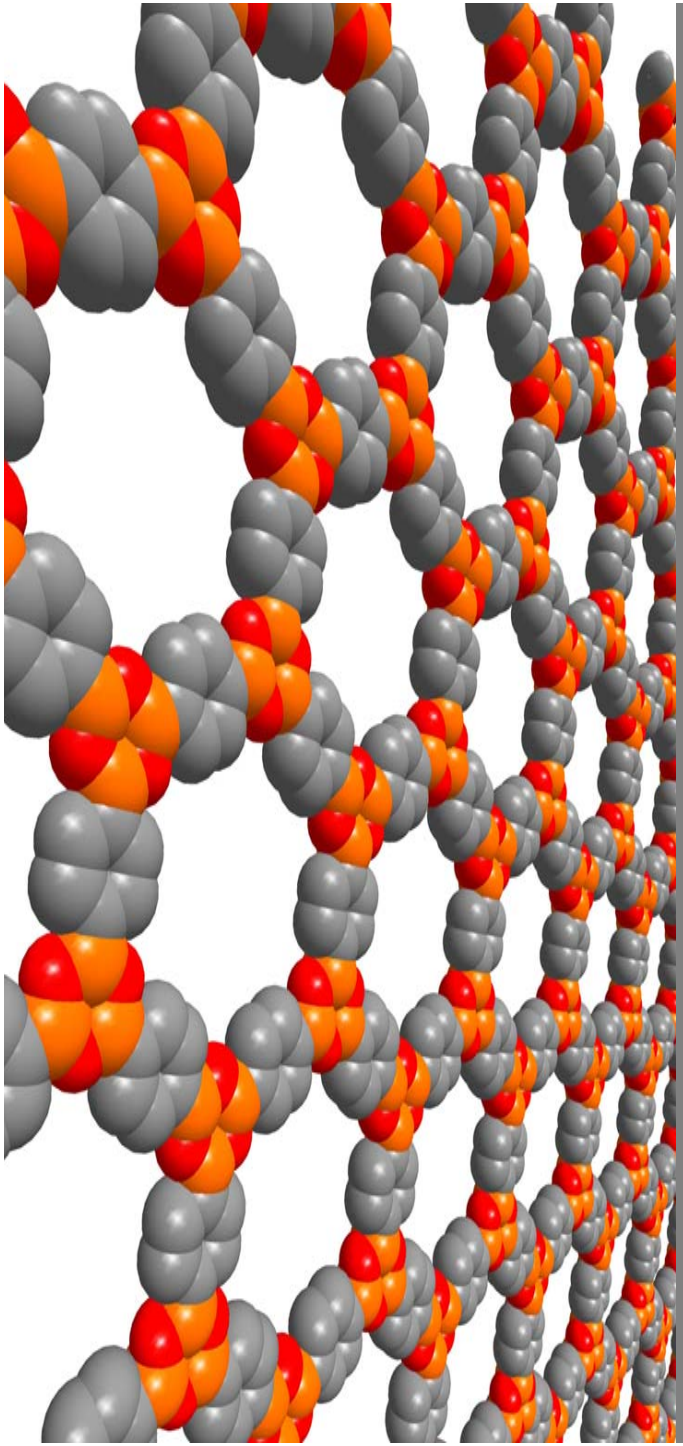

Porous Crystals For Carbon Dioxide Storage

Omar M. Yaghi

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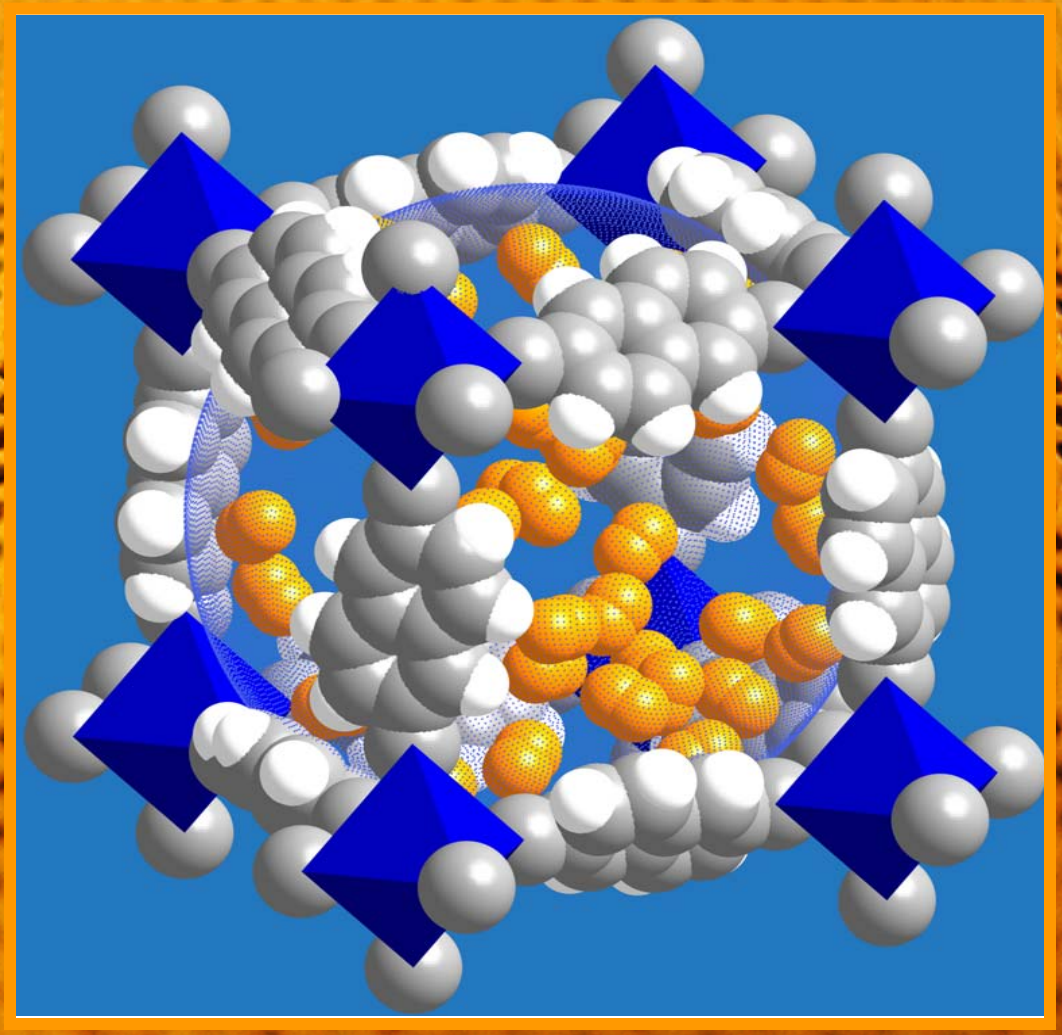
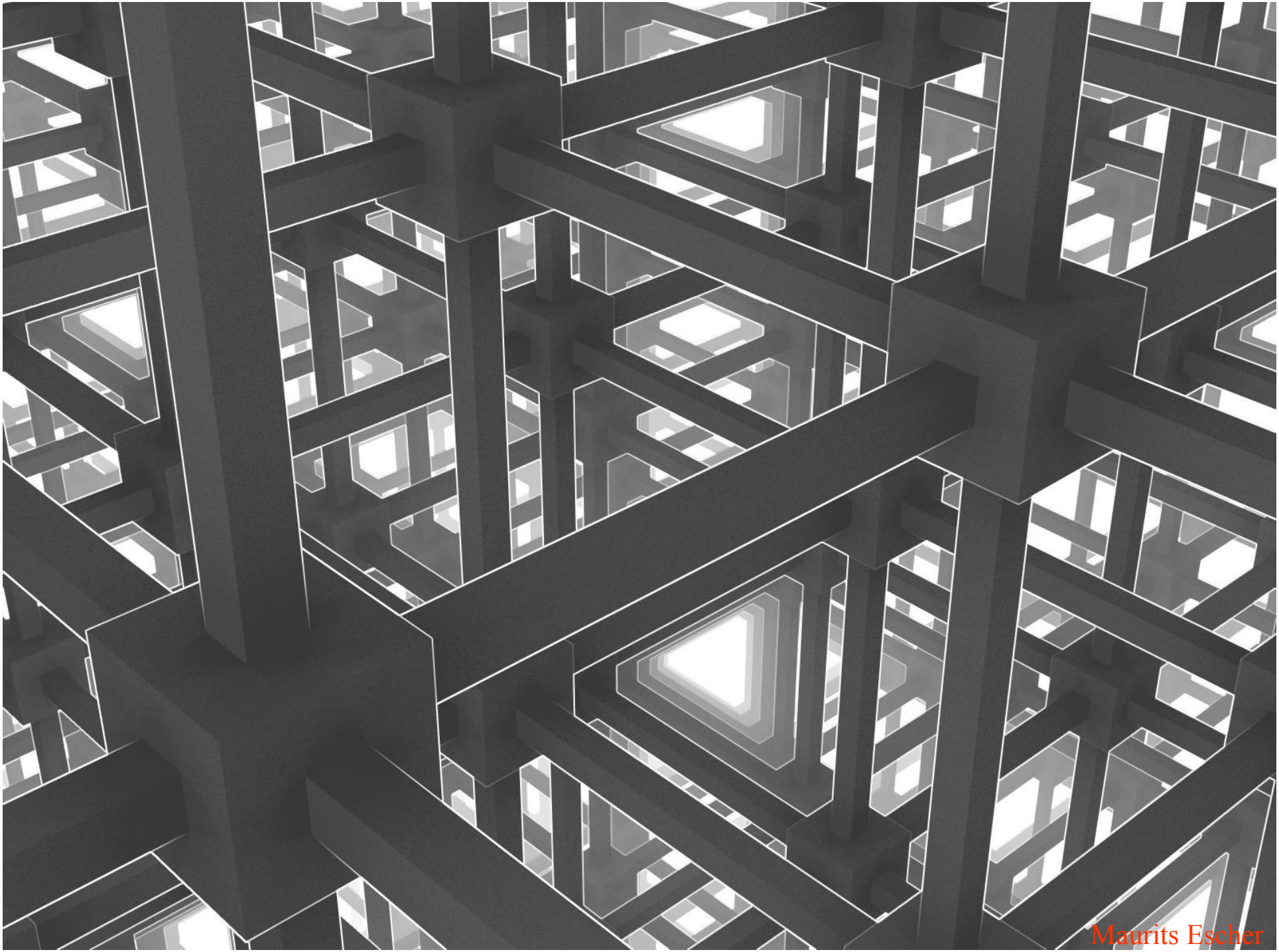
Center for Reticular Materials Research at
California NanoSystems Institute
UCLA

