Title: MOFs and their composites for environmental applications

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Metal-organic frameworks (MOFs) have gained significant attention for their versatile application in photocatalysis and environmental remediation.

In this study, PCN-222 was synthesised, characterized, and its photocatalytic efficiency was evaluated in two key processes: CO<sub>2</sub> photoconversion and photodegradation of organic pollutants in water. Meanwhile, pre-synthesized MIL-101-based materials were tested for phenol degradation via the Fenton process.

PCN-222 exhibited a good performance in the sorption and photodegradation of bisphenol A (BPA) and chlorophenols, with superoxide radicals (O<sub>2</sub>-) identified as the primary reactive species responsible for pollutant degradation. However, metal modification of PCN-222 with Zn, Mn, Co, Pd and Au, did not enhance photocatalytic activity as expected, indicating the need for further characterization and optimization of the modification process. Additionally, PCN-222 was immobilized on Al<sub>2</sub>O<sub>3</sub> foams, and it improved its recovery and potential reusability, although purification steps require refinement to remove residual contaminants. Furthermore, TiO<sub>2</sub> nanotubes were modified with PCN-222 for future photoelectrocatalysis experiments aimed at enhancing the efficiency of pollutants degradation.

In terms of  $CO_2$  photoconversion, the experiments revealed limited photocatalytic activity for the reduction of  $CO_2$  to formic acid, with PCN-222(Mn) achieving the highest efficiency (70  $\mu$ mol/g in three hours).

Regarding to Fenton process,  $NH_2-MIL-101(Fe)$  demonstrated superior efficiency compared to MIL-101(Fe), completing the process in less than five minutes. Conversely, the other MIL-101-based materials (with AI, Ti, Mn and Cr) exhibited no activity, likely due to their inability to activate  $H_2O_2$ , highlighting the role of iron in this process.

Overall, this study provides insights into the catalytic and photocatalytic behavior of MOFs for environmental applications, emphasizing the importance of material design, surface modifications, and experimental conditions in optimizing photocatalytic efficiency.

**Keywords:** MOFs, PCN-222, photocatalysis, CO<sub>2</sub> photoconversion, photodegradation of organic water pollutants, MIL-101, Fenton process.