

Poster Sessions

Ultra-high porosity in MOFs: One of the most important properties of metal-organic frameworks (MOFs) is their high porosity and high specific surface area, which has led to many applications concerned with gas storage, separations, and catalysis. An important consideration in maximizing the uptake of gases within porous MOF crystals is to increase the number of adsorptive sites within a given material. We have succeeded in preparing materials with ultra high porosity (10400 m²/g Langmuir) by combining octahedral SBUs with tritopic linkers, following the isoreticular expansion principle (MOF-180, -200). In addition, the combination of tritopic and ditopic linkers also led us to highly porous materials with new topologies (MOF-210, -205).

Multiple Functional Groups of Varying Ratios in Metal-Organic Frameworks (MTV-MOFs): We show that MOFs can incorporate a large number of different functionalities on linking groups in a way that mixes the linker, rather than forming separate domains. Our strategy to making MTV-MOFs is to assemble their structures from links with different functional groups whose orientation, number, relative position, and ratio along the backbone can be controlled by virtue of the unchanged length of the link and its unaltered connectivity. In this way, each of the pores within the MOF would have an array of functionalities pointing into its center.

Porous Materials with charge mobility and electrical conductivity:

We have prepared two covalent organic frameworks (COFs) with structures based on covalently linked porphyrin units to afford sheets in which the porphyrin units are stacked laterally to give an efficient conducting interface. The two porphyrin COFs (COF-66 and COF-366) have been found to be hole conducting with mobilities as high as 8.1 and 3.0 cm²V⁻¹s⁻¹. Such multifunctional conducting COFs combine thermal stability, electrical conductivity, high charge mobility, and pore accessibility and, as the first members of the COF family to exhibit such properties, represent an important step towards plastic electronics and optoelectronics.

By combining 1,2,3-triazole and divalent metal atoms, a new family of seven metal-triazolates, METs, has been prepared. The crystal structure of the compounds has been determined *ab initio* by applying the charge flipping method to powder X-ray diffraction data obtained from a laboratory X-ray source. The new compounds exhibit a dia network type, built up from tetrahedral secondary building units. All the materials are porous, having surface area in the range 480 - 1100 m²/g. The Fe(II)-MET material has proven to have electrical conductivity. Measurements carried out in a pressed pellet of Fe-MET reveals a conductivity value of 10⁻³ S cm⁻¹.

Keywords: porous, powder, MOFs

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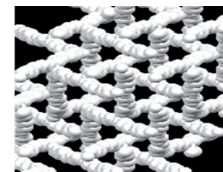
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A series of rarely observed all helical 3-D coordination polymers derived from various chiral amino acids :effect of amino acid side chain & their unique ability of separating cations & anions

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Design and synthesis of functional MOF is an active area of material research for their various potential applications viz. molecular storage, catalysis, magnetism, non-linear optical material, selective anion separation etc. Crystal engineering is a major support in developing different novel functional MOFs.[1] When these tailor-made MOFs engineered by crystal engineering approach are chiral then these become even more important for their immense possibility to be used as a promising functional material. Moreover chiral helical coordination polymers are also interesting for their fascinating supramolecular architectures. Four rarely observed all

helical 3-D coordination polymers (all belong to enantiomorphic P3₂1 space group) derived from chiral amino acid based viz. Phenyl alanine, alanine, leucine bis pyridyl bis amide ligands with Cu²⁺ are studied by single crystal X-ray diffraction. The study is undertaken in order to demonstrate the effect of amino acid side chain on overall supramolecular architecture. This is a part of our ongoing research efforts which include a detail and systematic study of amino acid side chain on overall supramolecular architecture within a coordination network[2]. The unique ability of those MOF to separate cations and anions are also worthwhile to be mentioned here.



General views of MOFs along c-direction

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Keywords: 3D, coordination, polymer

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Photonic materials: how protonation influence structure and properties

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Salt formation is the most common and effective method to increase solubility and dissolution rates of drugs. For compounds containing amino groups their protonation in presence of acids leads to formation of salts with better solubility than for neutral compounds. On the other hand, if consider compounds for potential application as photonic materials in photodynamic therapy, it should be taken into account that protonation might significantly influence molecular polarizability, and hence photonic properties of such materials. Series of neutral, mono- and triprotonated (dialkylammonio)-benzylidenepiperidones was structurally characterized and geometrical characteristics were compared with results of quantum-chemical computations. Spectroscopic evaluation of one and two-photon absorption properties, and hyperpolarizabilities values are compared with geometrical characteristics obtained for neutral and protonated materials.

Keywords: organic salts, NLO properties, benzylidenepiperidones

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Two Co(III) dioximates with unprecedented V-shape ligands in apical positions

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