Center for Gas Separations Relevant to Clean Energy Technologies

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Mission and Approach

The aim of the Center is to develop new strategies and materials that enable energy-efficient separations of gases, as required in the clean use of fossil fuels and in the generation of alternative fuels.

Particular emphasis will be placed on:

(1) Separation of CO_2 from power plant flue streams

(2) Separation of CO_2 from natural gas deposits

The research will involve close cooperation between three teams:

Materials Synthesis Team

- microporous metal-organic frameworks
- microporous polymers

Materials Characterization Team

Computational Separations Team

Metal-Organic Frameworks for Gas Separations

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Omar Yaghi
UCLA

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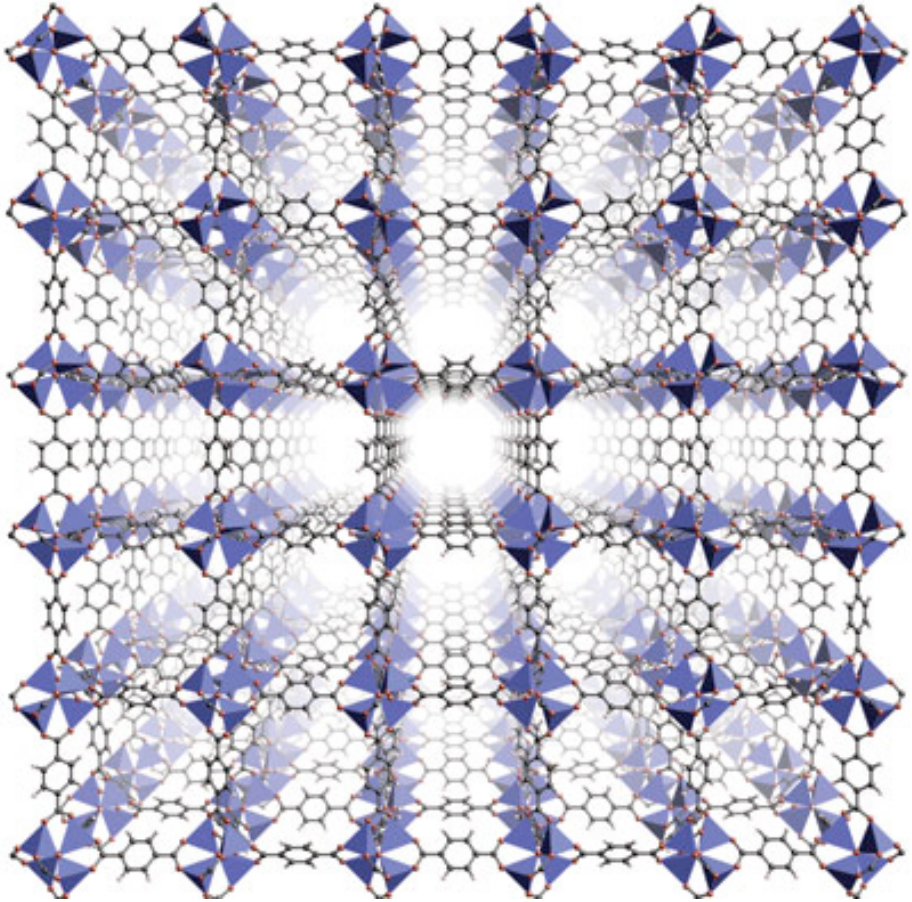
Texas A&M

Metal-Organic Frameworks



Zn_4O(1,4-benzenedicarboxylate)$_3$
(MOF-5)

