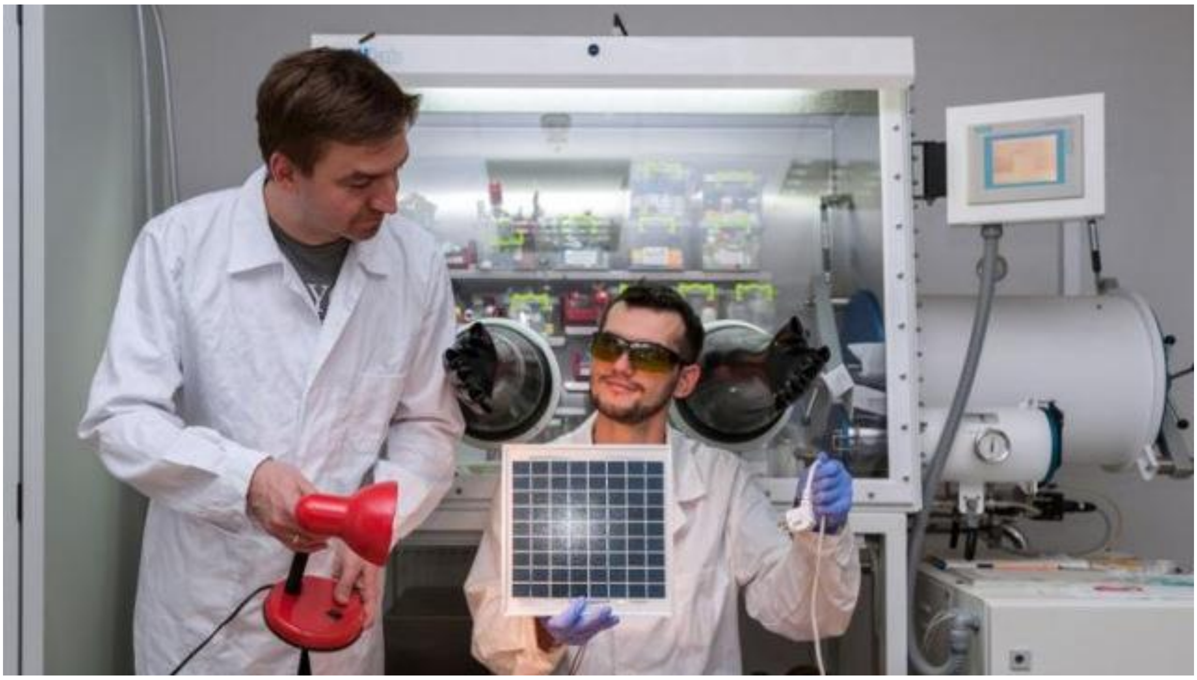
Mechanochemistry paves the way to higher quality perovskite photovoltaics



A Swiss-Polish team from the Institute of Physical Chemistry of the Polish Academy of Sciences (IPC PAS) in Warsaw and the Ecole Polytechnique Federale de Lausanne (EPFL) in Lausanne (Switzerland) co-operating within the GOTSolar project, implemented under the FET Open (Future and Emerging Technologies) programme in Horizon 2020, has demonstrated a perovskite cell with a significantly smaller number of structural defects.

The "unexpected" improvement of the photovoltaic performance was observed when perovskites produced by mechanochemistry were used for the construction of a typical photovoltaic cell.

According to researchers mechanochemistry is a rapidly developing field of science dealing with chemical reactions occurring directly between solid-phase compounds upon activation by mechanical force.

In laboratories, such processes are carried out in automatic ball mills. However, some mechanochemical reactions could be successfully performed at home, by manual grinding in ordinary mortars.

The researchers added that perovskites are a large group of materials with the general chemical formula ABX_3, characterized by a cubic crystalline structure. Atoms of A are located at the centre of the cube, in the middle of each wall there is an X atom, and the corners are occupied by the atoms of element B.

The name of this group of materials is derived from a naturally occurring mineral, calcium titanate $CaTiO_3$, named perovskite in honour of the Russian geologist Leo Perovski.

Over time, it has become apparent that the physicochemical properties of this material can be improved by replacing calcium, titanium and oxygen with other elements. Currently, the most commonly studied compound of the perovskite group is $(CH_3NH_3)PbI_3$. In this material, calcium, titanium and oxygen ions are replaced by methylammonium (in position A), lead (in position B) and iodide (in position X) ions, respectively.

