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

Subhadip Goswami, [†] Debmalya Ray, [‡] Ken-ichi Otake, [†] Chung-Wei Kung, [†] Sergio J. Garibay, [†] Timur Islamoglu, [†] Yuexing Cui, [†] Christopher J. Cramer, [‡] Omar K. Farha, [†, §], Joseph T. Hupp[†,*]

[†] Department of Chemistry, Northwestern University, 2145 Sheridan Road, Evanston, IL 60208, United States

[‡] Department of Chemistry, Chemical Theory Center, and Minnesota Supercomputing Institute, University of Minnesota, 207 Pleasant Street SE, Minneapolis, MN 55455

[§] Department of Chemistry, King Abdulaziz University, Jeddah 21589, Saudi Arabia

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 C_{60}, 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:

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