

# Design and Development of multi cation hybrid perovskites for photovoltaic applications

By

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This report, as well as all of the experimental details and results, were completed during my training in the Research Group of Prof. Dr. Dr. (h.c.) Sanjay Mathur at the Institute of Inorganic Chemistry, department for Chemistry, University of Cologne, under the supervision of professor Sanjay Mathur and the PhD student Niusha Hishmati, who supported me and provided me with all of the necessary information and experimental experience. I would like to thank everyone in the group for their help during my stay.

The training is separated into five different projects; each one is primarily concerned with the fabrication of a perovskite solar cell and perovskite material.

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## Project\_1:

### Perovskite layer development (increase grain size)

#### Introduction

The grain boundaries and interface characteristics in the active layers of perovskite solar cells (PSCs) have a significant impact on the device's performance. The quality of the perovskite active layer is the most important factor influencing the performance of PSCs. It has been shown that it is feasible to control the grain growth process in order to produce perovskite films with high crystallinity, large grains, few grain boundaries, low trap densities, and a high rate of carrier recombination [1].

Fast and unregulated crystallization produces relatively small grains and hence a significant number of grain boundaries, resulting in more flaws at grain boundaries or inside grains, as well as shorter carrier lifetime or diffusion length. Slowing down the crystallization process is therefore critical for producing highly efficient and stable perovskite and tandem solar cells [2].

Following the spin coating, the substrates was annealed using two annealing process:

- Normal annealing
- Close-space annealing (CSA) [17].

## Project\_2:

### Prepare Perovskite solar cells

#### Introduction

There are four stages of photovoltaic technical advancement that are now known; the first generations of solar cells are made from crystalline silicon, which has dominated the photovoltaic (PV) business for the past half-century. The processing cost of crystalline silicon-based solar cells. Furthermore, the residuals from the silicon wafer processing are harmful to the environment. The second generation of photovoltaic technology employs thin film inorganic compounds such as a-Si:H, CdTe, and CIGS, which frequently require vacuum vapour deposition in the creation of the film, which consumes a significant amount of energy. Third-generation PV technologies include light condensed cells, organic photovoltaic cells (OPV), and dye-sensitized solar cells (DSSCs), which are meant to achieve high power conversion efficiency at low device fabrication cost. The last generation of photovoltaics is the perovskite-based solar cells which outperforming expectations in terms of delivering high power conversion efficiency in a relatively short period of time [3].

#### About Perovskite Structure

Perovskite is formed by the combination of metal with organohalide molecules, with the usual reaction formula:  $AX + BX_2 \longrightarrow ABX_3$ , where A represents a protonated amino group such as  $MA^+$  or  $FA^+$ , B represents  $Pb^{2+}$  or  $Sn^{2+}$ , and X represents a halide such as  $I^-$ ,  $Br^-$ , or  $Cl^-$ .

#### Perovskite solar cell architectures

Perovskite solar cells (PSCs) are made out of a perovskite photoactive layer sandwiched between two electrodes. To facilitate charge transport operations, inter-facial buffer layers are frequently used between the active layer and the electrodes. In PSC device architectures, there are two types of inter-facial layers: electron transport materials (ETM) and hole transport materials (HTM), which can be organic or inorganic. In general, one of the electrodes must be a transparent conducting oxide (TCO), such as indium or fluorine-doped tin oxide (ITO or FTO). The device was completed by the deposition of a metal (top) electrode made of aluminum, silver, or gold. Furthermore, there are two separate charge collection strategies from PSC devices: normal (n-i-p) and inverted (p-i-n) architectures. The letters p, n, and I denote p-type, n-type, and intrinsic layers of materials, respectively. The primary distinction between the n-i-p and p-i-n architectures is that current flows in opposing directions. Moreover, the perovskite solar cell can be categorized as mesoporous or planar based on whether it comprises mesoporous material [3-7].

**Project\_3:**  
**Encapsulation of perovskite solar cells**

**Introduction**

Perovskites solar cells have exceptional optoelectronic properties and a high tolerance for defects, providing for low-cost, high-efficiency, solution-processable photovoltaic devices [8].

