**Influence of structural stability of porous nanoparticles on photocatalytic and photothermal performance**

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A key challenge with cancer therapy is its ability to regenerate after treatment, reducing the effectiveness of subsequent exposure as resistant cells survive. One potential solution is the use of agents that exert multimodal effects on tumor tissue, minimizing the likelihood of affected cells persisting and, in turn, lowering the risk of cancer recurrence.

Metal-organic frameworks (MOFs) are a class of hybrid porous materials consisting of metal nodes and organic ligands structured into a crystal lattice. MOFs are highly porous on a structural level, being able to entrap molecules within their crystal lattice, which combined with their ability to generate reactive oxygen species (ROS) through photocatalytic activity makes them a promising potential agent for photodynamic or combined therapy [1]. Additionally, the possibility of using MOF nanoparticles as photothermal nanomaterials is being actively studied [2].

The mechanism of ROS generation by MOFs is quite typical for semiconductor materials — after absorbing photons of energy larger than the bandgap formed by ligands and metallic nodes, an electron-hole pair is created and the charge migrates to the highly developed surface of the MOF. There, an electron reduction of oxygen to superoxide radical and hole oxidation of water to hydroxyl radicals occur. These reactive oxygen species then proceed to attack organic molecules, cleaving bonds and mineralizing them into CO2, water and simple ions, effectively destroying original compounds [3].

Despite there being a number of works on visible-light photocatalytic activity of MOFs, most focus on solar light-driven catalysis and optimization of MOFs to such conditions. An alternative approach using lasers to induce photocatalysis offers several advantages. These include the ability to detect and characterize even subtle photocatalytic activity of nanoparticles, as well as allowing to separate different modalities of exposure: the effect of laser irradiation on the dye, the catalytic activity of ROS generated by MOFs, and the photothermal effect of nanoparticles.

The aim of this work was to compare MOF nanoparticles of the same crystalline structure and different metal ions in their photocatalytic and photothermal performance. For this purpose, Al-, Fe-, and Cr-based MOFs were synthesized and characterized by using dynamic light scattering, UV-vis spectroscopy, scanning-electron microscopy and X-ray crystallography. The photocatalytic activity of MOFs under 450 nm laser irradiation was characterized on aqueous solutions of Rhodamine B by changes in the absorption spectra of the dye. The photothermal activity of MOFs was investigated using an infrared camera.

MOF nanoparticles have shown severely differing photocatalytic and photothermal performance, which is associated with the additional energy states in metal atoms, enabling oxidation reactions or thermal conversion of absorbed electromagnetic waves.

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**References**

1. Ni, K. [et al.]. Nanoscale Metal–Organic frameworks generate reactive oxygen species for cancer therapy // ACS Central Science. 2020. V. 6(6). P. 861–868.

2. Yin, X. [et al.]. Recent development of MOF-Based photothermal agent for tumor ablation // Frontiers in Chemistry. 2022. V. 10.

3. Wang, Y. [et al.]. Bimetallic UiO-66-NH2(Zr–Hf) synergistic photocatalytic and piezoelectric effects for the degradation of rhodamine // B. Dalton Transactions. 2023. 52(29), 10079–10088.