yaghi@chem.ucla.edu

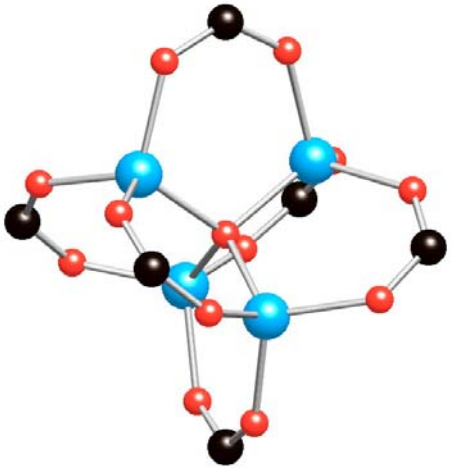
Reticular chemistry *is concerned with linking of molecular building blocks (organic molecules, inorganic clusters, dendrimers, peptides, proteins,...) into predetermined structures in which such units are repeated and are held together by strong bonds.*

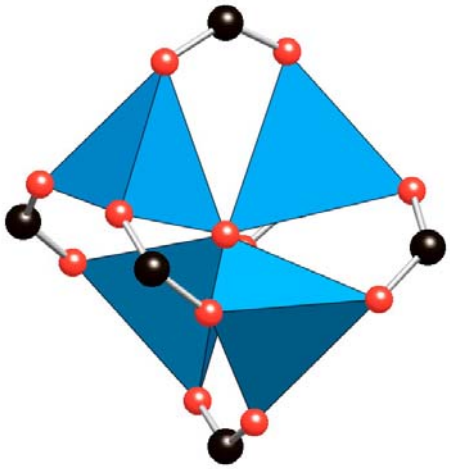
COMPACTING GASES IN POROUS CRYSTALS
‘molecular tanks’