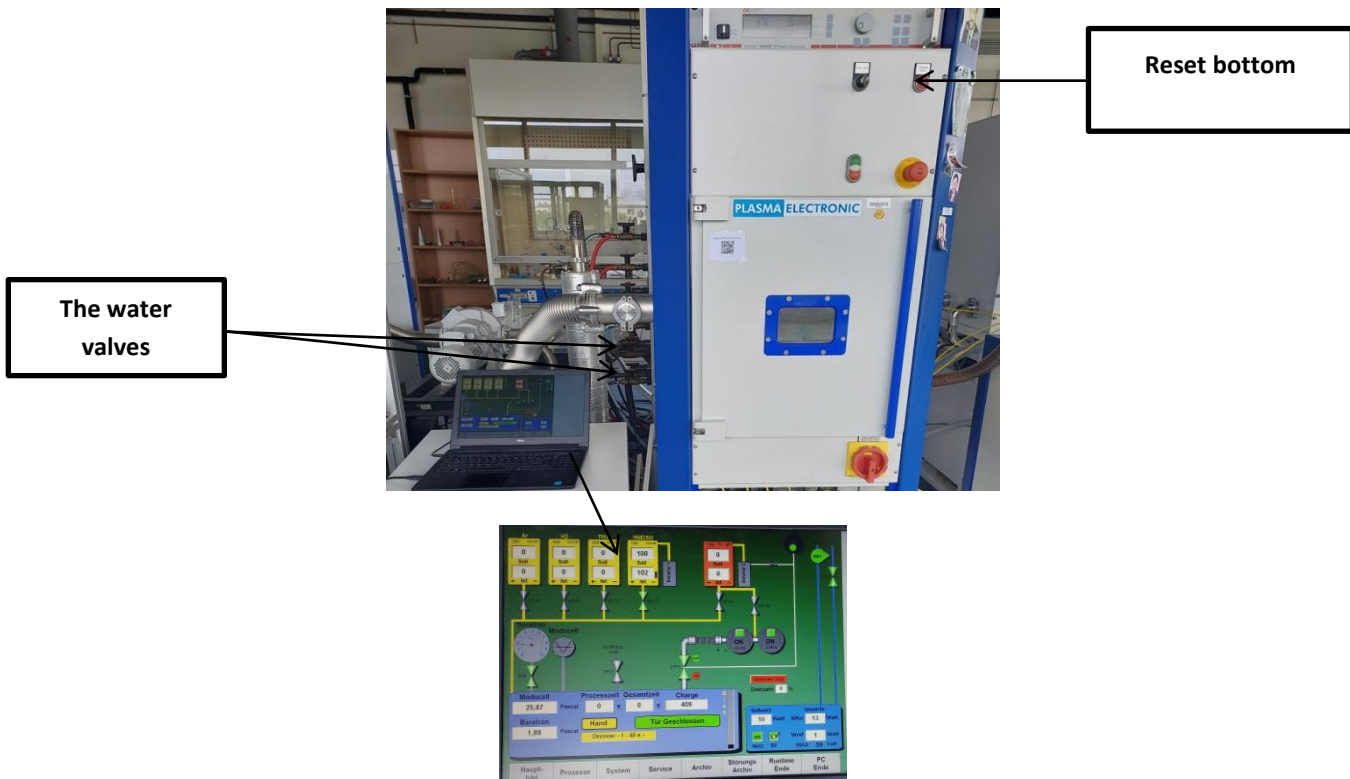
Their chemical instability, moisture sensitivity, and mechanical weakness, on the other hand, now limit their service lifetime and feasibility as a reliable solar technology. The focus of research has shifted away from boosting efficiency and toward enhancing stability, both at elevated temperatures and under operational conditions for up to a year [9-13].

**Materials used:**

1. PES solution
2. Hexamethyldisiloxane (HMDSO) / O<sub>2</sub> / tetramethylsilane (TMS)
3. Superhydrophobic solution with nanoparticles
4. Silicon elastomer + curing agent

**Encapsulation methods:**

- A. Spray coating PES solution:
- B. Superhydrophobic surface of SiO<sub>x</sub> film from O<sub>2</sub>/HMDSO by plasma enhanced chemical vapour deposition (PECVD):



C. **HMDSO by PECVD and Spray coating of superhydrophobic solution then solution PES solution:**

1. HMDSO has been coated our sample using PECVD method.
2. We spray coated the superhydrophobic solution on our sample and annealed the sample.

Then the PES solution has been coated and then annealed.

D. **Silicon elastomer and the curing agent (used for photoelectrochemical measurement application)**

The silicon elastomer was added to the curing agent with a mass ratio (10:0.5), they were mixing together then we put the mixing material in the desiccator to be evacuated and degased. We need to wait until all the bubbles disappeared.

For the encapsulation of our solar cell sample, we cover the needed area with the material and then heated the substrate.

