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In depth exploration of MOFs photophysics and application toward new scintillating materials

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Sub topic - MOF-derived functional materials, Photophysics, Sensors and Detection

Context

Scintillating materials are one of the cornerstone of radiation detection. A scintillator is a material able to convert an incoming ionizing radiation into a burst of photon that are detectable by conventional photomultiplier. The principal characteristic of organic scintillator is the presence of fluorescent molecules in their composition, which are most commonly aromatic or poly-aromatic. This family of molecules are also widely used as ligand in MOFs design due to their rigidity. Due to their modular chemistry, MOFs are then particularly interesting candidates for scintillating materials. As a first evaluation step, we explore the photophysics of MOFs and then used MOFs as starting materials for mixed organic/inorganic dense materials for radiation detection.

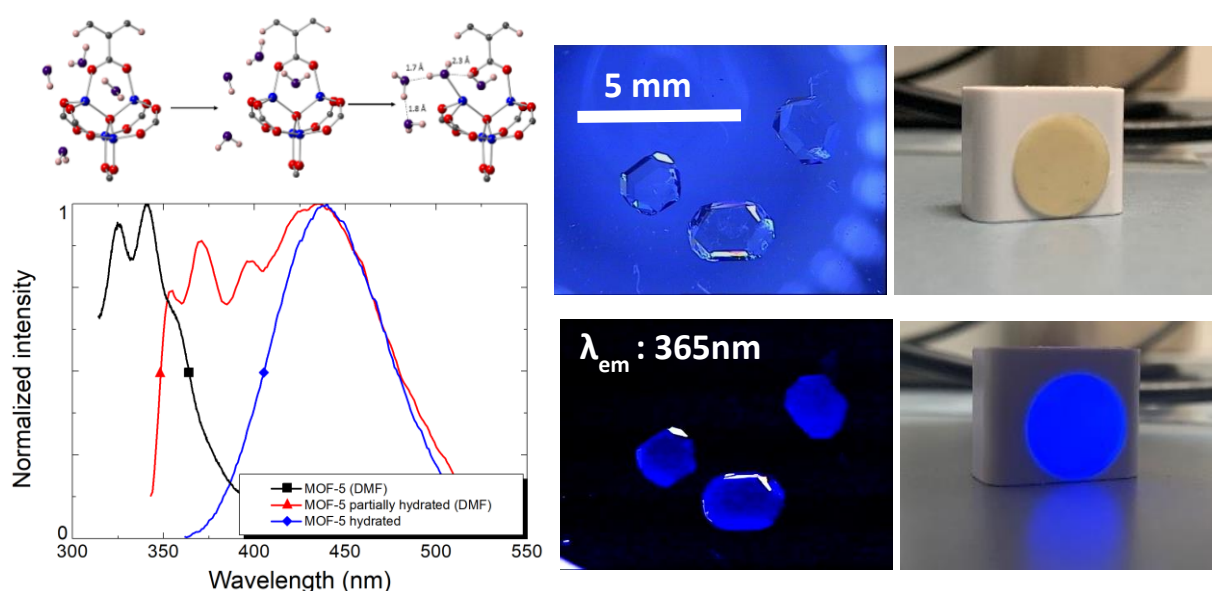


Figure 1: Fluorescence of MOF-5 and influence of hydration

Figure 2: Photos of MOF 205 as single crystal and pellet, under visible and UV lights

Objectives

This presentation will focus on the experimental observation of the true fluorescence of Zinc based MOFs. We will present our methodology that consist to performed photophysiques characterization on single crystal in different conditions. This experiment lead to observations on the effect of hydration on fluorescent MOF. Once these properties fully understood we proceed to the experimentation of MOF as scintillating materials. One of our approach was to use MOFs as a precursor for a compact scintillator. The core idea is to compress MOFs crystal into a scintillator pellet in order to make an organic scintillator with homogenous inorganic loading.

Results and discussion

Studying fluorescence of MOFs is a tough task. For example, the iconic MOF-5 fluorescence was study by three different teams with three different results and interpretation. Synthesis of iso-reticular MOFs based on Zn_4O nodes was performed and optimized in order to obtain pure phase millimetric single crystals. This allowed us to analyze their emission/excitation spectrometry and fluorescence decay time on single crystals under neutral and ambient atmosphere. We put forward two major results; the first one is the true fluorescence of MOF-5¹ that fit DFT prediction, the second one is the sensitivity of this fluorescence towards external factors which explain all the disparity found in the literature (*Figure 1*). This study was generalized towards some of the iso-reticular zinc based MOFs. Based on these results we took an approach to evaluate the scintillating properties of fluorescent MOFs. Most of the literature on this topic focus on the fabrication of MOFS/Polymer composites²; we took a different direction by compressing and heating the crystals in order to form a pellet. These samples exhibit the same photophysics properties of MOFs (*Figure 2*) despite the loss of structures and porosity. They showed scintillation properties in the same order of magnitude as other organic scintillators. The mixed nature (organic/inorganic) and density (1.5) of these materials make them more sensitive than classic organic scintillators, enabling Alpha/Beta/Gamma discrimination³.

¹ V Villemot, M Hamel, RB Pansu, I Leray, GHV Bertrand, RSC Advances 10 (31), 18418-18422

² Perego, J., Villa, I., Pedrini, A. *et al.* Composite fast scintillators based on high-Z fluorescent metal-organic framework nanocrystals. *Nat. Photonics* **15**, 393–400 (2021).

³ V Villemot, N Dufour, S Mauree, B Sabot, GHV Bertrand, M Hamel Advanced Photonics Research, 2100259