Prof. Janusz Lewinski (IPC PAS, Warsaw University of Technology) group is the first to demonstrate that polycrystalline halide perovskites, e.g., the afore-mentioned $(CH_3NH_3)PbI_3$ can be produced in mechanochemical reactions.

Recently, the group have also presented the mechanochemical production of mixed perovskites, i.e., those in which several different types of ions alternate in position A. This is an important achievement, because, by carefully altering the chemical composition of the perovskite materials, they can be adapted to specific applications in photovoltaics, catalysis and other fields of science and technology.

Professor Lewinski's team is conducting academic research on the synthesis of perovskites in Poland. The materials produced in this research announcement were assembled and tested at EPFL in collaboration with Prof. Michael Graetzel.

The laboratory photovoltaic cells, working on perovskite materials obtained by mechanochemistry, have just been constructed by Dr. Daniel Prochowicz (EPFL, IPC PAS).

Why are the electrical properties of perovskite cells obtained by grinding better?

The answer is not evident yet. It seems that the solvent used in production of perovskites plays a negative role. It can be incorporated into the structure of the material, and upon deposition of the perovskite on the substrate its residues may cause the formation of defects in the crystalline structure. Microscopic and electrical studies have shown that better quality of mechanochemically-synthesised perovskites (obtained without solvents) comes along with reducing the number of traps for charge carriers, formed at the junction of the material with the substrate.

The research was carried out within two projects of the Horizon 2020 programme of the European Union.

- GOTSolar is a part of FET Open action, one of the most prestigious grants for international consortia of academic institutions and companies for the development of cutting-edge technologies on the early stage.
- Additional part of this research was a part of a Maria Sklodowska-Curie Individual Fellowship (MSCA IF), which a prestigious scholarship for young researchers for the postdoctoral research.

> "In practice, the mechanochemical production of our perovskites is as follows. Two powders, e.g. white methylammonium iodide CH3NH3I and yellow lead iodide PbI2, are placed in a mill equipped with a few steel balls. Then, we grind them for several dozen minutes and... we pour out a homogeneous black powder of the perovskite (CH3NH3)PbI3, which can be directly used for the construction of photovoltaic cells. You do not need to use high temperature, organic solvents, or worry about waste. The whole process is really fast and efficient. It is green chemistry."
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> **Marcin Saski**, *PhD student at IPC PAS*

> "An important property characterizing the quality of a photovoltaic cell is the amount of electrical charge accumulating at the boundary of individual cell layers. If there is too much, the cell undergoes degradation more rapidly. Perovskites obtained by mechanochemistry formed a very homogeneous layer, which reduced the number of defects in the structure impairing the work of the cell and reduced the amount of charge deposited on the surface."
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> **Dr. Prochowicz**, *conducting research under a Maria Sklodowska-Curie Individual Fellowship in Prof. Graetzel's group**

Reduction in the Interfacial Trap Density of Mechanochemically Synthesized MAPbI3

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Abstract

Organo-lead halide perovskites have emerged as promising light harvesting materials for solar cells. The ability to prepare high quality films with a low concentration of defects is essential for obtaining high device performance. Here, we advance the procedure for the fabrication of efficient perovskite solar cells (PSCs) based on mechanochemically synthesized MAPbI3. The use of mechano-perovskite for the thin film formation provides a high degree of control of the stoichiometry and allows for the growth of relatively large crystalline grains. The best device achieved a maximum PCE of 17.5% from a current–voltage scan (J–V), which stabilized at 16.8% after 60 s of maximum power point tracking. Strikingly, PSCs based on MAPbI3 mechanoperovskite exhibit lower "hysteretic" behavior in comparison to that comprising MAPbI3 obtained from the conventional solvothermal reaction between PbI2 and MAI. To gain a better understanding of the difference in J–V hysteresis, we analyze the charge/ion accumulation mechanism and identify the defect energy distribution in the resulting MAPbI3 based devices. These results indicate that the use of mechanochemically synthesized perovskites provides a promising strategy for the formation of crystalline films demonstrating slow charge recombination and low trap density.