Lead-free organic-inorganic stable materials with enhanced photoconversion efficiency for solar cells and photodetectors

Considering the limited resources of fossil fuels in the world, other ways of generating electricity than those using them are sought. One possibility is to convert solar energy into electricity. In devices that convert photons into electrons flowing in an electrical circuit, it is necessary to use materials with specific properties. First of all, they must be semiconductors with a band gap (in the band model) corresponding to the energy of the incident photons (1 - 3 eV). This is not a sufficient condition. To obtain the highest photoconversion efficiency (PCE – power conversion efficiency), a sufficient number of electrons in the semiconductor can be excited into the conduction band. In other words, there must be an appropriate number of energy levels for electrons near the valence band (VB) maximum and the conductance band (CB) minimum. In the nomenclature of the band model, this is called the density of states (DOS). The ideal material for the active layer in an electronic device for photoconversion, in addition to the features as mentioned above, must be characterized by the high mobility of current carriers (electrons and holes) and their long free path. Another difficulty that must be overcome in producing a suitable photoconversion material is that the resulting exciton (electron-hole pair) is rapidly recombined. So the electron-hole pair must be separated quickly in order to participate in the current flow. The key issue is the binding energy value of the exciton, it should not be too large. In addition, the condition for the separation of the electrons and the holes is the presence of an electric field. The electric field can be created by using *p*-type and *n*-type semiconductors on one and the other side of the active layer, respectively. Another option is to use a ferroelectric material with built-in spontaneous polarization (positive and negative charges appear on opposite sides of the active layer). Another problem is the selection of metals for electrical contacts. On the one hand, the metal should have good adhesion to the semiconductor layer. On the other hand, the work function of the electron from the metal should ensure ohmic contact because it sometimes happens that an energy barrier is created for electrons (the so-called Schottky barrier), which prevents their flow. All these requirements for materials for active layers in photoconversion devices made us decide to systematically search for this type of materials in the promising group of organic-inorganic hybrids (OIH). These materials belong to the widely understood perovskites, which include their most famous representative $(CH_3NH_3)PbI_3$. Unfortunately, the latter is toxic due to its lead content and is unstable in the air. It is known that the use of a different metal, a halogen and an organic molecule allows the modification of the bandgap width and concentration of carriers and the increase of stability. And by using appropriate organic cations (e.g. containing π-conjugated electrons) it is possible to generate appropriate conduction paths for electrons. In this way, we expect to obtain a material with high air stability, semiconductor, good bandgap width and suitable for commercialization efficiency of conversion of photons into electric current. Our research will include the determination of the crystal structure of the material. It is important, for example, to determine the dimensionality of the anionic network - 3D, 2D, 1D or 0D. Of course, the most advantageous from the point of view of conductivity is the three-dimensional (3D) network, but it should be expected that the use of appropriate organic cations will enable better conduction of electricity also in structures with lower dimensions. Of course, it will be important to determine the semiconductor parameters: bandgap width, the density of states, mobility of current carriers and their free path. These quantities can be determined experimentally but also by theoretical calculations. Determining these values in a wide range of temperatures will allow describing the usefulness of the obtained materials for use in electronic devices (photodetectors, photovoltaic cells, *p-i-n* diodes, etc.) The research proposed as part of the project belongs to current global research trends and opens new perspectives and possibilities in synthesizing and characterizing perovskites based on organic-inorganic hybrids. As a result, the obtained results will provide new clues for producing stable and efficient photodetectors.