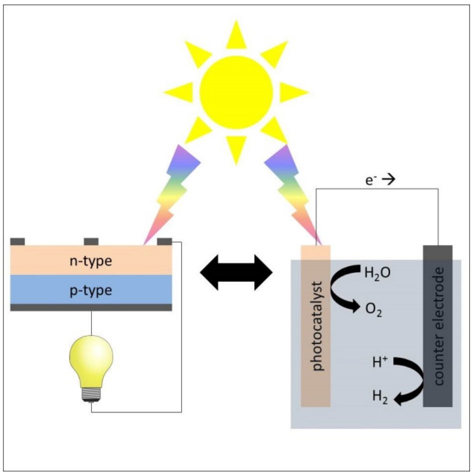
PROGRAMUL DE COOPERARE ELVEȚIANO-ROMÂN
SWISS-ROMANIAN COOPERATION PROGRAMME

Small band-gap nanostructured perovskite materials for photovoltaic and photocatalytic hydrogen generation applications

Starting Date 01.01.2013
Duration 36 Months
Discipline Material Science

Main Goals

Today's demand to provide more sustainable energy requires materials and devices with improved or even new functionalities. Harvesting solar energy, using stable, cheap, and environmentally friendly materials, with photovoltaic cells and photocatalysis for solar water splitting is an attractive approach (see scheme). An optical band gap in the visible range is needed to allow a more efficient use of the solar spectrum. Examples of promising materials are perovskites such as $LaTiO_2N$, $BiFeO_3$, and Y or La doped $BiFeO_3$. The main goal of this project is to prepare thin films of these materials as model systems to correlate the crystallographic and morphologic properties with the photovoltaic and photocatalytic performance.



Activities

The fabrication of the thin films is performed by pulsed laser deposition. Parametric studies on the deposition conditions have been performed to obtain epitaxial thin films. The physical and chemical properties of the layers are investigated using different techniques: X-ray diffraction is used to study the crystalline properties and the surface orientation, while Rutherford backscattering spectrometry and elastic recoil detection analysis are used to determine the chemical composition of the thin films. The band gap can be changed by doping and the overall optical properties of the thin films are determined by spectrometric ellipsometry. Model heterostructures, involving different bottom and top electrodes, such as TiN, Pt, or Al doped ZnO, are created to characterize the photoelectrochemical and photovoltaic properties of the different materials. These heterostructures are applied as photoelements (for photovoltage, photocurrent, and external quantum efficiency measurements) using a solar sun simulator, while the photocatalytic activity is studied by photoelectrochemical experiments.

Expected results

The properties of the thin films will be correlated with chemical and physical characteristics, such as the chemical composition, crystalline structure or surface orientation. An increase of the light absorption from the solar spectrum by the deposited thin films due to a decrease of the band gap is the main expected result. This band gap decrease can be achieved by Y or La doping of $BiFeO_3$ or by tailoring the N content in $LaTiO_{3-x}N_x$. An enhancement of the photovoltaic and photoelectrochemical (water splitting) properties should be achieved for these designed materials.

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