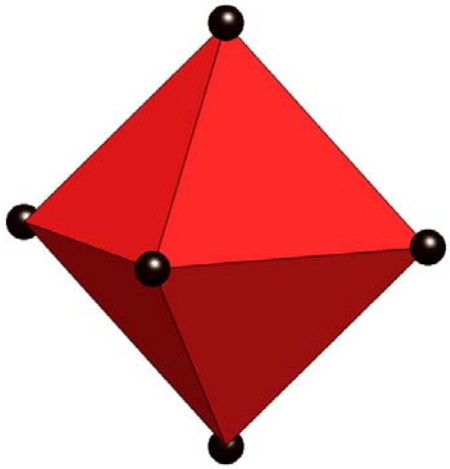



Maurits Escher

Basic Zinc Acetate

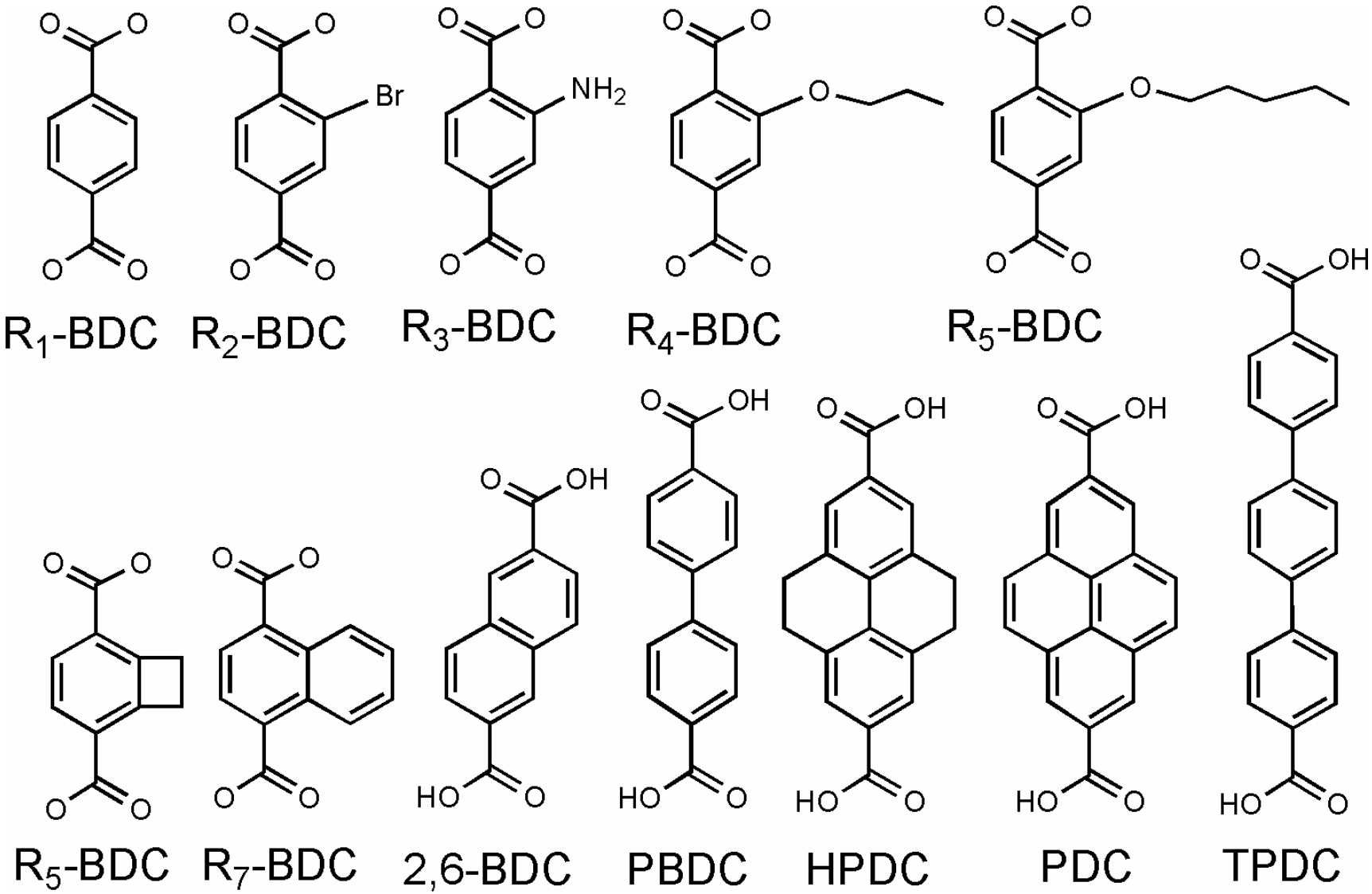




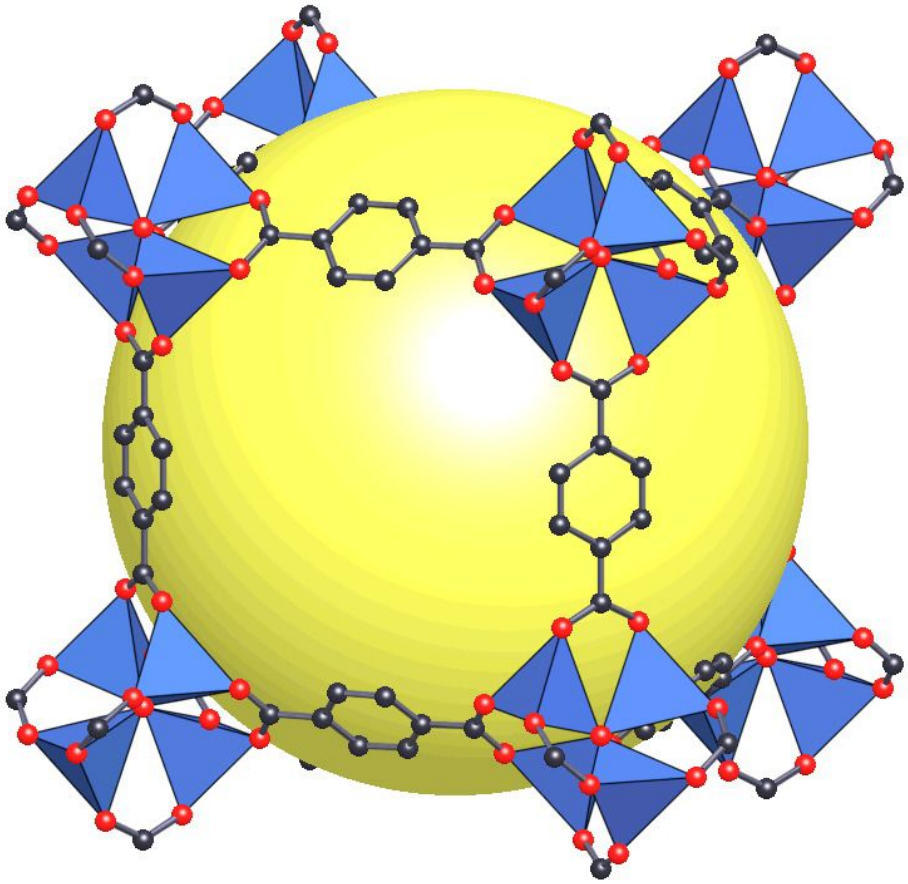


red, O; blue, Zn; black, C

Linkers “struts”

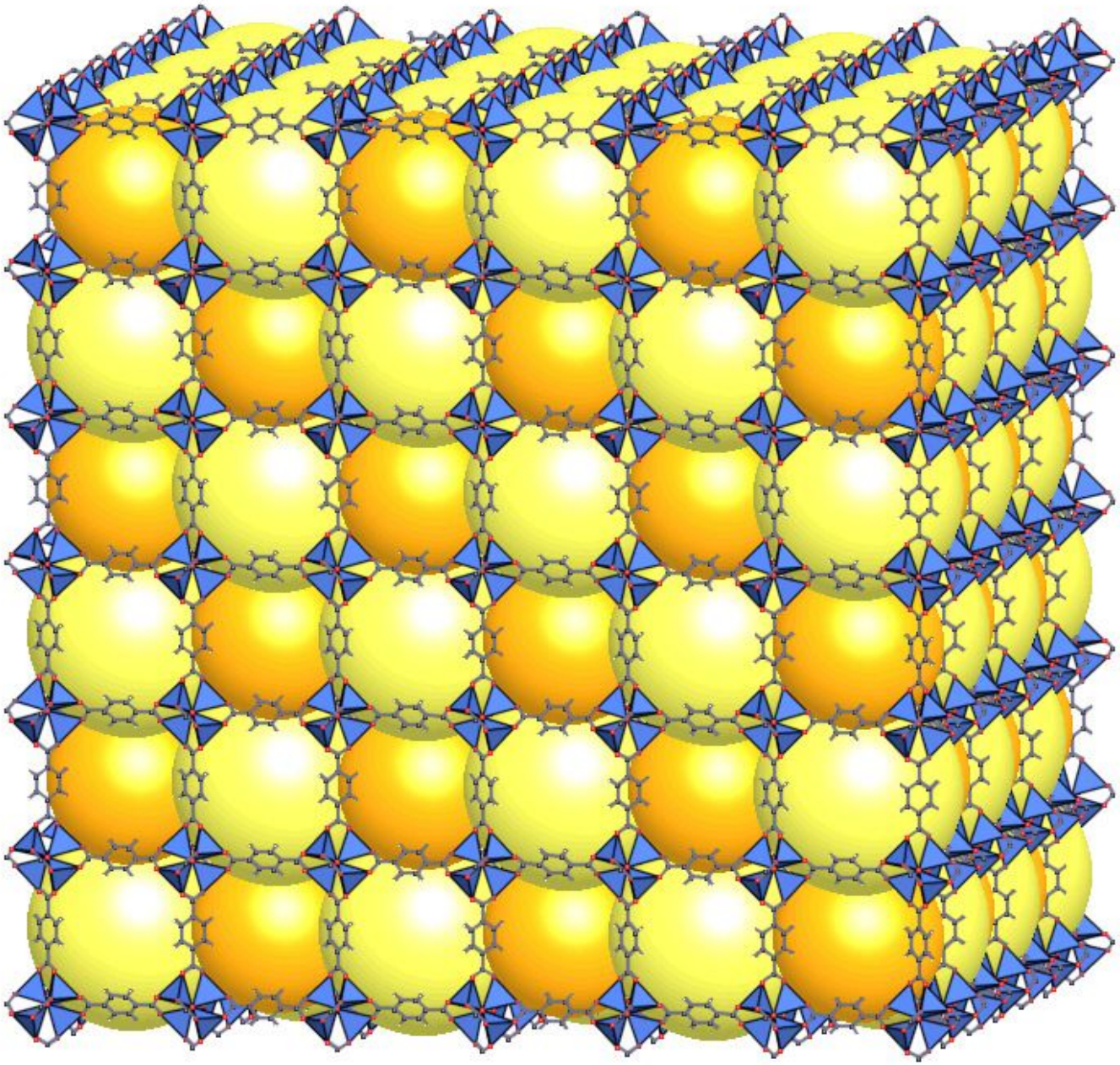


$$H_2BDC + Zn(NO_3)_2 \bullet 4H_2O \xrightarrow{\text{DEF (12mL)}} Zn_4O(BDC)_3 \bullet (DEF)_7$$

