Scintillating hetero-ligand metal organic frameworks (MOF) nanocrystals with engineered Stokes shift for photonics activated by ultrafast energy transfer.

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The Stokes shift is an important property of luminescent materials, crucial in photonic devices, that sets how much an emitter would be affected by reabsorption of its luminescence. Thus, reabsorption-free materials are desirable for several applications, including the realization of scintillation detectors of ionizing radiation showing maximum output without effects on the light pulse timing. [1] [2]

Fast and large Stokes shift emission is obtained in *hetero*-ligand MOF nanocrystals. Two conjugated polyacene ligands of equal molecular length and connectivity, yet complementary photophysical properties, are co-assembled by metal oxy-hydroxy clusters, generating the nanocrystals. The fast diffusion of singlets excitons in the framework, coupled to the fine matching of co-ligands electronic properties, enables to achieve an ultrafast activation of the low energy emitting ligands by a diffusion-mediated non-radiative energy transfer in the picoseconds time scale. [3] [4] In the optimized composition, MOF nanocrystals show a fluorescence yield of ~60% with a Stokes shift of 1.3 eV. This allowed to realize prototypal scintillating surpassing both the corresponding *homo*-ligand nanocrystals and several commercial systems. [3] [4]

[1] *Nature Photonics* **15**, 393 (2021)
[2] *Nature Photonics* **17**, 672–678 (2023)
[3] *Nature Communications* **13**, 3504 (2022)
[4] *Adv. Funct. Mater*. 2404480 (2024)