BET surface areas up to 4800 m^2/g

Density as low as 0.4 g/cm^3

Adjustable pore sizes of up to 5 nm

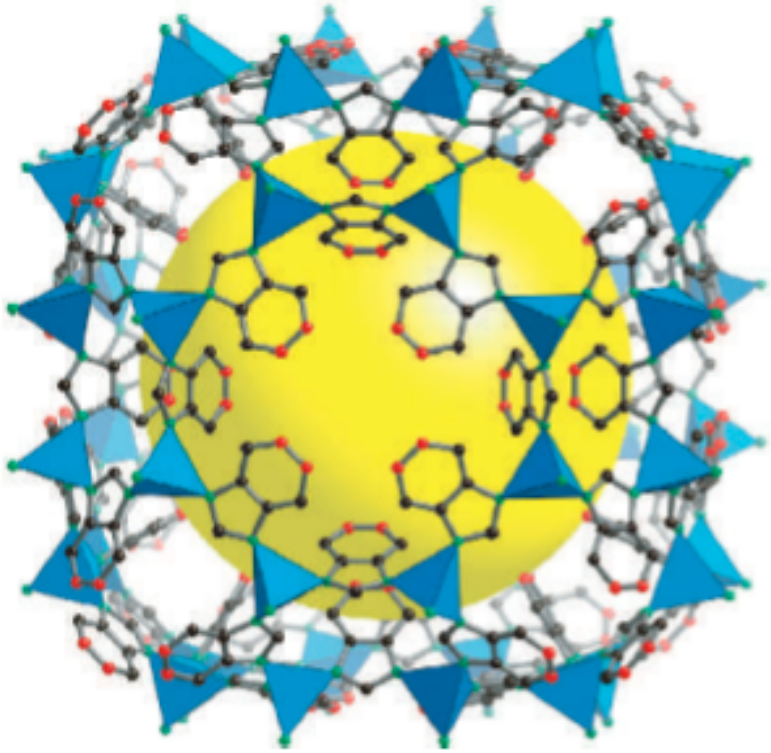
Channels connected in 1-, 2-, or 3-D

Internal surface can be functionalized

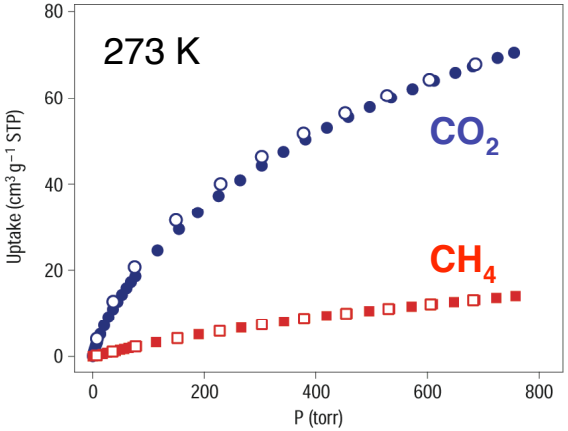
Can these porous, high-surface area materials be used for gas separations?

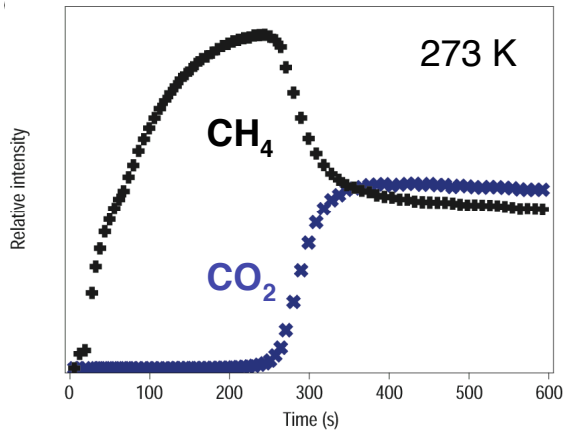
Yaghi et al. *Nature* **2003**, *423*, 705

