Effect of water vapor partial pressure on the perovskite film formation via chemical vapor deposition

Introduction

A **perovskite solar cell** is a type of solar cell which includes a perovskite structured compound, most commonly a hybrid organic-inorganic lead halide-based material, as the light absorber (Figure 1a). Such perovskite absorbers, with an ABX_3 crystal structure where A can be Cs^+, $CH_3NH_3^+$ (MA^+), $CH(NH_2)_2^+$ (FA^+) cations, B site is usually Pb^{2+} and X is typical I^-, Br^- or Cl^- (Figure 1b), stand out among light absorbers in the last decade. Power conversion efficiency (PCE) for single junction perovskite solar cell rapidly increases from 3.8% in 2009 to **24.2%** (certified) on a laboratory scale (0.1 cm^2), already surpassing the other well-established commercial photovoltaic technologies, e.g., multi-crystalline silicon (22.3%) and thin film copper indium gallium selenide (CIGS) (23.35%).[1] Taking efforts from the scientists in the big perovskite community, over 10000 scientific papers have been published, including 41 papers published in *Science*.

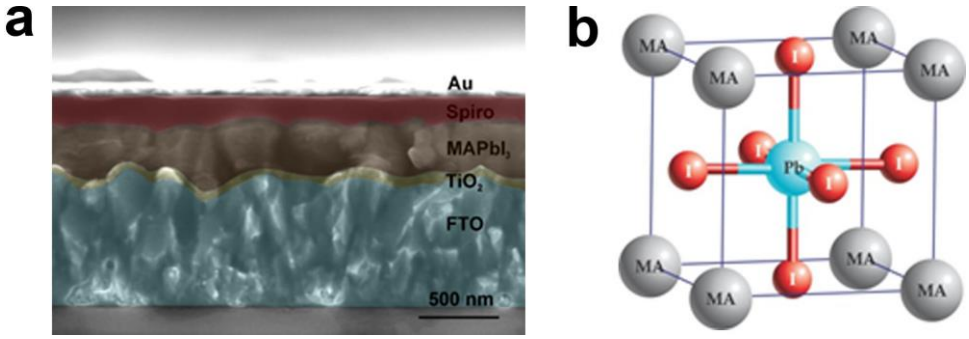

Figure 1. (a), Cross-section SEM image of a perovskite solar cell. (b), crystal structure of the $MAPbI_3$ perovskite. [2,3]

By far, most of the perovskite films showing high solar cell PCE are prepared by non-scalable methods on small active area. These methods are difficult to transfer to industrial manufacturing. Therefore, one of the main challenges is to develop reliable perovskite deposition technologies that show homogeneous perovskite film over a large area and would allow mass production in the industry. Among the scalable deposition methods developed by research laboratories and industry companies, hybrid chemical vapor deposition (CVD) shows several advantages, such as compatibility with processing methods of existing photovoltaic technologies, high PCE and low PCE loss per increased solar cell active area.[4] For the hybrid CVD method, a PbI_2 film is first deposited on the substrate by thermal evaporation and then converted to perovskite in a furnace under the vapors of organic halides, such as methylammonium iodide (MAI), formamidinium iodide (FAI), formamidinium bromide (FABr), etc. By adjusting the partial pressure of the organic halide vapor and the reaction temperature, the perovskite formation rate can be finely tuned. However, perovskite films prepared by hybrid CVD usually show a **shorter carrier lifetime** than the state-of-the-art spin-coating-processed perovskites, limiting the solar cell performance.

Humidity is reported to play an important role during the perovskite formation for solution-processed perovskite film.[5] Appropriate humidity conditions during annealing of perovskite precursor films lead to

larger perovskite grain sizes, lower carrier recombination rate and therefore higher solar cell PCE and lifetime. However, the effect of humidity on the formation of perovskite via CVD is not fully clear. During the CVD process, the conversion to perovskite usually happens under low vacuum, e.g., 100 Pa in N_2 atmosphere. For some cases when the conversion happens under low vacuum with air containing certain humidity as a carrier gas, the partial pressure of water vapor is relatively low, leading to little effect. Therefore, a systematic study on the effect of water vapor partial pressure during perovskite formation via CVD will be important and it has the potential to improve the carrier lifetime, and therefore the solar cell PCE.

Project task:

The candidate will deposit the PbI_2 films by thermal evaporation, and convert it to perovskite via CVD method under several different water vapor partial pressure conditions. The candidate will systematically investigate the phase composition, morphology, and optoelectronic properties of the perovskite film by XRD, SEM, UV-Vis spectroscopy, steady-state and time-resolved PL measurements. The optimal PVD/CVD grown perovskite absorber will be integrated into the complete perovskite solar cell and characterize its photovoltaic performances.

Duration: 4-6 months (Master thesis)

Starting date: ASAP

Required skills: Education background in Materials Science/Physics/Chemistry/Electrical engineering

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Reference

1. Solar cell efficiency chart. (accessed on Dec. 2018) https://www.nrel.gov/pv/assets/pdfs/pv-efficiency-chart.201812171.pdf.
2. Jiang. Y. et al. Post-annealing of MAPbI3 perovskite films with methylamine for efficient perovskite solar cells *Mater. Horiz.* **3**, *548–555* (2016).
3. Perovskite solar cell. (accessed on Dec. 2018) https://en.wikipedia.org/wiki/Perovskite_solar_cell.
4. Jiang. Y. et al. Combination of Hybrid CVD and Cation Exchange for Upscaling Cs-Substituted Mixed Cation Perovskite Solar Cells with High Efficiency and Stability. *Adv. Funct. Mater.* **28**, 1703835 (2018).
5. Huang, J. et al. Impact of H_2O on organic–inorganic hybrid perovskite solar cells. *Energy Environ. Sci.* **10**, 2284-2311 (2017).