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# How Photoelectron Spectroscopy can be used to investigate organic-inorganic perovskites? Chemical, Electronic Structure Characterization and Stability Behavior

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## Abstract

The use of organic/inorganic perovskite as solar cells material constitutes one of the main breakthrough of this last five years in solar energy research. The so-called perovskite structure adopts the general formula  $ABX_3$  where A and B are two cations and X an anion.  $CH_3NH_3PbI_3$  belongs to this family (A =  $CH_3NH_3^+$ , B =  $Pb^{2+}$ , and X = I<sup>-</sup>) and was the material that initiates this breakthrough. This material was relatively quickly outperforming the common dye-sensitized solar cells (DSSCs) technology reaching in 2012 the symbolic efficiency line of 10%. A lot attention has since been devoted to the development and improvement of these organic/inorganic perovskite materials. Alternative chemistry have been proposed i.e. different nature of the halide (X), the metal (B), or the cation group (A), combination with hole conductors as well as the development and optimization of novel fabrication/deposition techniques that all together brought certified efficiency up to 21% in 2016.

While these materials are usually characterized through their structure (XRD) and performance within solar cell communities, not so much attention is devoted to their surface chemical composition and, specifically, the surface composition. Photoelectron spectroscopy (PES) can easily fulfill this task, and, in addition to chemical information, PES provides an overall picture of the electronic structure of the perovskite and its relation to the scaffold layer used (e.g.  $TiO_2$ ,  $Al_2O_3$ ).when studied with hard X-rays.Through various recent examples, we will present how PES can be used to investigate perovskite solar cells materials based on different metals ( $Pb^{2+}$ ,  $Bi^{3+}$ ), anion (I<sup>-</sup>, Br<sup>-</sup>, Cl<sup>-</sup>) or cation (Cs<sup>+</sup>, MA<sup>+</sup>, FA<sup>+</sup>). [1][2][3]

The main drawback towards a commercialization of these devices remains their poor stability. We have exposed the classical  $CH_3NH_3PbI_3$  to various environments, such as water, temperature, and long-time storage in air and argon, and followed changes of the surface composition with PES. The main result of the different exposures is that the perovskite

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is decomposed into PbI<sub>2</sub>, but an important point is that this degradation seems to occur already at 100 °C and is not only related to large humidity level. Indeed, even in an inert atmosphere such as argon, a slow degradation to PbI<sub>2</sub> is observed. [4]

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