A Porous, Electrically Conductive Hexa-Zirconium(IV) Metal-Organic Framework

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Engendering electrical conductivity in high-porosity metal-organic frameworks (MOFs) promises to unlock the full potential of MOFs for electrical energy storage, electrocatalysis, or integration of MOFs with conventional electronic materials. Here we report that a porous zirconium-node-containing MOF, NU-901, can be rendered electronically conductive by physically encapsulating C₆₀, an excellent electron acceptor, within a fraction (ca. 60%) of the diamond-shaped cavities of the MOF. The cavities are defined by node-connected tetra-phenyl-carboxylated pyrene linkers, i.e. species that are excellent electron donors. The bulk electrical conductivity of the MOF is shown to increase from immeasurably low to 10⁻³ S cm⁻¹, following fullerene incorporation. The observed conductivity originates from electron donor-acceptor interactions, i.e. charge-transfer interactions – a conclusion that is supported by density functional theory calculations and by the observation of a charge-transfer-derived band in the electronic absorption spectrum of the hybrid material. Notably, the conductive version of the MOF retains substantial nanoscale porosity and continues to display a sizable internal surface area, suggesting potential future applications that capitalize on the ability of the material to sorb molecular species.

References:

Goswami et. al, Chemical Science, 2018, DOI: 10.1039/c8sc00961a