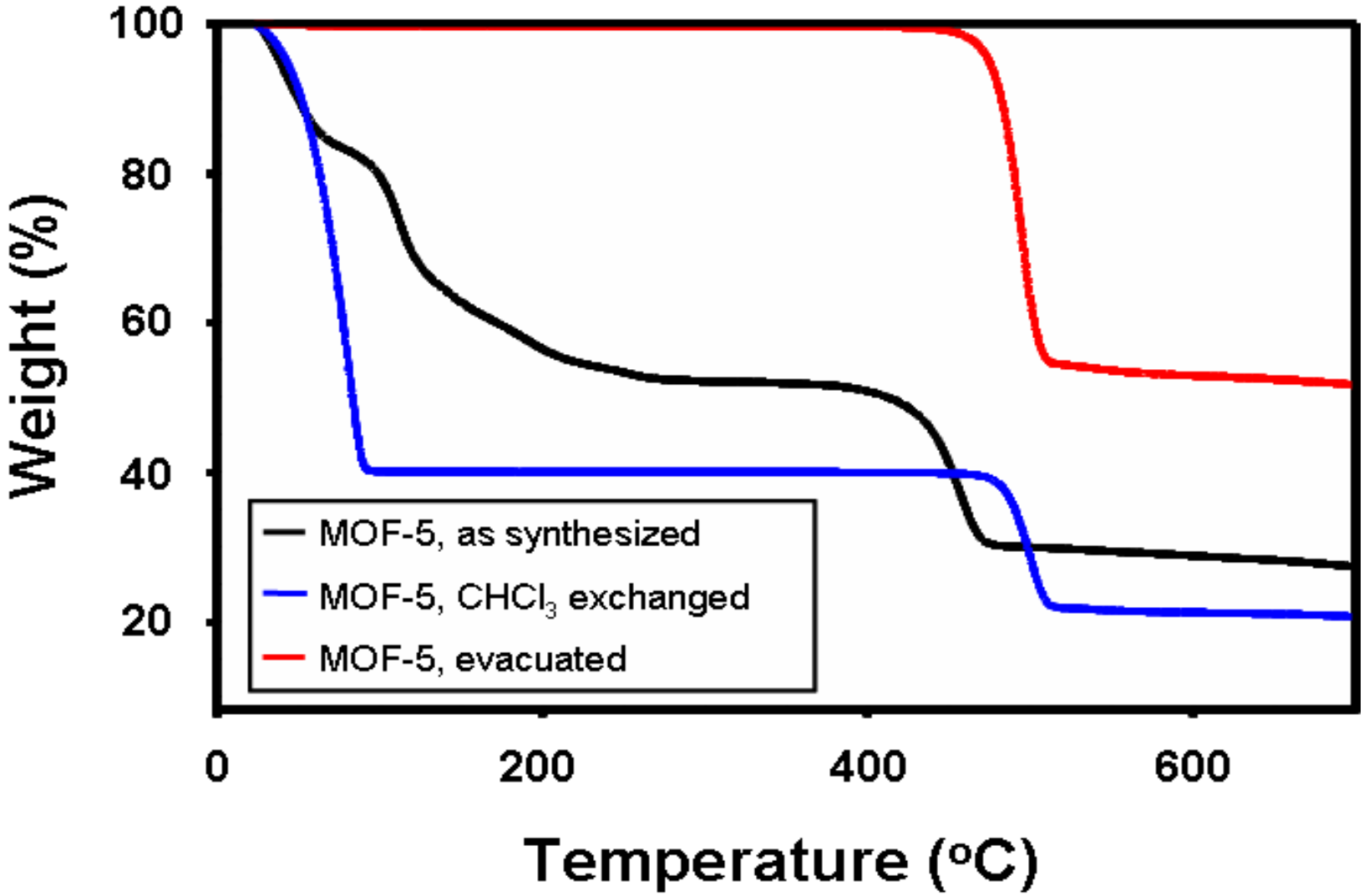


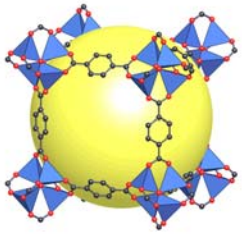
$Zn_4O(O_2C\text{-}C_6H_4\text{-}CO_2)_3$: MOF-5