Demonstration of CO_2/CH_4 Separation



ZIF-20

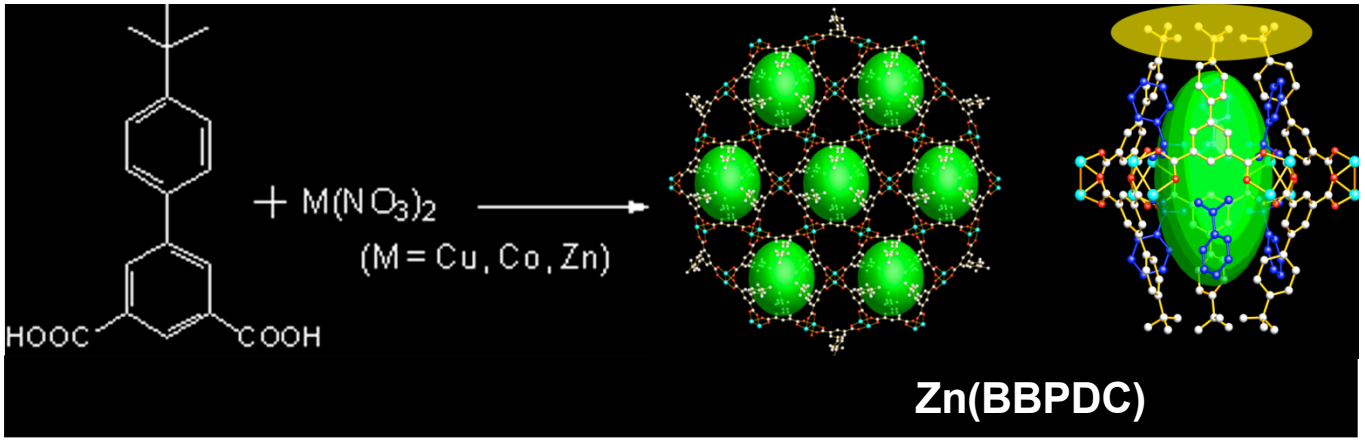


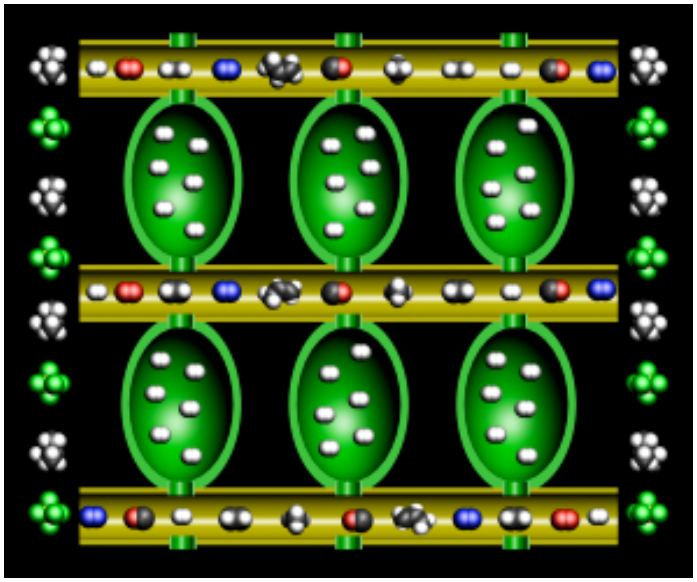


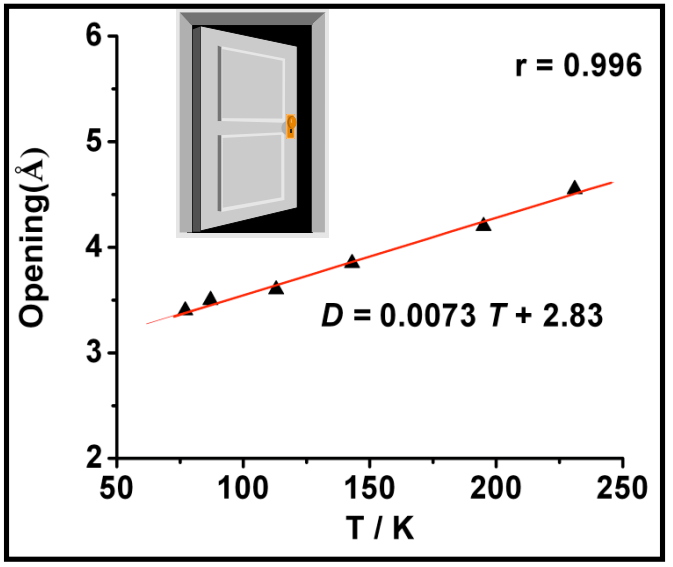
- Purinate functionality appears to be key in carrying out the separation
- Mechanism (pores size versus chemical interaction) is not yet known

