

VABILO NA PREDAVANJE V OKVIRU DOKTORSKEGA ŠTUDIJA KEMIJSKE ZNANOSTI / INVITATION TO THE LECTURE WITHIN DOCTORAL PROGRAMME IN CHEMICAL SCIENCES

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z naslovom / title:

New insights into the synthesis and properties of organic-inorganic perovskites

v četrtek, 27. 3. 2025 ob 15. uri v predavalnici 1 v 1. nadstropju Fakultete za kemijo in kemijsko tehnologijo, Večna pot 113 / on Thursday, 27. 3. 2025 at 15.00 in lecture room 1, 1st floor at the Faculty of Chemistry and Chemical Technology, Večna pot 113

Vljudno vabljeni! / Kindly invited!

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Abstract:

Hybrid organic-inorganic perovskites (HOIPs) are likely to be the materials of the future due to their unique properties and wide variety of applications. One prominent example is their use in solar cells, thanks to their exceptional light-harvesting capabilities. The increasing demand for clean energy has driven the search and synthesis of new perovskite compounds. The first study on the application of organic-inorganic perovskites for photovoltaic purposes was conducted by Kojima *et al.*, achieving solar cells with efficiencies of up to 3.8%. Over the last decade, intensive research on perovskite solar cells has led to an efficiency increase of up to 33%.

The effectiveness of organic-inorganic perovskites (designated by the general formula ABX₃) is primarily related to the metal-halogen bonds (B–X) within the octahedral coordination polyhedra, which serve as their main structural motif. In the perovskite structure, the octahedra form cubooctahedral cavities in which the A-cation is located, resulting in an ideal cubic structure. In organic-inorganic perovskites, the A position is usually occupied by a small organic cation, the B site by a metal cation at the center of the octahedra, and X by an inorganic anion, typically a halogen element. Many combinations of cations and anions can be used while retaining the perovskite structure, allowing for the modeling of perovskite compositions and the tuning of their properties.

Most recently studied HOIPs feature methylammonium (MA) and formamidinium (FA) cations in the A position, though other cations such as guanidinium, hydroxylammonium, hydrazinium, imidazolium, pyrrolidinium, azetidinium, and others have also been used to synthesize these hybrid materials. Despite variations, the typical corner-sharing perovskite motif is maintained, though different kinds of deviations from the ideal cubic structure may lead to lower symmetry and/or dimensionality. Today, perovskites are known to belong to different crystal classes and possess 3, 2, 1, or 0-dimensional structures.

The focus of this lecture will be on the various methods of synthesizing organic-inorganic materials and the potential for obtaining quality crystals for investigation using single-crystal X-ray diffraction (XRD). Additionally, the influence of different solvents and synthesis conditions will be considered and explained. The lecture will also explore the possible analysis to understand and explain the structural properties of the organic-inorganic perovskites currently being investigated.