H. Li, M. Eddaoudi, M. O'Keeffe, O. M. Yaghi. *Nature* (1999) *402*, 276-279

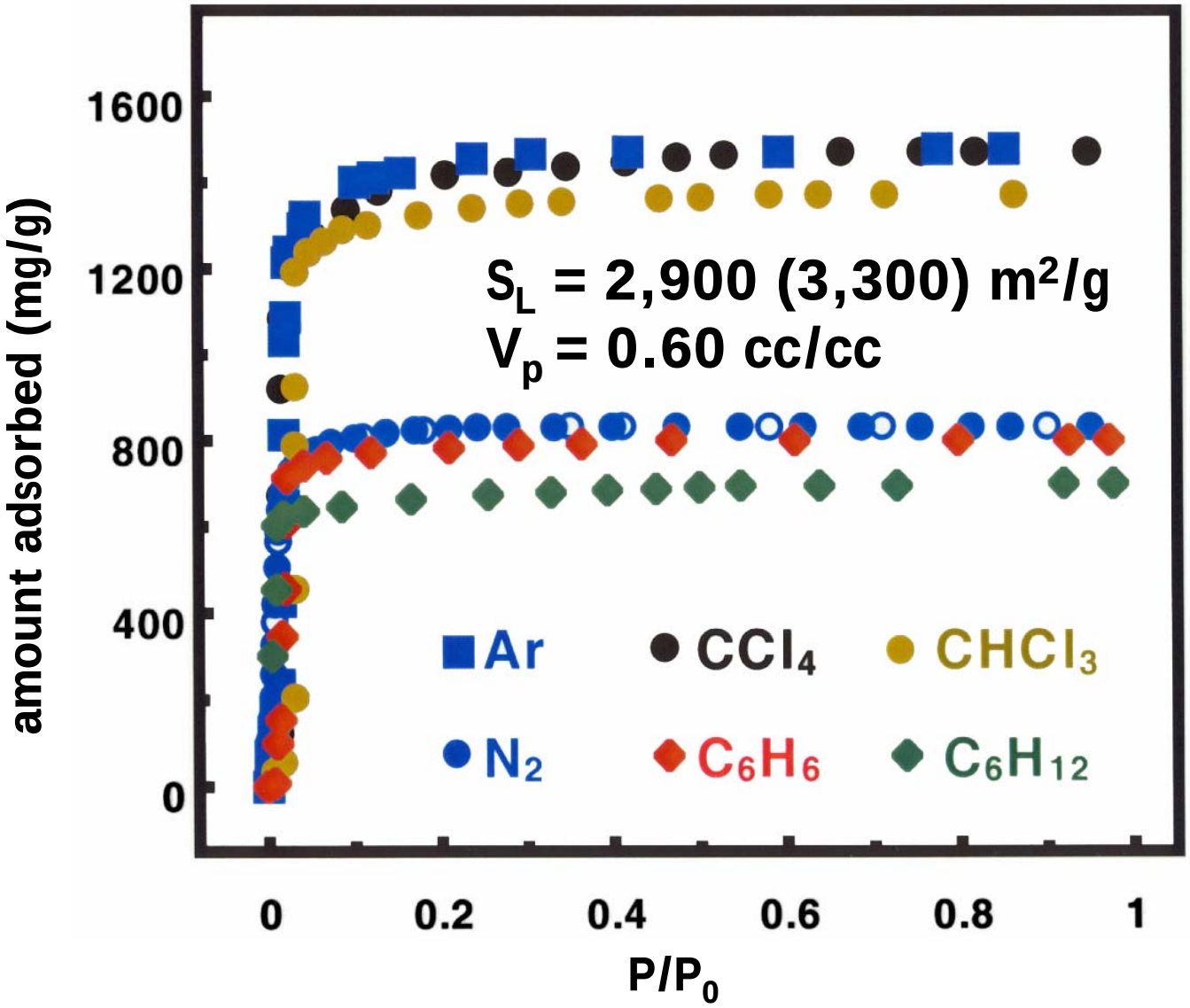


Thermal stability of MOF-5





Porosity of MOF-5

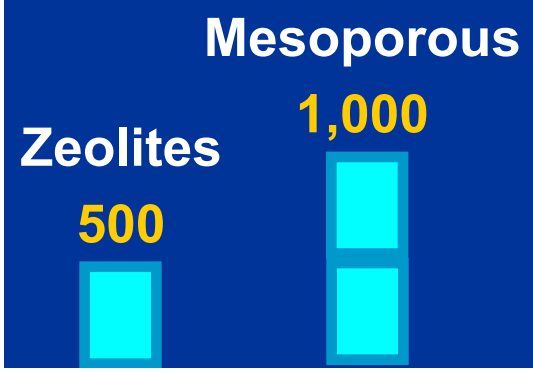


Typical Surface Areas (m^2/g)

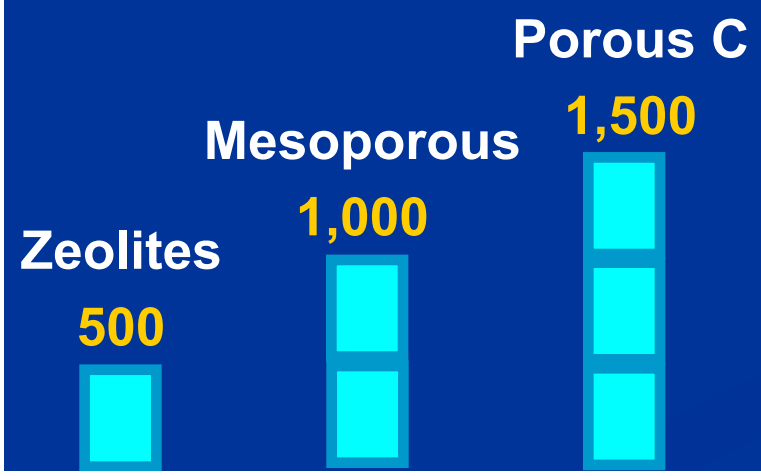
Zeolites

500

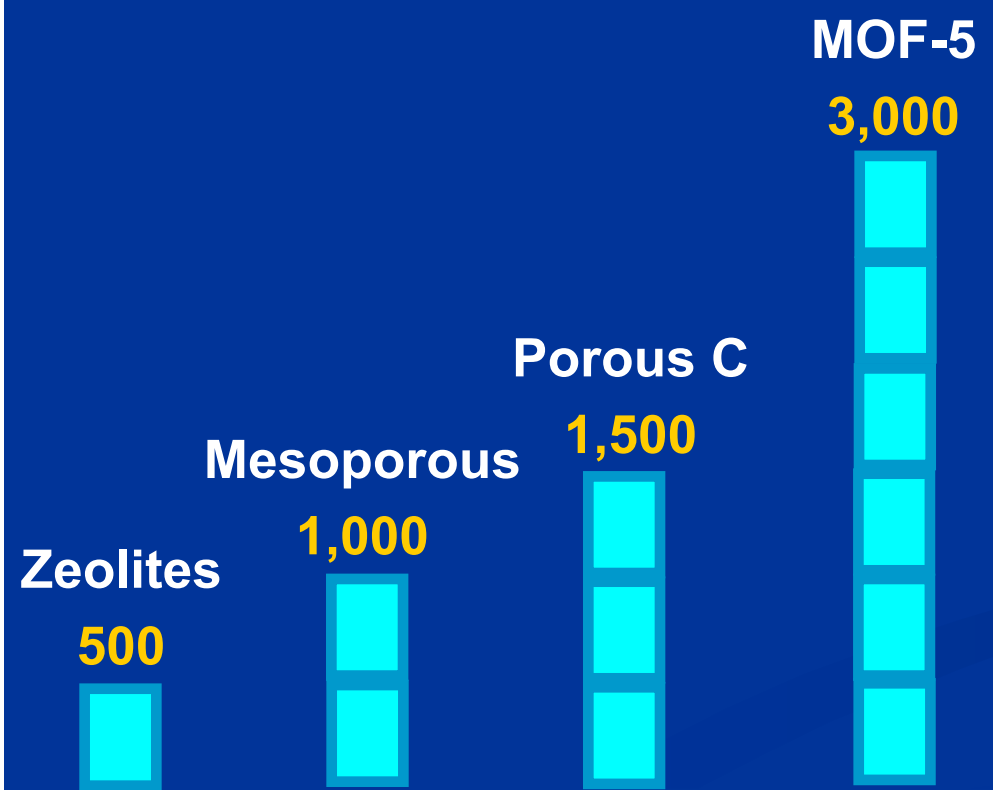
Typical Surface Areas (m^2/g)



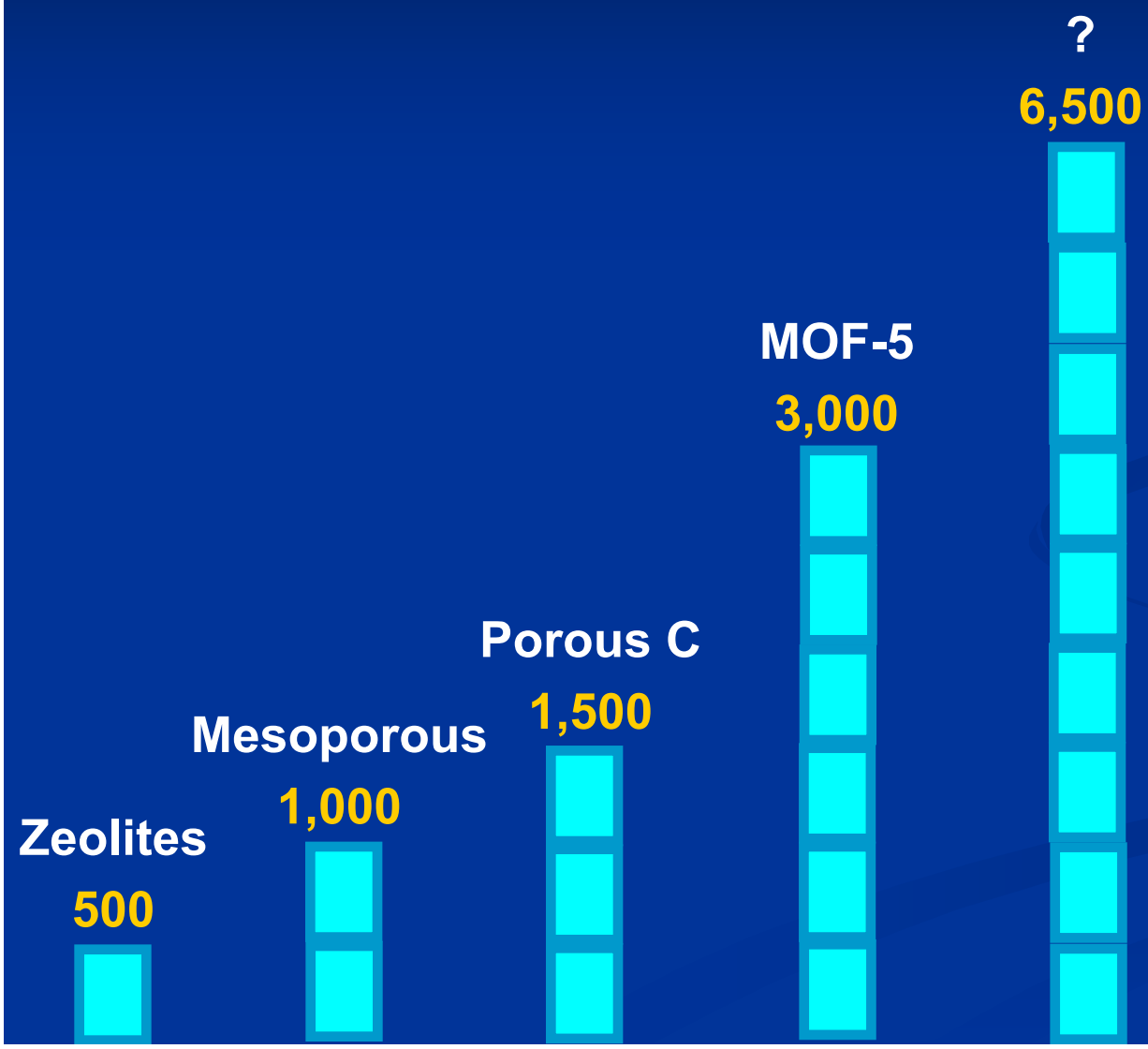
Typical Surface Areas (m^2/g)



