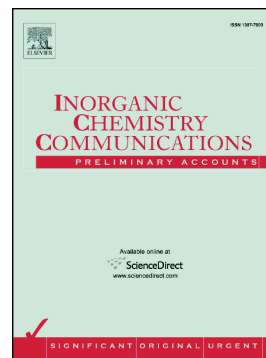


Accepted Manuscript

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PII: S1387-7003(18)30781-0
DOI: doi:[10.1016/j.inoche.2018.09.025](https://doi.org/10.1016/j.inoche.2018.09.025)
Reference: INOCHE 7116
To appear in: *Inorganic Chemistry Communications*
Received date: 21 August 2018
Revised date: 14 September 2018
Accepted date: 15 September 2018

Please cite this article as: Fumin Wang, Weicong Liu, Saying Li, Robert W. Gable, Huarui Zhong, Qiuxia Xu, Gaoxiang Huang, Amita Singh, Jianqiang Liu, Abhinav Kumar, A polyhedral metal-organic framework based on rigid precursor for photocatalytic properties. Inoche (2018), doi:[10.1016/j.inoche.2018.09.025](https://doi.org/10.1016/j.inoche.2018.09.025)

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A polyhedral metal-organic framework based on rigid precursor for photocatalytic properties

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Abstract

A 3D polyhedral metal organic framework, $[\text{Cu}_4(\text{L})_2(\text{H}_2\text{O})_4 \cdot 5\text{DMF}]_n$ (**1**) (H_4L = 3,5-di(3,5-dicarboxyphenyl)nitrobenzene), has been designed and successfully synthesized. **1** shows a 3D *mfi* topological framework with 1D triangular channels. The UV diffuse reflectance spectroscopy of the MOF indicates its semiconducting nature which induces photocatalytic property in the MOF. The photocatalytic property of **1** in photo-degradation of organic dyes viz. methyl violet and Rhodamine B have been investigated. The possible mechanism for the photocatalytic activity of **1** against organic dyes has been addressed using density of states (DOS) and partial DOS (pDOS) calculations.

Keywords: tetracarboxylate; photocatalysis; calculation

Photocatalysis is a new technology for the treatment of all kinds of industrial dyes and this area have received considerable research attention in the field of catalysis [1-2]. Recently, metal– organic frameworks (MOFs) have been demonstrated to be an efficient photocatalyst in the green degradation of organic pollutants [3]. However, industrial applications of MOFs in ultraviolet-light-driven photocatalysis are just commenced to emerge. To synthesize inexpensive, stable, and efficient MOF photocatalyst is still a big challenge [4].

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