

## Research Topic for the ParisTech/CSC PhD Program

**\*Field (cf. List of fields below):**

2. Chemistry, Physical Chemistry and Chemical Engineering
4. Energy, Processes.
8. Materials Science, Mechanics, Fluids

**Subfield:** Chemistry

**Title:** *Development of new hybrid perovskites for advanced applications.*

**ParisTech School:** Chimie-Paristech

**Advisor(s) Name:** Dr. Thierry PAUपोर्टÉ

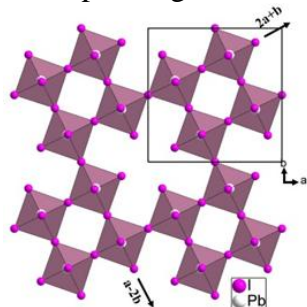
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### **Short description of possible research topics for a PhD:**

Recently, hybrid halogen perovskites (HPs) have emerged as fascinating materials and highly versatile semiconductors. These compounds can be prepared as 3D materials of  $ABX_3$  general formulae which composition can be varied over some extent. This ensures the possible tuning of their optoelectronic properties. Their properties make them attractive photoactive materials for photodetectors, solar cells, light-emitting diodes, and lasers. Recently, we have discovered a new family of 3D perovskite materials in which  $BX^+$  groups are partly replaced by a monovalent organic cation (see Ref-1 ° and Figure). Their advantages are the possibility of stabilizing certain phases, to go beyond the Goldschmidt tolerance factor and to get superior properties: high stability, finely tunable opto-electronic properties while keeping the 3D structure and a high electric conductivity.

The aim of the Ph.D will be to investigate this new family of materials. The B(II) cation will be varied (Pb, Sn, Ge). Various large replacement organic cations will be investigated. These new perovskites will be prepared as thin films. They will be designed and their properties will be tuned to integrate them in efficient and stable perovskite solar cells (PSC) and photodetectors. The work will include the full characterization of the HP layers, the fabrication of the solar cells and photodetectors as well as the characterizations of the corresponding devices.



**Required background of the student:** Material science, Chemistry, if possible Physics of semiconductors, photovoltaics.

**A list of 5(max.) representative publications of the group:** (Related to the research topic)

- 1 °) A. Leblanc, N. Mercier, M. Allain, J. Dittmer, V. Fernandez, T. Pauport é *Lead and iodide deficient MAPI, d-MAPI: the bridge between 2D and 3D hybrid perovskites*. *Angew. Chem. Int. Ed.*, 56 (2017) 16067 –16072.
- 2 °) Thierry Pauport é "Synthesis of ZnO Nanostructures for Solar Cells- A Focus on Dye-Sensitized and Perovskite Solar Cells." In “*The Future of Semiconductor Oxides in Next-Generation Solar Cells*” (2017) Chap. 1, pp.3-43.
- 3 °) M. Ulfa, P. Wang, J. Zhang, J. Liu, W. Daney de Marcillac, L. Coolen, S. Peralta, T. Pauport é *Charge Injection and Electrical Response in Low Temperature SnO<sub>2</sub>-Based Efficient Perovskite Solar Cells*. *ACS Appl. Mater. Interfaces*, (2018) DOI: 10.1021/acsami.8b10979.1.
- 4 °) M. Ulfa, T. Zhu, F. Goubard , Th. Pauport é *Molecular versus Polymeric Hole Transporting Materials for Perovskite Solar Cell Application*. *J. Mater. Chem. A.*, 6 (2018) 13350 - 13358
- 5 °) D. Pitarch-Tena, T.T. Ngo, M. Vallés-Pelarda, Th. Pauport é I. Mora-Ser ó, *Impedance Spectroscopy Measurements in Perovskite Solar Cells. Device Stability During the Measurement and Noise Reduction*. *ACS Energy Lett.*, 3 (2018) 1044–1048.