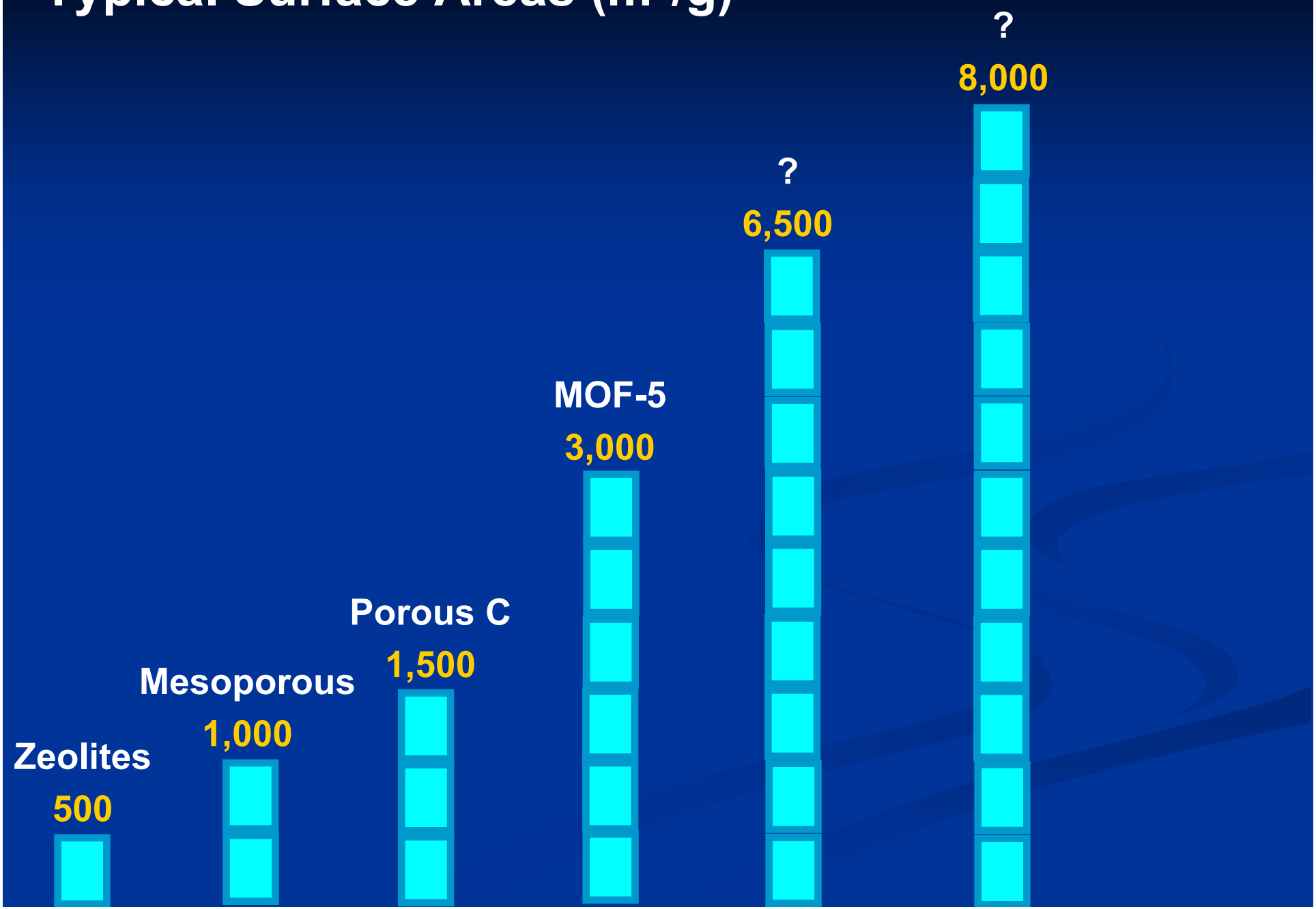
Typical Surface Areas (m^2/g)



