), and as a consequence to alter their physicochemical properties as well as possible interactions between IL and solute, and between ILs molecules. At the same time, ionic liquids have an ability to interact with photocatalyst particles playing a role of the structuring agent during the preparation route. Appropriate selection of the ionic liquid structure will enable preparation of new systems with interesting morphologies and desired properties (three-dimensional features, high surface area and high photocatalytic activity, etc.).

The proposed solution allow to **develop a new efficient photocatalysts**, and thus allows the use of renewable sources of energy (solar radiation) to produce hydrogen. Moreover, the mode of action proposed in the project combines computational methods with experimental studies should allow in the future for modern design of new nanomaterials with enhanced functionality and to reduce the cost of experimental research. Results of the project will contribute to **a progress in the fields of** material science, ionic liquids and photocatalysis.

3. Research methodology

It is proposed to enhance the effectiveness of hydrogen generation under UV-Vis or visible light irradiation in the presence of new developed nanomaterials such as: **$AgTaO_3$, $AgNbO_3$, $SrSnO_3$, $SrTiO_3$, $GaFeO_3$ and $FeVO_4$**. Photocatalysts will be synthesized during the hydrothermal process in the presence of ionic liquids. Characterization of obtained samples will include measurments of: surface area, crystal structure and phase composition, atomic composition, absorption spectra, FT-IR and Raman spectra, photoluminescence spectra, size, shape, surface topography. The theoretical model - connecting surface properties of series photocatalysts with photoactivity in hydrogen generation- will be developed