Design Cellulose/Metal-organic Framework Hybrids for Functional Adsorbents and Luminescent Sensors

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[ORAL PRESENTATION] Metal-organic frameworks (MOFs) emerge as appealing nanoparticles because of their high surface area and porous structure functionality. However, the intrinsic agglomeration and inferior processibility of MOF particles often restrict their applicability and recyclability in the real world. To address these limitations, cellulosic biopolymers are explored as a flexible and sustainable supporting material to hybridize MOFs. The combination of cellulose and MOFs enables the design of tangible and processible materials with remarkable synergic features of both building components. We have achieved the designing and engineering of a new type of cellulose/metal-organic frameworks (Cello-MOF) hybrid using sulfonated cellulose nanofibrils (SCNF) as a biopolymer and template. This judicious design is based on the hypothesis that sulfonate groups increased the electronegativity and enhanced the dispersibility of the cellulose fibers and the negatively charged sulfonates could be manipulated as anchors for metal ions to initiate the *in situ* growth of MOFs along the surface of cellulose fibers. We have achieved the synthesis of three types of SCNF/MOF hybrids, namely, SCNF/ZIF-8, SCNF/ZIF-67, and SCNF/HKUST-1. Additionally, we have developed a portable 2D sensing pad by integrating cellulose nanofibers with luminescent MOF featuring aggregation-induced emission properties. The resulting hybrid material exhibits fluorescent properties under UV exposure, which can be used to identify and quantify commonly used methyl parathion pesticides. Time-dependent Density Functional Theory calculations were employed to elucidate the underlying mechanisms of the cellulose-MOF assembly and the molecular host-guest interactions. Our study offers a versatile and robust biopolymer substrate for templating a wide array of MOFs with promising applications as adsorbents, sensors, catalysts, and beyond.