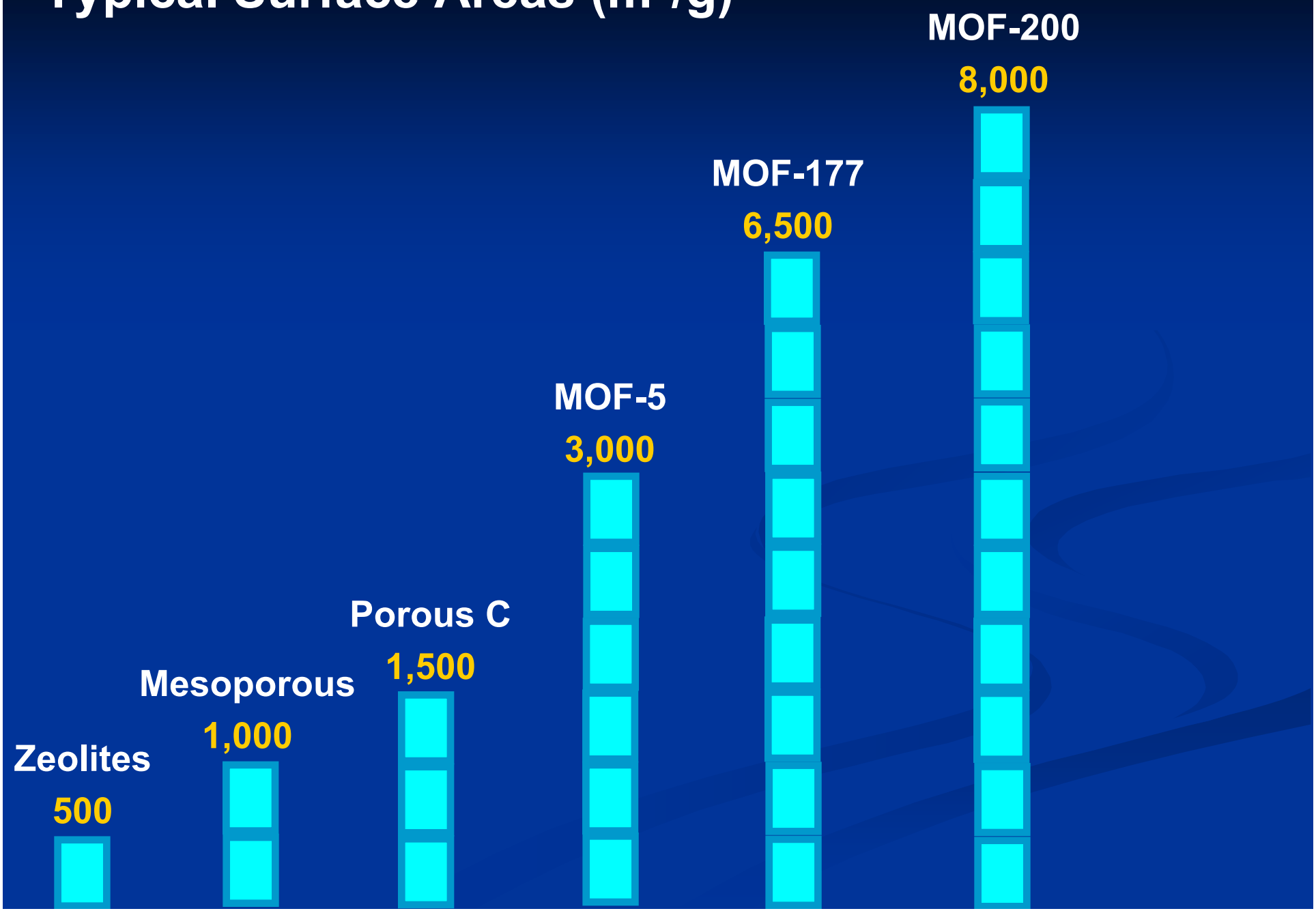
Typical Surface Areas (m^2/g)

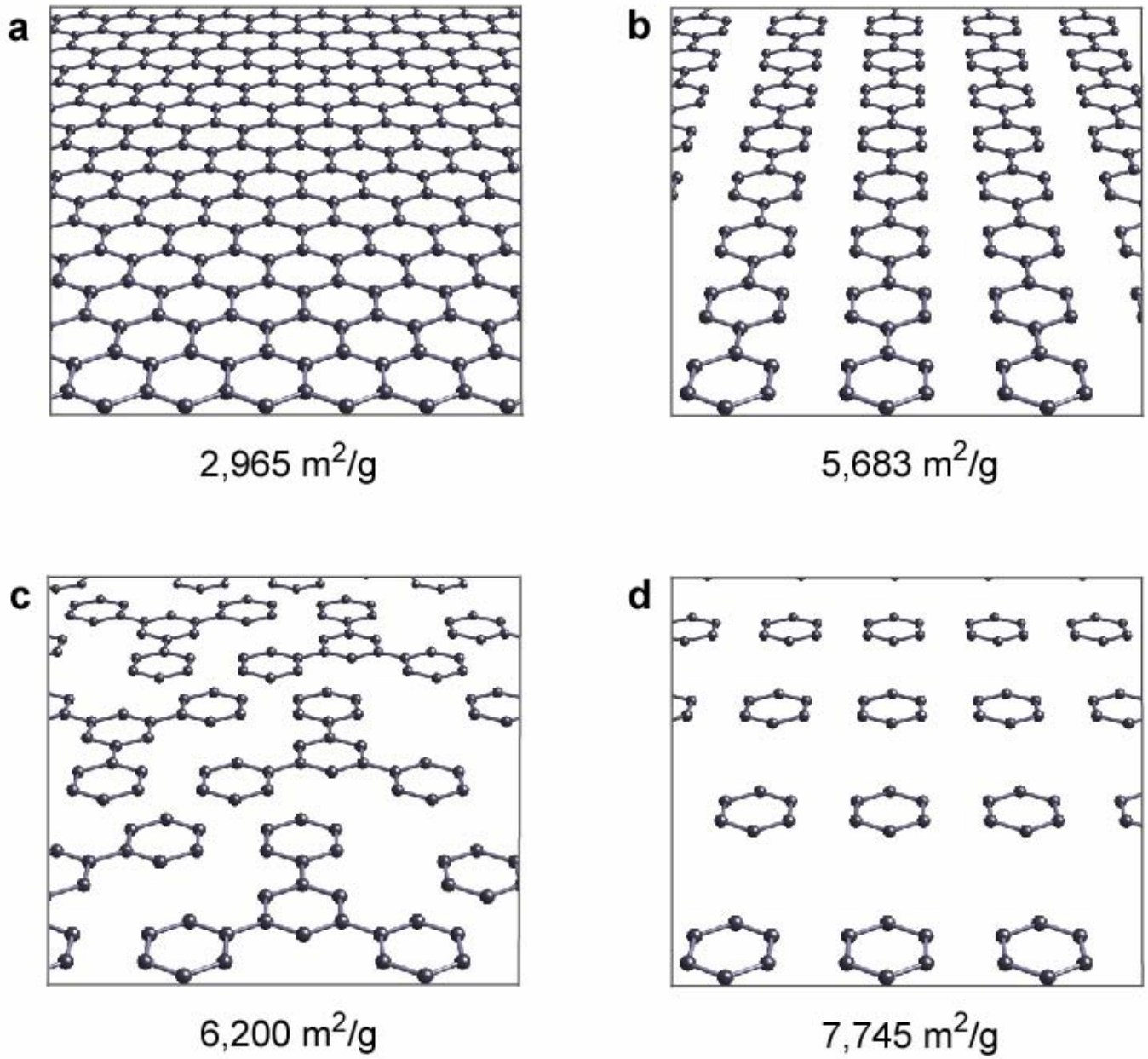


Typical Surface Areas (m^2/g)



