Ordered TiO_2 nanotubes modified by conjugated copolymers for hydrogen generation

One of the most important challenge and necessity for human is finding a new energy source, which could avoid to utilize fossil fuels. One of the way to obtain hydrogen is photocatalytic water splitting process, which require to the photocatalyst – a material which is active under irradiation.

The major group of photocatalysts is active only under UV light. To reduce cost of photocatalytic process it is necessary to find materials active under visible light. By apply suitable substances used as a photocatalyst it is possible to obtain hydrogen under solar light in water splitting process. However finding a good photocatalyst with a suitable properties is quite difficult. There are four important features, which the photocatalyst has to have to be applied in the photocatalytic water splitting process utilizing irradiation from the visible range: (*i*) band gap lower than 3.0 eV, (*ii*) suitable position of valence band (VB), conduction band (CB) of the semiconductor, (*iii*) suitable position of the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) of the organic compounds conjugated with semiconductor; and (iv) high stability and durability during prolonged photoreaction.

The aim of this project is synthesis of the photocatalyst, active under UV-Vis and Vis light. It was supposed that application of different ways, which decrease band gap value, allow to obtain the macromolecule active under visible light. Combination this polymers with NPs-TiO_2 nanotubes create suitable materials for water splitting.

The proposed materials contain conjugated copolymers at the TiO_2 nanotubes surface. The macromolecules was obtained from EDOT, 2,1,3-benzothiadiazol and their derivatives. This type of composite has not been described in the literature. The TiO_2 nanotubes was proposed because of good photocatalytic activity, developed surface area and possibility of control the dimension of nanotubes (diameter, length, space between nanotubes). Conjugated copolymer contains acceptor and donors units in the chain. The interaction between HOMOs of acceptor and donor as well as LUMOs of acceptor and donor, allow to obtain materials with smaller band gap. The presence of highly electronegative atoms in the donors units enhance decreasing of the band gap. The selected method of the electrodeposition of copolymers layer at TiO_2 nanotubes surface is cyclic voltammetry. This way allow to control the chains length by the numbers of cycles. The materials obtained by the combination of TiO_2 nanotubes and conjugated copolymers will be suitable to generation of hydrogen by water splitting process under visible light. Optimization of synthesis of copolymers at the nanotubes surface. The morphology of TiO_2 nanotubes, molar ratio of used monomers and substituent effect for efficiency of hydrogen generation *via* water splitting process. Additionally the stability of photocatalyst during irradiation and the influence of wavelength of irradiation on quantum efficiency of H_2 generation will be investigated.