Hayashi, Côté, Furukawa, O'Keeffe, Yaghi *Nature Mater.* **2007**, *6*, 501

Mesh-Adjustable Molecular Sieves

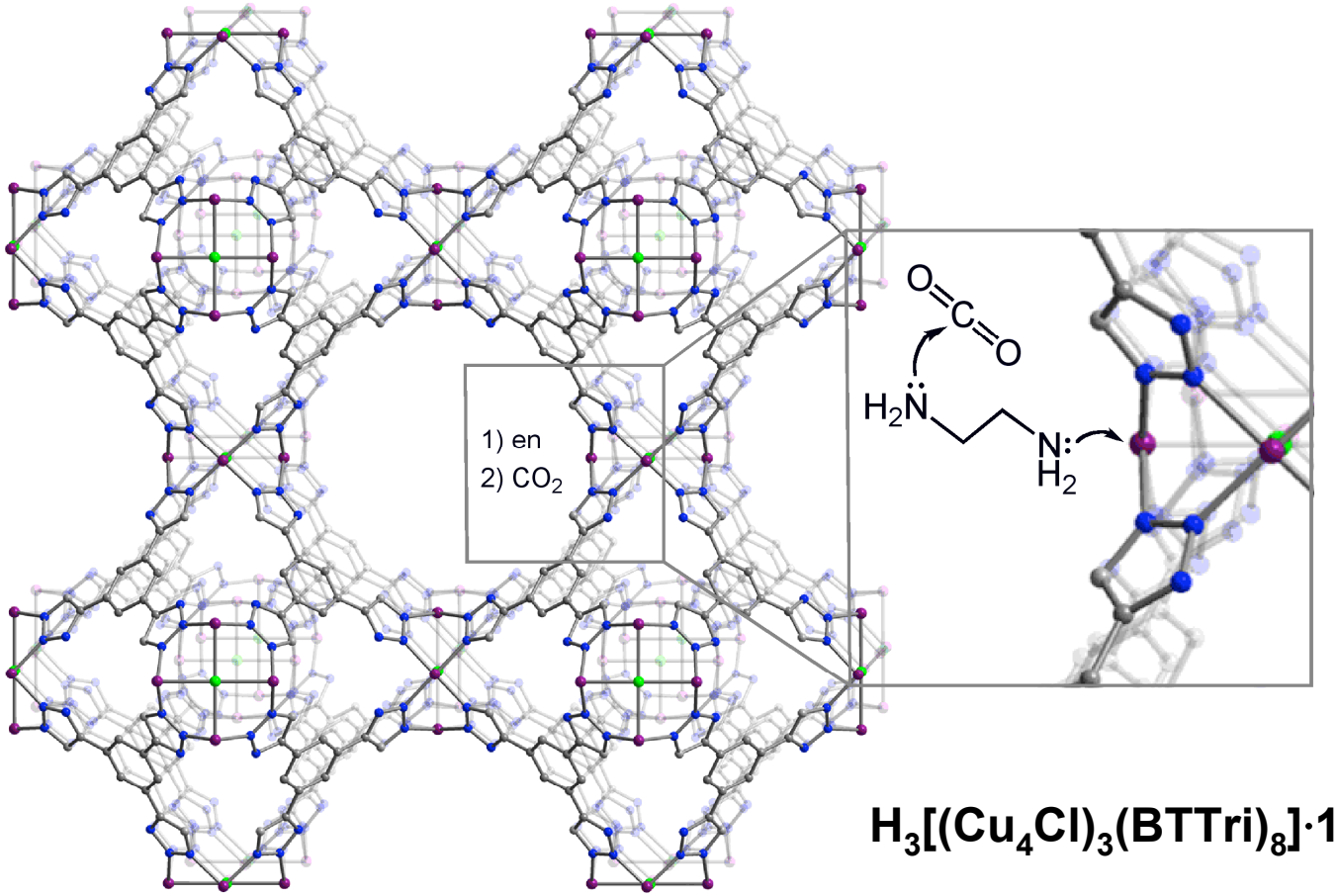






Ma, Sun, Wang, Zhou *Angew. Chem., Int. Ed.* **2007**, *46*, 2458

Alkylamine-Functionalized MOF Surfaces

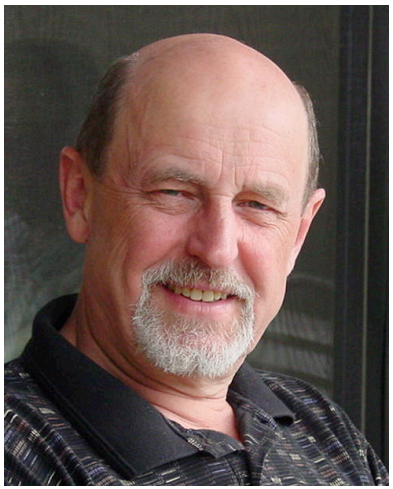


$H_3[(Cu_4Cl)_3(BTTri)_8]\cdot 12en$

- Initial isosteric heat of CO_2 adsorption of -90 kJ/mol observed
- Methods for directly functionalizing bridging ligands are under development

