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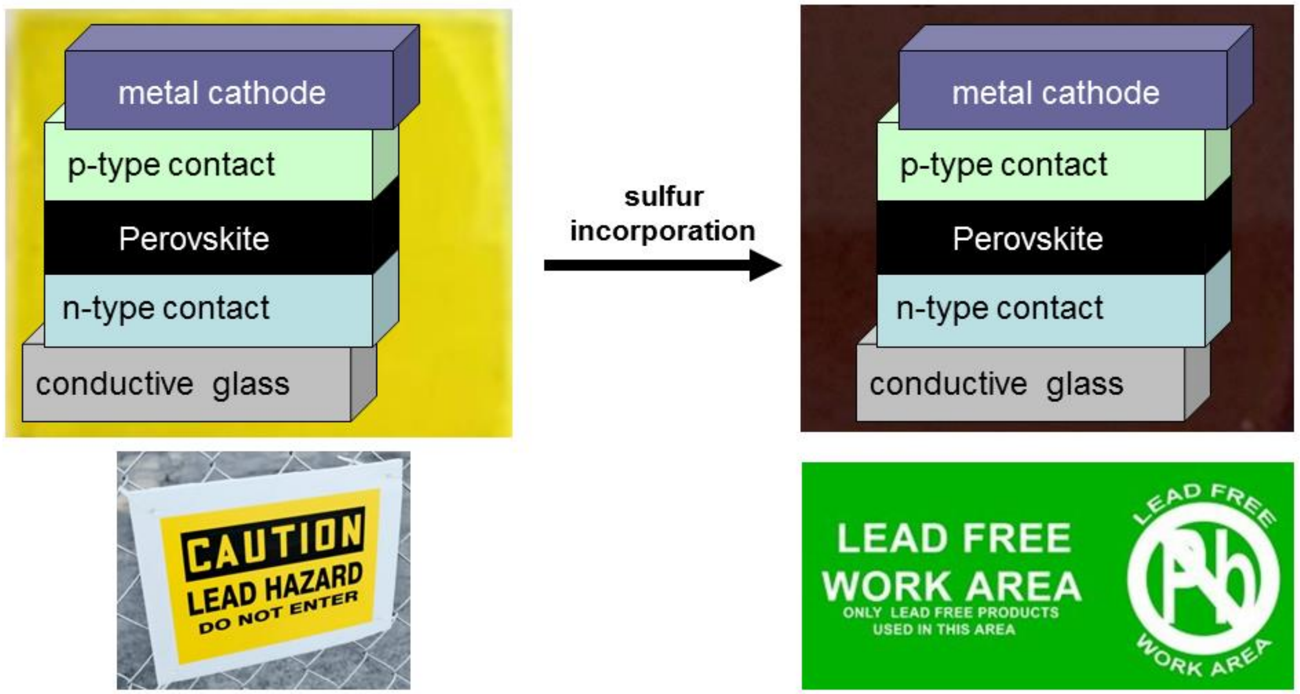
# Description of the funded research project

## 1st Call for H.F.R.I. Research Projects to Support Faculty Members & Researchers and Procure High-Value Research Equipment

## Title of the research project:

**Consolidating perovskite photovoltaics through sulfur incorporation**




## Principal Investigator: **Thomas Stergiopoulos**

## Reader-friendly title: **SUL-FUR COAT**

## Scientific Area: **Natural Sciences**

## Country: **Greece**

## Host Institution:

**National Centre of Scientific Research "Demokritos"**

**Institute of Nanoscience and Nanotechnology**

## Budget: **199,980.00 €**

## Duration: **36 months**

# Research Project Synopsis

Lead halide perovskite solar cells manifest as a new generation of optoelectronic devices which combine high power conversion efficiencies and low cost, but at the expense of robustness and environmental compatibility. This presents two major challenges which this research addresses directly. First, solar cells with improved stability should be developed. Second, excessive use of lead should be restricted. To tackle these challenges, SUL-FUR COAT proposes to develop viable perovskite photovoltaics through the incorporation of sulfur which has been proven to improve the optoelectronic quality of perovskites via its interaction with $Pb^{2+}$ and organic cations (such as methylammonium) as well as to provide semiconductors (such as PbS) with relatively strong air/moisture-stability. To achieve this, SUL-FUR COAT has set the following objectives: (i) ) devising means to effectively passivate perovskite films and interfaces so as to slow-down degradation kinetics, (ii) designing and developing lead-free, chalcogenide perovskite thin films that have never been explored before through solution-processing, and (iii) implementing optimized materials into boundary-pushing photovoltaic devices.

