ANR-18-EURE-0012

Offre de thèse en CHIMIE

Titre de la thèse : Congruent Melting Halide Perovskites for Lighting Applications

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Déroulement de la thèse : début : Septembre 2022 ; localisation: Angers et Nantes (2 x 1.5 an ou en alternance, à discuter)

Sujet de thèse :

In lighting applications, the demand for new phosphors has been rising strongly in the past years owing to their key role in white Light-Emitting Diodes (LEDs). LEDs have high potential of energy saving since they are forecasted to save 75% of the energy consumed for lighting by 2035. In this context, halide perovskites (HP) show a great potential, in particular in white light emission in the case of layered HP.[1-3] Emission properties of HP (intensity, rendering color,..) depend on the nature and structural features of the perovskite layers. Optimizing emission properties requires to tune the composition of HP.[4] However, the design of such materials is very challenging because their preparation is mainly achieved from solutions. This phD project aims to take advantage of congruent melting perovskites at moderate temperature, recently discovered at MOLTECH-Anjou, to prepare solvent-free halide perovskites. This solvent-free route between a molten phase and solids appear greener than the synthesis using solvents (such as the toxic N,N,dimethylformamide) which generates a lot of waste. And above all, this unprecedented type of reaction will lead to new materials which could not be obtained through a classical solution route and will allow a good control of their chemistry (solid-solution, doping, …) in order to optimize the photoluminescence properties.

The main objective of this project is the design of HP materials exhibiting specific emission properties (mainly broad band emission) for their integration in pc-LED. The first step will be the search of HP exhibiting a low melting temperature (T_m) and interesting emission properties. Following the strategy used in our recent discovery of a bromoplumbate hybrid perovskite exhibiting a congruent T_m as low as 151 °C and a broad band type emission, we will search for other HP with such low T_m and possessing a high stability in the molten state. The second step will consist in tuning the emission properties of the HP emitters with low T_m discovered in the first step. Taking advantage of their stability in the molten state, these HP materials will be modified through reaction with additional reagents. This solvent-free synthesis approach, which has never been considered up to now in the field of HP, will allow the design of emitting halide perovskites which could not be obtained through a classical solution route. Finally, in the third step, the most interesting materials will be used to prepare phosphor converted-LEDs.

[1,2] : M. Ben Haj Salah, N. Mercier et al. : **J. Mater. Chem C 2019**, 7, 4424; **Angewandte Chemie 2021**, 60, 834.
[3] R. Gautier et al **Advanced Materials 2019,** 31, 1807383
[4] H. Yuan, R. Gautier et al. **Angewandte Chemie 2020,** 132, 2824-2829.

Expected skills :

- Synthesis of materials.
- Crystallography and X-ray diffraction techniques : single crystal X-ray diffraction, from data collection to structure determination ; powder X-ray diffraction (thermodiffractometry, unit cell determination)
- Spectroscopy (photoluminescence, …)