Demmesence, D'Alessandro, Foo, Long *J. Am. Chem. Soc.* **2009**, *131*, 8784

Microporous Polymers for Gas Separations



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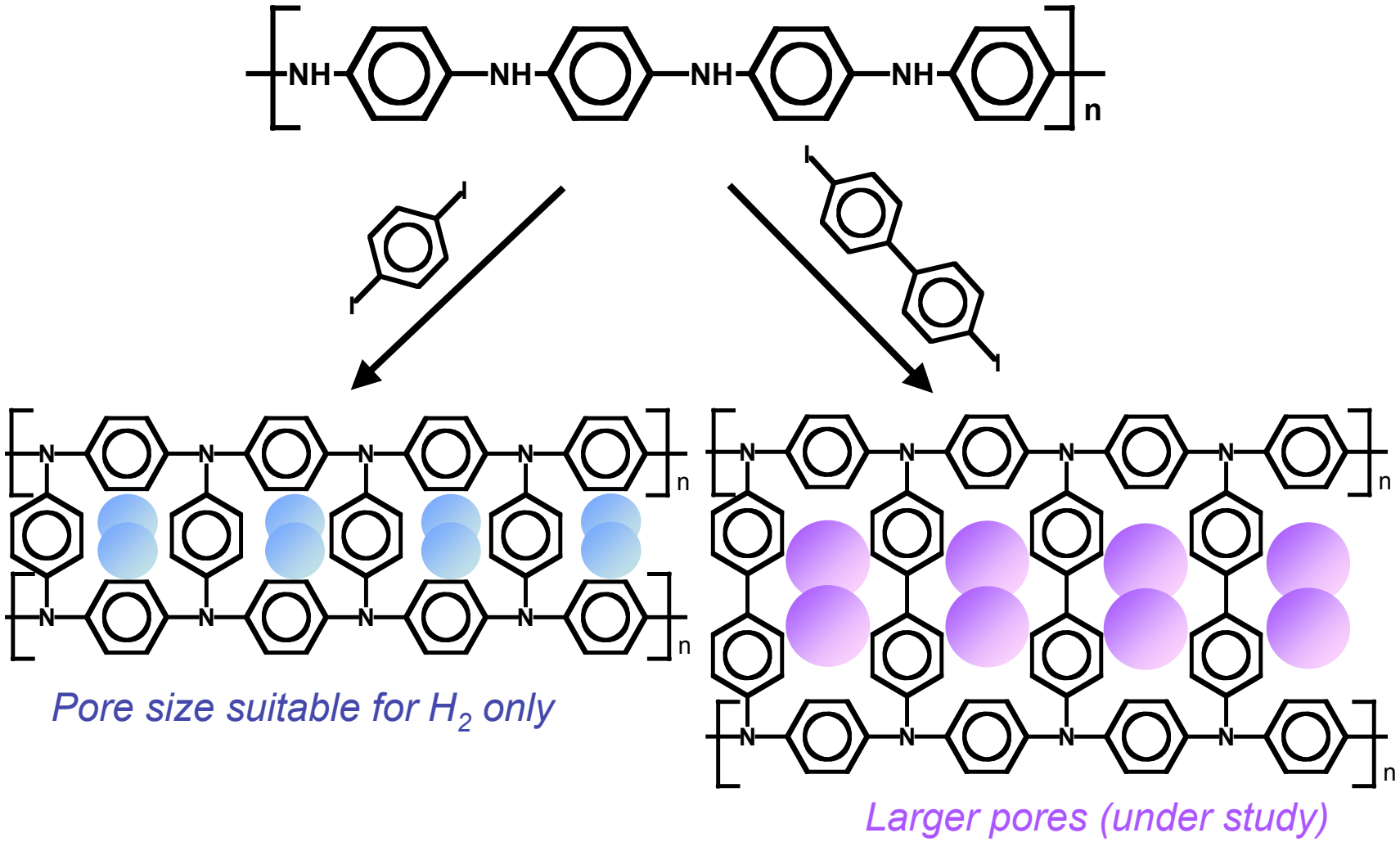
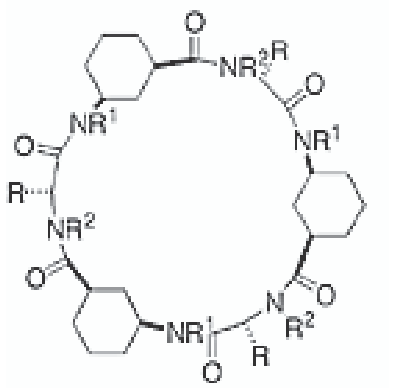
Selective Gas Uptake in Hypercrosslinked Polymers

