'Physique et Chimie des Matériaux' – ED 397 – année 2017

Proposition pour allocation de recherche,

Envoi impératif par mail (*PDF exclusivement*) avant le lundi 20 mars 2017 à 12h à :

christian.bonhomme@upmc.fr,

! Attention : après cette date, aucun sujet ne sera pris en compte !

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Nombre de doctorants actuellement encadrés et années de fin de thèse (*: ligne à renseigner obligatoirement) : 1,5 (2018 et 2019)
Co-encadrant éventuel :

Thème* (A,B,C,D,E) : B

Titre de la thèse: Lead-Free Organic-Inorganic Halide Perovskites for Solar Cells

Description du projet (max. 1 page) : The recent introduction of methylammonium metal halide perovskite nanocrystalline compounds (structure see **Figure 1**) has stimulated a number of ground breaking developments suggesting themselves as one of the most important candidates for third-generation solar cells.[1] These perovskites was initially applied in dye-sensitized solar cells acting as a high-performance photon absorber. Subsequently, they have been applied in a variety of solid-state structures, including planar thin film *p-i-n* cells, by various chemical and physical deposition techniques. Astonishing photovoltaic performance has been achieved in these systems with power-conversion efficiency more than 22%,[1] approaching that of single crystalline silicon solar cells.

So far most perovskite solar cells were demonstrated based on methylammonium lead halide perovskite compounds. Despite their excellent performance, the use of heavy metal such as lead poses significant obstacles for their fabrication in large-scale. By comparison, organo-tin or organo-germanium halide perovskites, of a similar crystal structure as their lead counterparts, are the key determining the fate of this technology due to their much reduced toxicity. While it is possible to use other metal cations to replace lead, there have only been limited studies on lead-free perovskite systems. The initial application of organo-tin halide perovskites in solar cells resulted inferior performance compared to that from lead-containing perovskites.[2]

Objectives. In this PhD project, we aim to explore the synthesis and application of organometal halide perovskite nanocrystalline compounds in solar cells. In particular, comparison studies between lead-free halide perovskites and their lead counterparts will be performed to investigate possible directions to improve the their photovoltaic performance in comparison to lead perovskite solar cells. Practically, this project will (1) start with learning the synthesis of a few lead-free organa-metal halide perovskite compositions (e.g. methylammonium tin iodide, formamidinium tin iodide, cesium tin bromide…etc.). The candidate will compare different synthetic methods, notably the direct formation route of thin films from organic precursors and the 'two-step' route of formation of colloidal nanocrystals first and then nanocrystals into thin films. It will then involve (2) fabrication of solar cells (relevant equipments and techniques acquired in our team at LPEM[3]), (3) in-depth device characterizations of solar cells; and (4) the study of structure-property relationship in these systems.

Innovating Aspects. While there are plenty of materials and photovoltaic device studies on methylammonium lead halide perovskite compounds, studies on lead-free organometal halide perovskites are still rare. The physical origins accounting for the inferior solar cell performance based on them compared to lead halide perovskites as well as ways to circumvent the obstacles limiting their performance remain obscure but important scientific topics. Fundamental understandings in their optimal synthetic routes, optical properties, structural evolution (e.g. crystallization from solution deposition, composition homogeneity, morphology, interfacial conditions), and charge generation (upon photon absorption) are keys in order to further develop their application in solar cells. As the use of heavy metals in lead halide perovskites is not likely to enable themselves for commercial applications in large-scale, knowledge in lead-free organometal halide perovskites will lead to important innovative progress in this field.

Summary. It can be anticipated that through this study we will gain fundamental understandings on the physical origins accounting for the different characteristics between solar cells based on lead-free halide perovskites and their lead-containing counterparts. We will gain knowledge on how composition, synthesis methods, morphologies, the combination with different charge transport layers and the interfacial conditions can affect the charge generation, transport and extraction in lead-free organo-metal halide perovskite solar cells. With the knowledge obtained in this thesis, we expect to find solutions in both the material and device aspects to circumvent the issues limiting their performance and provide directions for optimized nanomaterial systems for efficient and inexpensive solar cells.

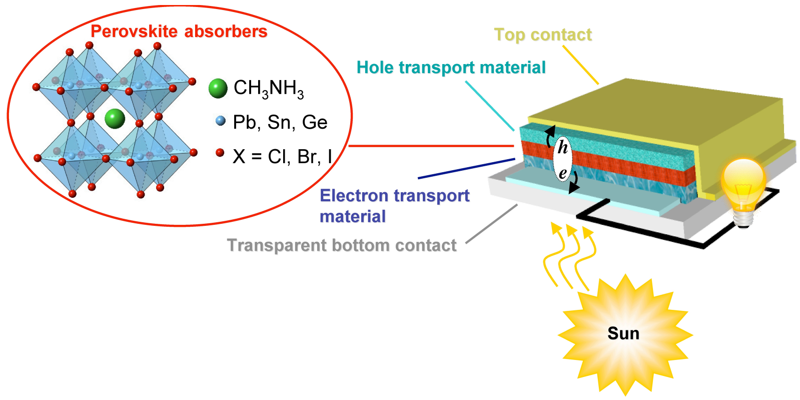

Figure 1. Schematic of the perovskite solar cell architecture.

References:
[1] W. S. Yang et al. Science 348, 1234-1237 (2015); M. A. Green et al. Prog. Photovolt: Res. Appl. 24, 905-913 (2016).
[2] W. Liao et al. Advanced Materials, 28, 9333-9340 (2016); S. Gupta et al. ACS Energy Lett., 1, 1028-1033 (2016).
[3] A. A. Bakulin et al. ACS Nano, 7, 8771-8779 (2013); Z. Sun et al. Scientific reports, 5, 10626 (2015); Z. Sun et al. Nanoscale, 8, 7377-7383 (2016).