Discovery of new hybrid perovskites for optoelectronic applications assisted by machine learning

Vers la découverte de nouveaux pérovskites hybrides avec l'aide de l'intelligence artificielle

Introduction:

The world's population is projected to reach eleven billion by 2100. One of the main challenges facing the human being is related to the production, storage and use of clean, sustainable and affordable energy. This problem is getting worse these days with the combined energy and pollution crises. Because of that, there is an urgent need to **supply sustainable electricity** with low CO_2 emission and in parallel **optimize and decrease our global electricity consumption**. For this aim, Hybrid Metal Halides perovskites with adjustable optoelectronic properties, represent promising and interesting materials with high photoluminescence efficiency and tunable bandgaps, providing wide range of applications as photovoltaic absorbers, light-emitting diodes, photodetectors, waveguides or nanolasers.[1-2] These compounds offer a very rich variety of crystal structures from dense 3D to low dimensional 0D structure classified by the arrangements of the metal halides octahedra. A typical hybrid halide perovskites structure has a 3D arrangement with a general formula of ABX_3 as reported in the case of methylammonium lead iodide material [$CH_3NH_3^+PbI_3^-$] MAPI) where A stands for $CH_3NH_3^+$, B = Pb_2^+ and X = I^-. Its crystal structure consists of PbI_6 octahedra sharing corners in the three spatial directions with the organic molecules filling the void. The famously known "MAPI" compound was reported to have a high-power conversion efficiency (PCE) around 25.5 %.[3-4] This behavior results from the interaction of the metal halides octahedra with low binding energy and long-range carrier transport. Lowering the dimensionality of these materials will drastically affect the excitonic migration by limiting it, allowing a more efficient radiative de-excitation pathway, increasing by so the photoluminescence quantum yield. The (TDMP)$PbBr_4$ (TDMP =trans-2,5-dimethylpiperaziniium) offers, for example, an optimized PLQY close to 60%.[5-6] A screening of the structures reported in the Cambridge Structural Data base (CSD), shows that the lead hybrid halides have 4% of 3D, 55% of 2D, 33% of 1D and 8% of 0D while most of the promising materials are 3D and 0D.

Project:

This limitation in the stabilization of such materials comes from the lack of reliable synthesis protocols. In a recent collaboration between IRCELYON, IMN we recently discovered new ways of synthesis offering the possibility to **tune and reveal unknown optoelectronics and the photonics** properties of new organic metal halides. Regarding our primary results, we expect our approach to possibly lead to the discovery of more than 300 new compounds during the 3 years PhD work period. However, if we follow a conventional path to characterize the obtained samples in terms of their crystal structures and optoelectronic properties, a huge amount of time is needed and 3 years duration of the PhD will not be enough. Therefore, in our PhD proposal we intend to develop a new method based a machine learning approach to optimize our synthesis and characterization effort to identify/optimize **0D and or 3D** materials which will be thus fully characterized in priority. In this purpose we recently developed a method based on machine learning allowing the possibility to identify from PXRD data whether the synthesized compound belongs to the perovskites family or not. [7] The synthesis, structure characterization and primary screening will be performed at IRELYON in Villeurbanne. Luminescence properties and machine learning activities will be performed at IMN Nantes.

Candidate: The PhD student will have to possess strong background in synthesis and structure characterization of new materials (inorganic, organic-inorganic) using different techniques available at

IRCELYON such as XRD (powder and single crystal), SEM, UV-VIS. In addition, the candidate has to show high interstets to the topics related to the field of luminescence.

Good organizetion and communication skills will be highly appreciated

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References:

1. Correa-Baena, J.-P.; Saliba, M.; Buonassisi, T.; Grätzel, M.; Abate, A.; Tress, W.; Hagfeldt, A., Promises and challenges of perovskite solar cells. *Science* **2017,** *358* (6364), 739-744.
2. Lin, K.; Xing, J.; Quan, L. N.; de Arquer, F. P. G.; Gong, X.; Lu, J.; Xie, L.; Zhao, W.; Zhang, D.; Yan, C.; Li, W.; Liu, X.; Lu, Y.; Kirman, J.; Sargent, E. H.; Xiong, Q.; Wei, Z., Perovskite light-emitting diodes with external quantum efficiency exceeding 20 per cent. *Nature* **2018,** *562* (7726), 245-248.
3. Kojima, A.; Teshima, K.; Shirai, Y.; Miyasaka, T., Organometal Halide Perovskites as Visible-Light Sensitizers for Photovoltaic Cells. *Journal of the American Chemical Society* **2009,** *131* (17), 6050-6051.
4. https://www.nrel.gov/pv/cell-efficiency.html.
5. Gautier, R.; Massuyeau, F.; Galnon, G.; Paris, M., Lead Halide Post-Perovskite-Type Chains for High-Efficiency White-Light Emission. *Advanced Materials* **2019,** *31* (14), 1807383.
6. Yuan, H.; Massuyeau, F.; Gautier, N.; Kama, A. B.; Faulques, E.; Chen, F.; Shen, Q.; Zhang, L.; Paris, M.; Gautier, R., Doped Lead Halide White Phosphors for Very High Efficiency and Ultra-High Color Rendering. *Angewandte Chemie International Edition* **2020,** *59* (7), 2802-2807.
7. Massuyeau, F.; Broux, T.; Coulet, F.; Demessence, A.; Mesbah, A.; Gautier, R., Perovskite or Not Perovskite? A Deep Learning Approach to Automatically Identify New Hybrid Perovskites from X-ray Diffraction Patterns. *Advanced Materials n/a* (n/a), 2203879.