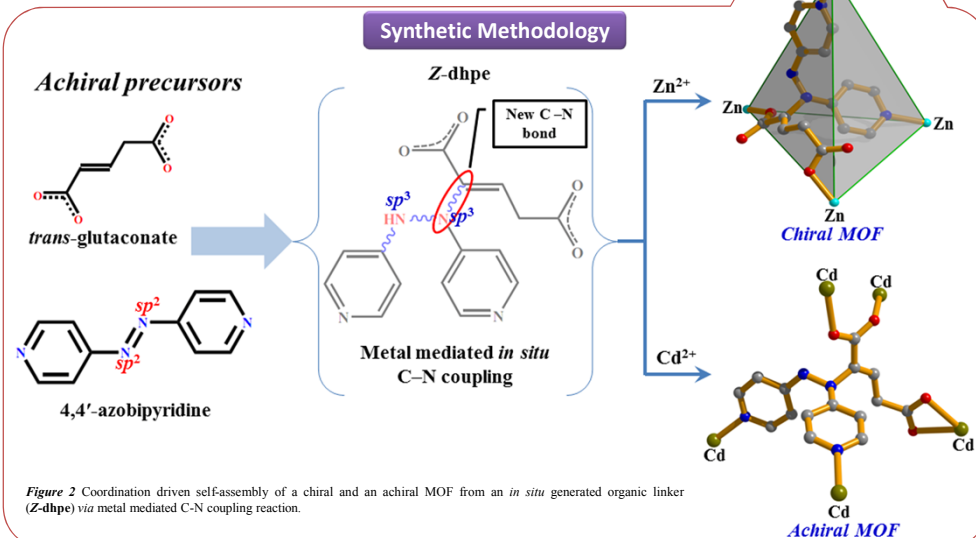
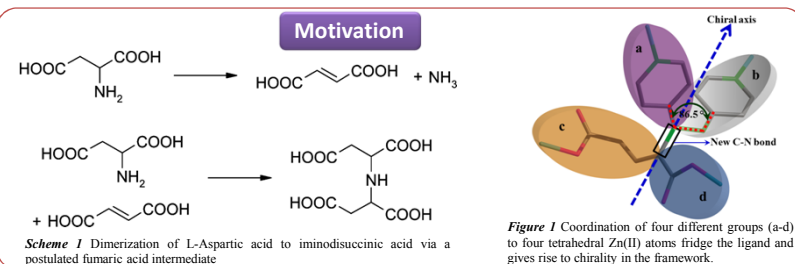
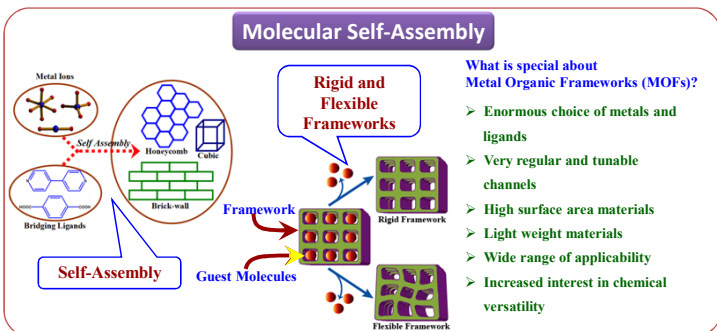


