

# Contaminants Removal From Fuel Cells for Aerospace Applications

Jack Y. Lu

**Abstract**—Research has been focused on the rational design and synthesis of new metal-organic fibers (MOF) materials for a polymer electrolyte membrane (PEM) FC fuel processing system in which the MOF material is an integral component and the key for contaminant removal in hydrocarbon or ammonia fuel processors. Design and synthesis of desirable MOF materials for uses in fuel processors will have immediate impact on a wide range of space applications.

**S**YNTHESIS OF FUNCTIONAL materials represents one of the great challenges in current research. Coordination polymers have found a wide range of applications, such as molecular separation and pollution prevention in air, liquid, and water systems, where they can be used as ion exchangers and molecular sieves. The objective of the research is to design and develop robust metal-organic framework (MOF) materials that may selectively remove small molecule contaminant(s) produced by the fuel processing system of a fuel cell.



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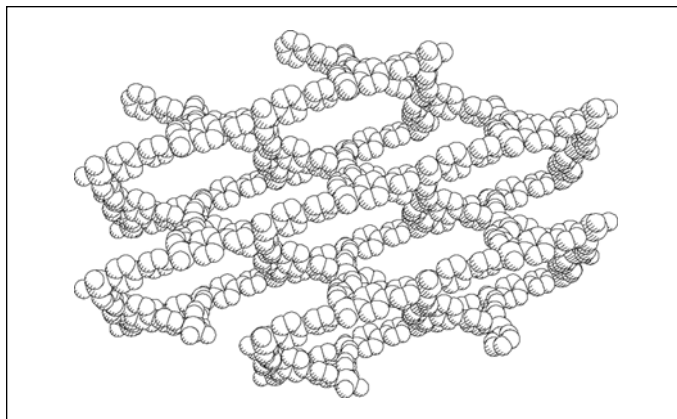


Figure 1. The Open Channel Structure

## Experimental Activity, Results and Discussion

Among the metal-organic coordination polymers synthesized in our laboratory  $[Cu(BPY)(NO_3)_2]_n$  (BPY = 4,4'-bipyridine)<sup>1</sup> is a new metastable coordination polymer. It was further reacted with additional 4,4'-bipy, resulting in a new self-assembled MOF featuring the first two-fold interpenetrating 3-D  $4^2.8^4$  network structure:  $\{[Cu(BPY)_2(H_2O)_2][Cu(BPY)_2(H_2O)(NO_3)]\}(NO_3)_3 \cdot 12H_2O$ .<sup>1</sup> The two independent 3-D networks in this compound, when minimally interpenetrating, enable this 3-D open-channel structure to accommodate a large amount of water molecules and nitrate anions. Such inclusion phenomena in interpenetrating open-frameworks are very suggestive of practical applications, especially in those open-channel structures with minimum interpenetrating frameworks (Fig. 1).

The reactions of  $Cd(NO_3)_2 \cdot 4H_2O$  with imidazol-4,5-dicarboxylic acid and 4,4'-bipyridine under hydrothermal reaction conditions resulted in two new metal-organic polymers.<sup>2</sup> The hydrogen-bonding linked 3-D structure of complex **2** composed of covalent pleated sheets. The pleated sheet conformation here is derived from the bonding-mode of the tetradentate HIDC<sup>2-</sup>

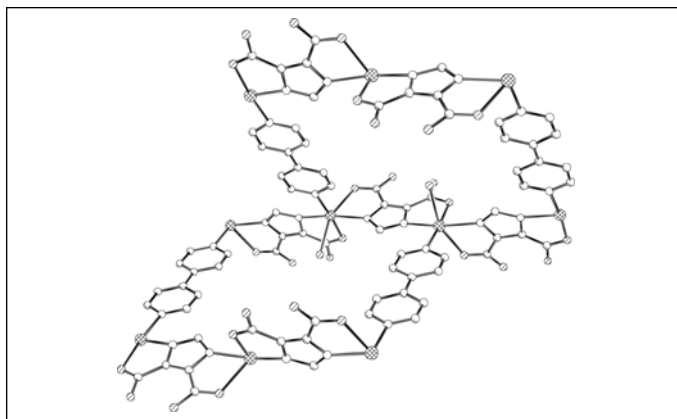


Figure 2. View of the Rectangular Grids in the Structure

ligands and the rigid BPY spacers. The rectangular grids (BPY-Cd-HIDC<sup>2-</sup>-Cd-HIDC<sup>2-</sup>-Cd-BPY-Cd-HIDC<sup>2-</sup>-Cd-HIDC<sup>2-</sup>-Cd) in the 2-D covalent pleated sheet conformation network have corner metal-to-metal distances of  $13.564 \times 11.754 \text{ \AA}$  (Fig. 2).

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### References

<sup>1</sup>J. Y. Lu, W. A. Fernandez, Z. H. Ge, and K. A. Abboud, "A Novel Two-Fold Interpenetrating 3-D  $4^2.8^4$  Network Self-Assembled from a New 1-D Coordination Polymer," *New J. Chem.* 29 (2005): 434.

<sup>2</sup>J. Y. Lu and Z. H. Ge, "Synthesis and Structures of Two New Metal-Organic Polymers Containing Imidazoldicarboxylate Ligands for Hydrogen Bonding Networks, One with a Covalent Pleated Sheet Conformation," *Inorg. Chim. Acta* 358 (2005): 828.

### Publications

Lu, J. Y. and Z. H. Ge. "Synthesis and Structures of Two New Metal-Organic Polymers Containing Imidazoldicarboxylate Ligands for Hydrogen Bonding Networks, One with a Covalent Pleated Sheet Conformation," *Inorg. Chim. Acta* 358 (2005): 828.

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