## Project\_4:

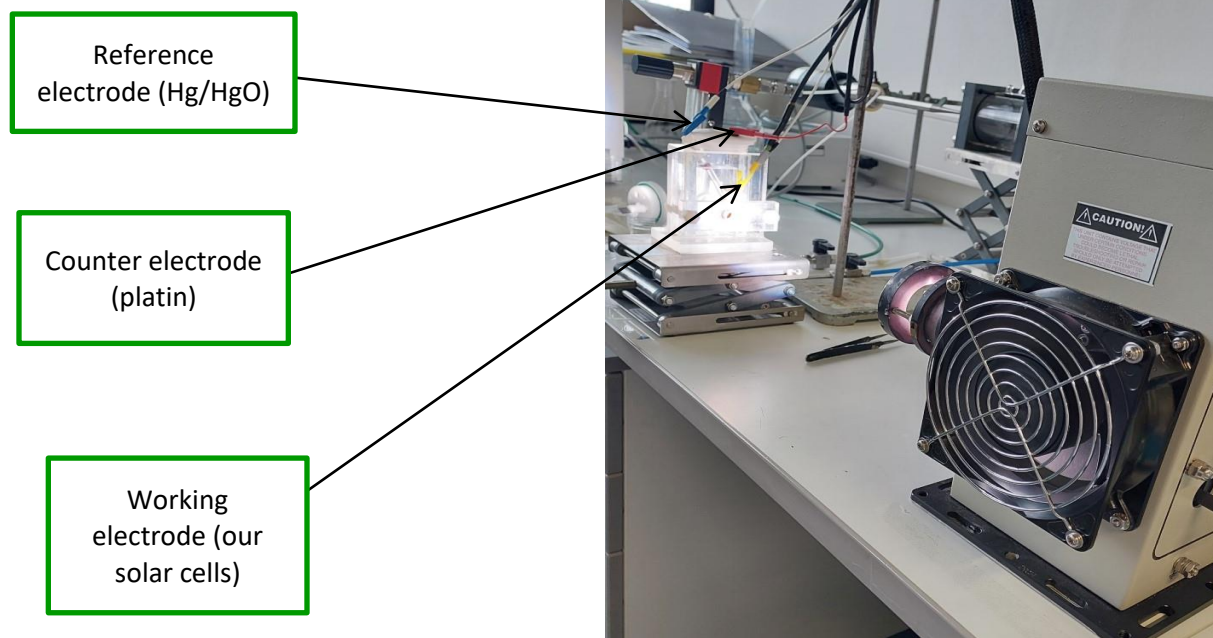
### Perovskite solar cell applied in an electrochemical cell for hydrogen evolution reaction and water splitting

#### Introduction

In recent decades, photoelectrochemical (PEC) water splitting has demonstrated technological and commercial viability. PEC is regarded as a promising method of overcoming the lack of reliable of solar energy conversion systems and an effective method of reducing the greenhouse effect. The most appealing light harvester for solar cells is organic-inorganic hybrid halide perovskite [14].

Perovskite's excellent characteristics may also make it a viable choice for PEC water splitting. Despite this, perovskite is particularly sensitive to environmental factors such as water and heat. Encapsulation strategies are required to overcome the instability in the PEC system in order to use perovskite directly in an aqueous solution [15, 16].

#### Experimental setup





## Conclusion and outlook

### Conclusion:

- Successful encapsulation of perovskite solar cells (PSC) have been demonstrated with a 4-cation  $\text{PbBr}_3$  PSC, using HMDSO and superhydrophobic solution.
- The superhydrophobic solution and silicon elastomer encapsulation are the suitable encapsulation process for a complete 4-cation  $\text{PbBr}_3$  PSC in water splitting application
- In comparison to encapsulated cells, the bare PSC was degraded when in contact with a water drop within seconds.
- HMDSO and the superhydrophobic solution are the suitable process for depositing materials on top of a complete 4-cation  $\text{PbBr}_3$  PSC.

### Outlook:

- Working extensively on perovskite solar cell stability measurement.
- Finding new ways to improve the grain size of the perovskite layer will help to boost the carrier lifetime.



## Equipment that I trained on and used during the experiments

<b>Fabrication process</b>	Spray Pyrolysis
	Spin coating
	Dip coating
	Electrode deposition
	PECVD
	Sample preparation inside the Glove box
<b>Characterization</b>	Optical characterization using: UV-Vis, FTIR
	Photovoltaic characterization
	Contact angle measurement

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## Time and destinations for socializing and sightseeing

### Hiking to Ahrtal



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