# Coordination Driven Axial Chirality in a Microporous Solid Assembled from an Achiral Linker via *In Situ* C-N Coupling

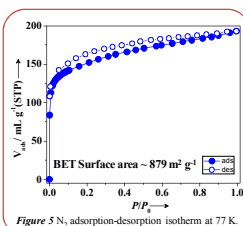
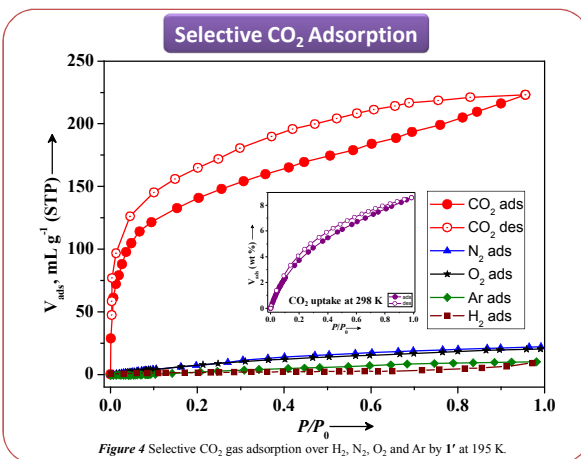
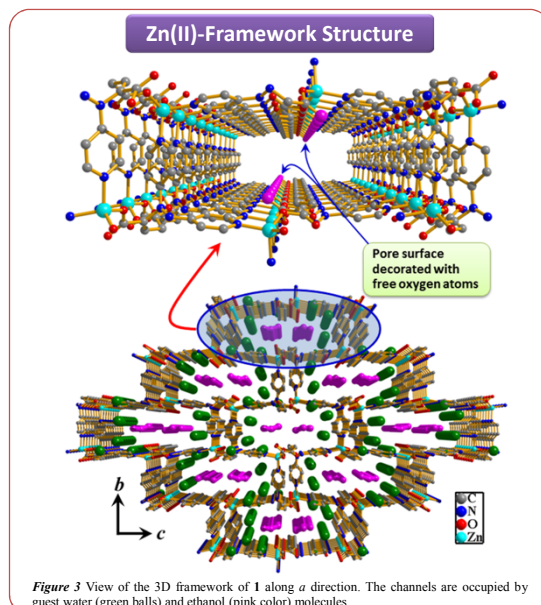
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**Figure 2** Coordination driven self-assembly of a chiral and an achiral MOF from an *in situ* generated organic linker (Z-dhpe) via metal mediated C-N coupling reaction.



**Table 1** Summary of crystal data and refinement results.

Samples	Space group	<i>a</i> (Å)	<i>b</i> (Å)	<i>c</i> (Å)	<i>R</i>	<i>R<sub>w</sub></i>	Flack
Crystal 1	<i>P</i> <sub>2</sub> <sub>1</sub> <sub>2</sub> <sub>1</sub>	8.741(5)	14.796(5)	19.340(5)	0.086	0.2689	0.00(3)
Crystal 1a	<i>P</i> <sub>2</sub> <sub>1</sub> <sub>2</sub> <sub>1</sub>	8.7423(6)	14.7183(11)	19.3742(15)	0.0843	0.2300	0.01(6)
Crystal 1b	<i>P</i> <sub>2</sub> <sub>1</sub> <sub>2</sub> <sub>1</sub>	8.7726(4)	14.7582(9)	19.3159(10)	0.0797	0.2428	0.02(4)
Crystal 1c*	<i>P</i> <sub>2</sub> <sub>1</sub> <sub>2</sub> <sub>1</sub>	8.7611(8)	14.7839(16)	19.353(2)	0.0811	0.2286	0.05(5)
Crystal 1d*	<i>P</i> <sub>2</sub> <sub>1</sub> <sub>2</sub> <sub>1</sub>	8.7562(6)	14.8244(11)	19.3329(14)	0.0798	0.2285	-0.01(5)

Crystals with and without \*mark have opposite handedness.

## Conclusions

- ❑ We show that Zn(II) mediates *in situ* C-N coupling reaction during construction of a MOF.
- ❑ The unusual distorted tetrahedral geometry of the newly *in situ* formed ligand, with a *Z*-configuration, and its asymmetric coordination with Zn(II) directs the structure in all the three crystallographic axes to generate a chiral 3D framework structure.
- ❑ The chirality in compound 1 is of axial type and is completely coordination driven.
- ❑ The microporous nature of the framework has been established by gas adsorption studies. More interestingly, the compound shows selective adsorption of CO<sub>2</sub> gas over H<sub>2</sub>, N<sub>2</sub>, O<sub>2</sub> and Ar at 195 K.

**Acknowledgement:** Financial supports from ICAM-I2CAM, 1 Shields Avenue, Davis, CA 95616 (NSF Grant Number DMR-0844115) and Council of Scientific and Industrial Research, Govt. of India are highly acknowledged.

**Reference:** Prakash Kanoo, Ritesh Halder, Soumya T. Cyriac and Tapas Kumar Maji, Submitted, 2011.



# THANK YOU