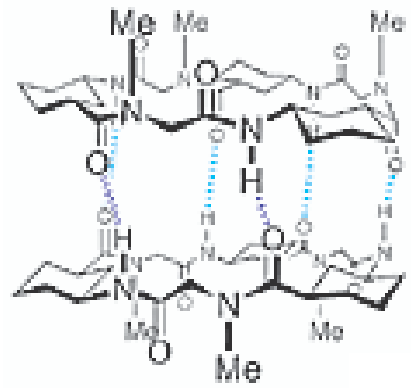


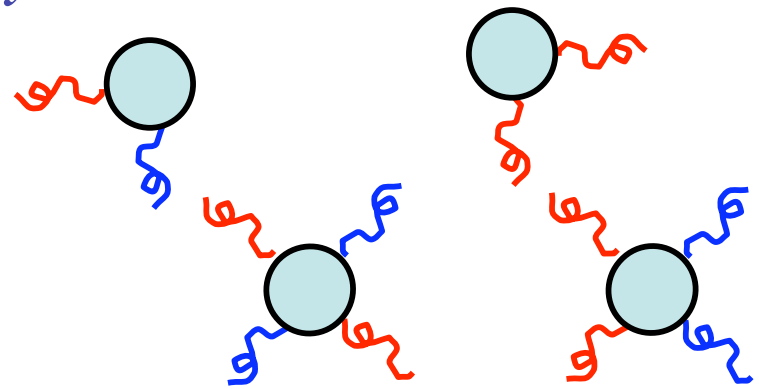
Germain, Fréchet, Svec *Chem. Mater.* 2008, *20*, 7069

Hierarchical Peptide-Based Block Copolymers

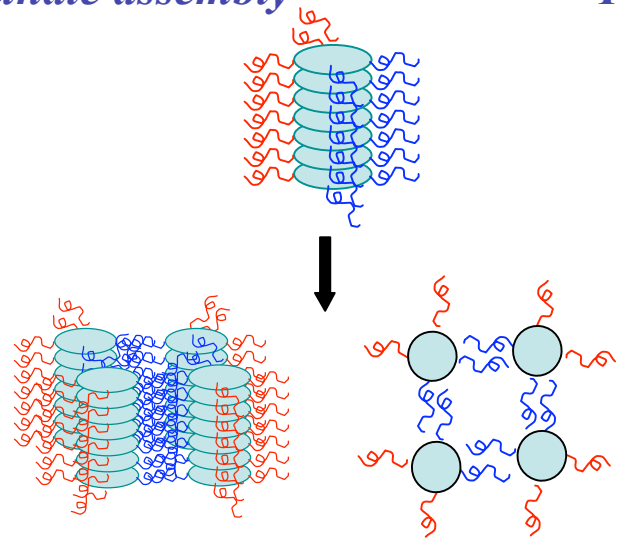
Cyclic peptide-polymer conjugates assembly



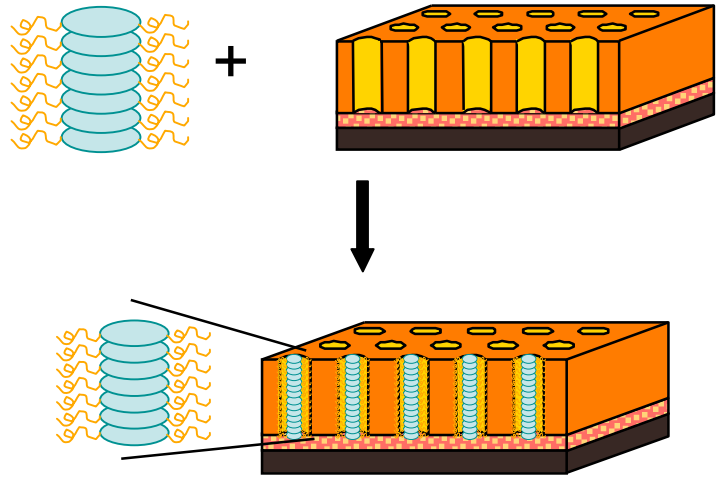




Tubular bundle assembly



Template assisted assembly



Helms, Xu, and coworkers

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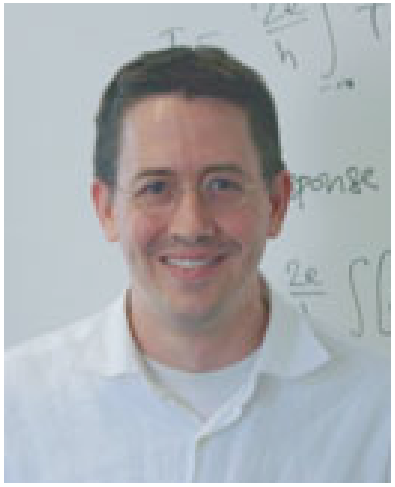

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