# Project originality

The motivation for the proposed research originates from the failure of other methodologies to suggest perovskites with long operational lifetime and acceptable environmental friendliness. Our proposed approach draws on the universality of sulfur compounds to passivate perovskites and also make novel, lead-free perovskites. To reach the ambitious goals of the project, SUL-FUR COAT proposes several methodological innovations that go substantially beyond the state-of-the-art.

In terms of trap passivation, attempts have been realized in order to passivate traps in the bulk, at grain boundaries and at interfaces in perovskite solar cells. Typical universal trap healing agents have been recognized to be iodide and chloride through coordinate and ionic bonding. Another strategy to eliminate killer defects at the surface of perovskite is the conversion of grain boundaries to produce a favorable heterojunction. However, in both cases, films suffer from intrinsic stability issues. Here we will employ an uncommon strategy, which is a holistic approach, testing various sulfur passivation strategies (coordinate, ionic bonding and chemical conversion) to heal traps at every area of the perovskite film or perovskite solar cell. We argue that stronger coordination of sulfur in comparison with halides, may lead to better stability.

In terms of environmental compatibility, successful efforts have been devoted to replace some of the toxic lead (e.g. 60%) with tin. However, 40% of lead is still far more than the maximum concentration of lead allowed in each homogeneous material contained in any electronic devices. Another example of failure is the lack of combined stability and efficiency in halide perovskites of variable structural dimensionality, metal ions and oxidation states. To tackle this challenge, here we will examine the unexplored class of lead-free chalcogenide perovskites, consisted of an inorganic core with more covalent bonding character than halides. which will may lead to enhanced moisture stability.

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# Expected results & Research Project Impact

The research methodology employed by SUL-FUR COAT will enable: (i) the development of passivated perovskites with minimum recombination (presenting photoluminescence lifetimes at the μs scale), (ii) the development of uniform pinhole-free chalcogenide perovskite films of high optoelectronic quality (with bandgap ≤1.7 eV and recombination lifetimes of at least 10 ns) and (iii) the fabrication of photovoltaic devices with long-term stable performance higher than those of current state-of-the-art lead halide perovskite devices.

Significant scientific breakthroughs can be expected such as: a) effectively passivate traps by sulfur will pave the way towards full commercial viability of solar cells and will be the spring board to the photovoltaic revolution b) attain efficiencies for chalcogenide solar cells higher than those attained by currently best $Sn^{2+}$-based technologies will manifest them as a novel family of reliable, lead-free perovskites with great potential.

This new family of devices will manifest as smart and green alternatives for established emerging photovoltaic technologies. The true applications can then go way beyond, such as in LEDs, lasers, light and X-Rays detectors, phototransistors or even beyond optoelectronics, in systems such as water splitting, batteries and supercapacitors. With this, SUL-FUR COAT will directly contribute to preservation of a sustainable society with renewable sources, reduced carbon emissions and reliance on fossil fuels, cleaner environment and less global warming.

# The importance of this funding

SUL-FUR COAT is the sole project that the Research Team in Demokritos has on perovskite solar cells, which is the current expertise of the Principal Investigator. With this funding, three research associates (one post-doc research assistant and two pHD students) will be hired and significant equipment (glovebox for controlled oxygen/humidity environment) will be bought, establishing a strong team and environment for the fabrication/characterization of emerging optoelectronics in our laboratory. In addition, the travel budget will cover the cost of research visits to work with Prof. Dr. Michael Saliba at the Institute for Photovoltaics of the University of Stuttgart in order to fabricate highly-stable solar cells based on multication perovskites.

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