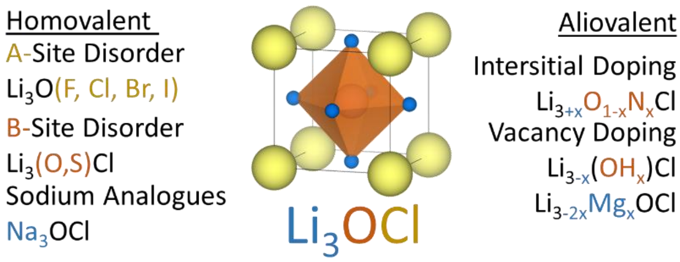
# Synthesis and Characterization of Antiperovskite Ion Conductors for Solid-State Batteries

Solid-State batteries represent one of the most promising next-generation electrochemical energy storage technologies to power the transition towards renewable energies and the electrification of transport[1]. The development of solid-state batteries is contingent on the development of solid materials with high ionic conductivities and stable with both electrodes under operating conditions[1]. Anti-perovskite materials; related to the archetype $Li_3OCl$; have recently been synthesized[2] and proposed as being stable against lithium metal[3]. In addition, their intrinsic ionic conductivity and low synthesis/processing temperatures show great promise. The proposed project entails the **rational design, synthesis and characterization** of such **anti-perovskite ionic conductors**.

**Design:** The stability and promise of a particular composition can be estimated by straightforward structural considerations involving the size of the ionic constituents and their electronegativity. This allows the identification of promising strategies in terms of homovalent or aliovalent doping or substitutions.

**Synthesis:** Novel solid-state synthesis routes are being developed in LRCS to produce antiperovskite samples of high purity. The candidate will be trained to perform inorganic synthesis and rationally adapt it to each desired product.

**Characterization:** The project will capitalize on the expertise of LRCS in advanced structural and electrochemical characterization. The intimate links between crystal structure and ionic conductivity will be investigated. The candidate will gain insight on both synthetic and structural chemistry; generally applicable in a multitude of fields.




<u>Techniques to be used</u> :

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| Synthesis: | *Solid-state, Mechanochemical, Melt-Quenching, Spark-Plasma Sintering* |
| Characterization: | Structure Determination- *X-Ray Diffraction, Infrared and Raman Spectroscopies* |
| | Ionic Conductivity- *Electrochemical Impedance Spectroscopy* |
| | Electrochemical Stability- *Cyclic Voltammetry, Galvanostatic Cycling* |
| | Thermal Stability- *Differential Scanning Calorimetry, Thermogravimetric Analysis* |

<u>Recent publications related to the topic :</u>

1. Janek, J. & Zeier, W. G. A solid future for battery development. *Nat. Energy* **1,** 16141 (2016).
2. Zhao, Y. & Daemen, L. L. Superionic Conductivity in Lithium-Rich Anti-Perovskites. *J. Am. Chem. Soc.* **134,** 15042–15047 (2012).
3. Emly, A., Kioupakis, E. & Van der Ven, A. Phase Stability and Transport Mechanisms in Antiperovskite $Li_3OCl$ and $Li_3OBr$ Superionic Conductors. *Chem. Mater.* **25,** 4663–4670 (2013).

The 6-month internship, supported by the RS2E network will be based in the Energy Hub, the brand new home of the Laboratoire de Réactivité et Chimie des Solides (LRCS) in Amiens, France. The work will be performed under the supervision of T. Famprikis and Prof. C. Masquelier. Interested candidates following a master-level course in materials science, physical chemistry or related, should direct informal inquiries or official applications to theo.famprikis@u-picardie.fr no later than **November 30th**, 2018.