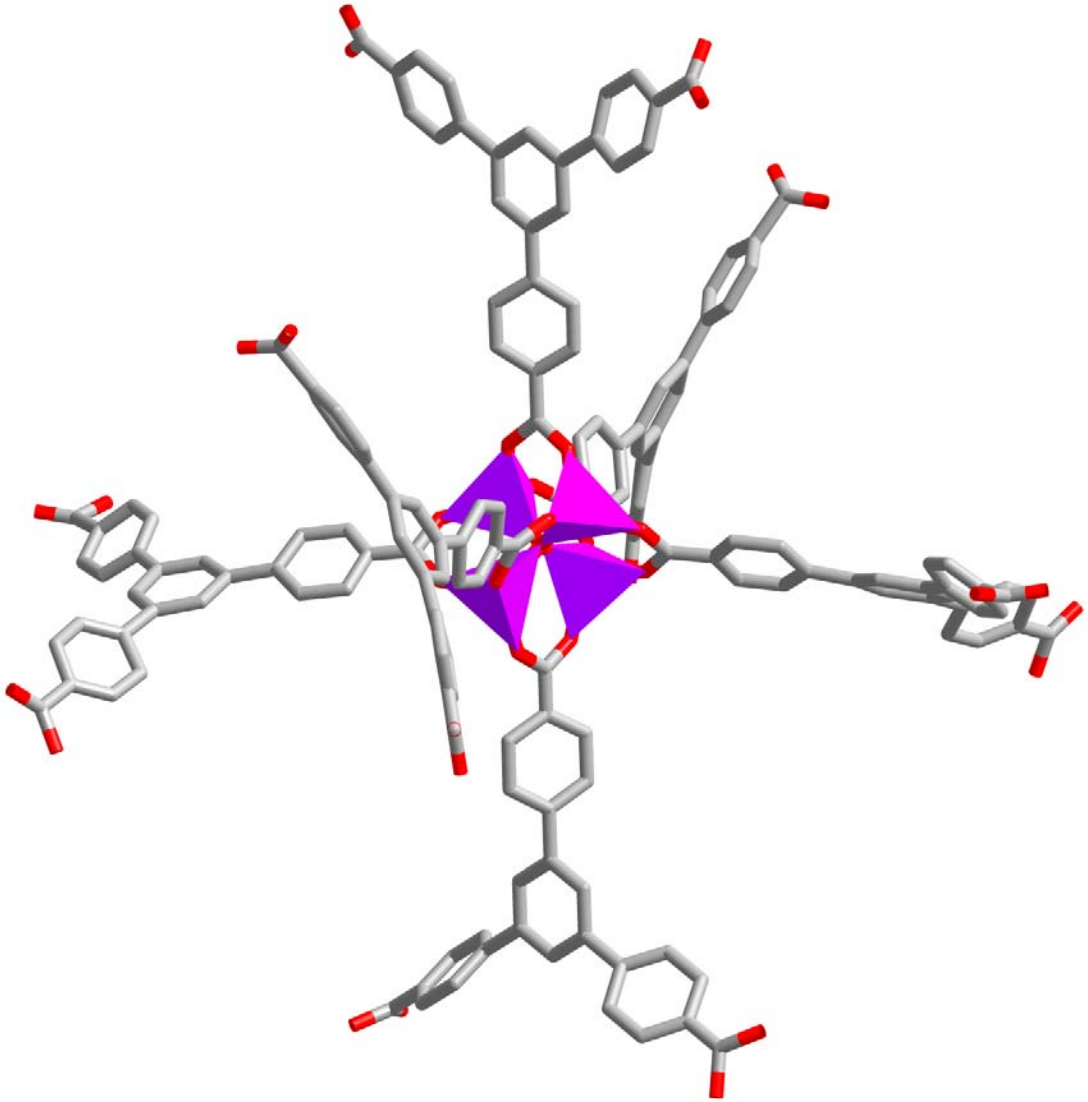
Typical Surface Areas (m^2/g)

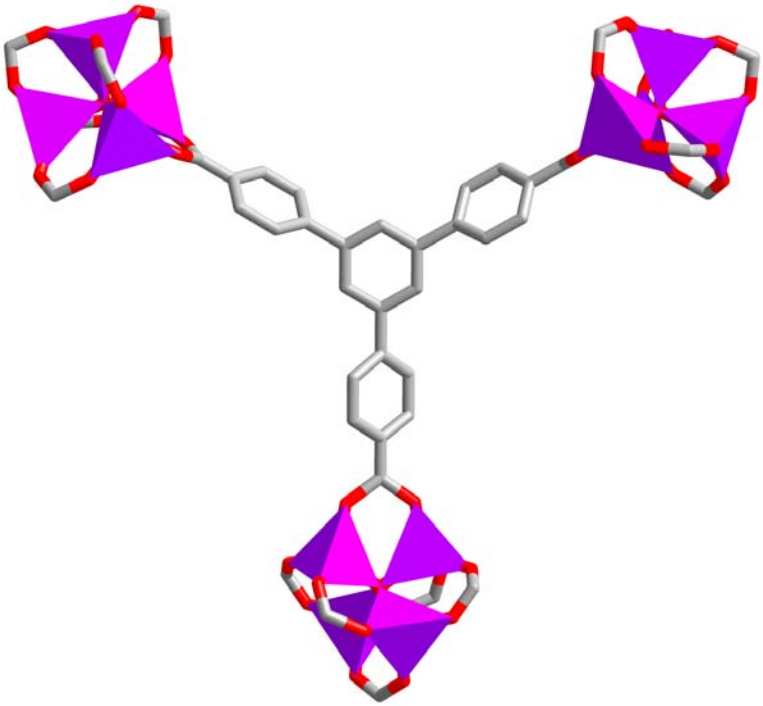




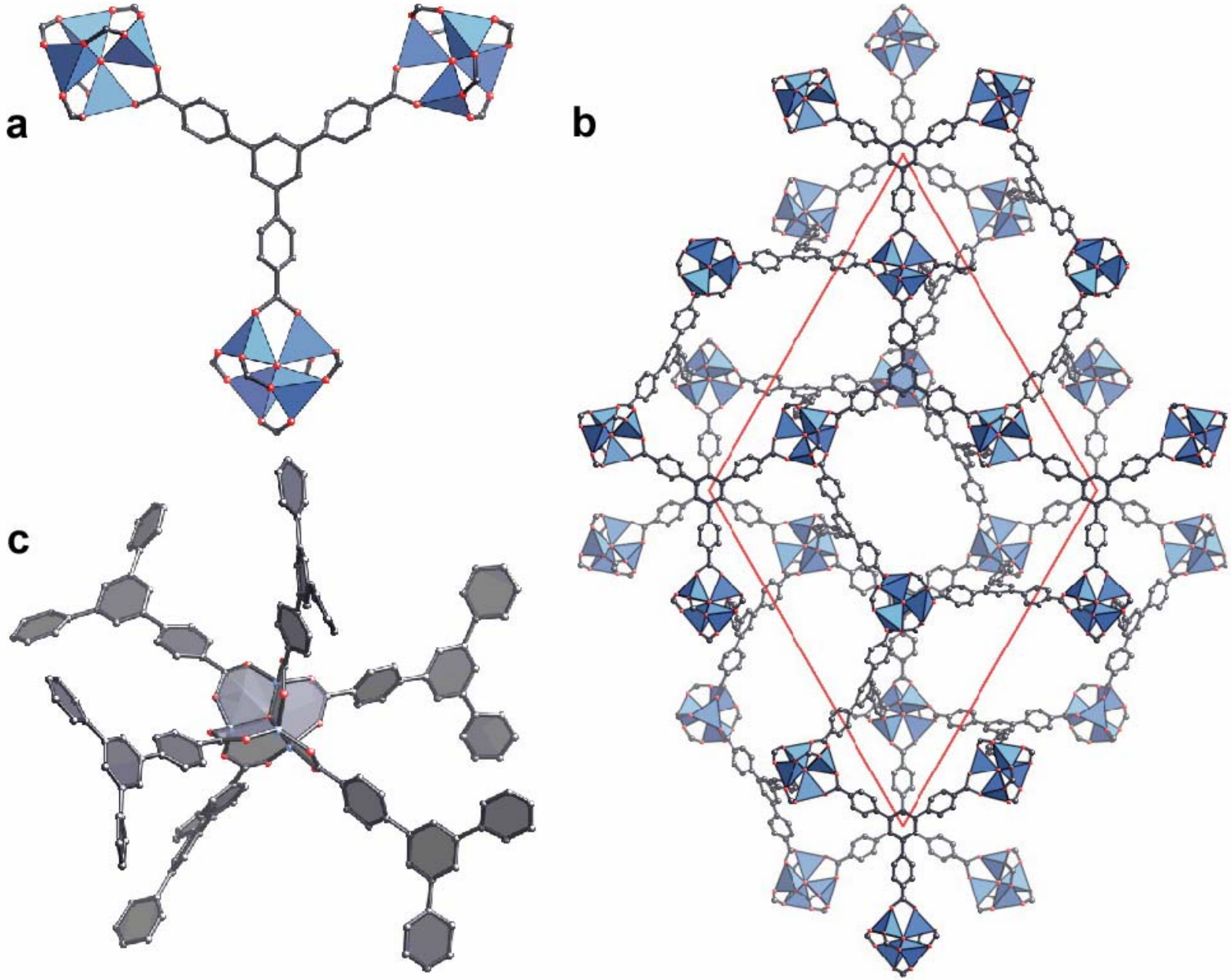
Calculated surface areas

$Zn_4O(BTB)_2 \bullet (DEF)_{15}$

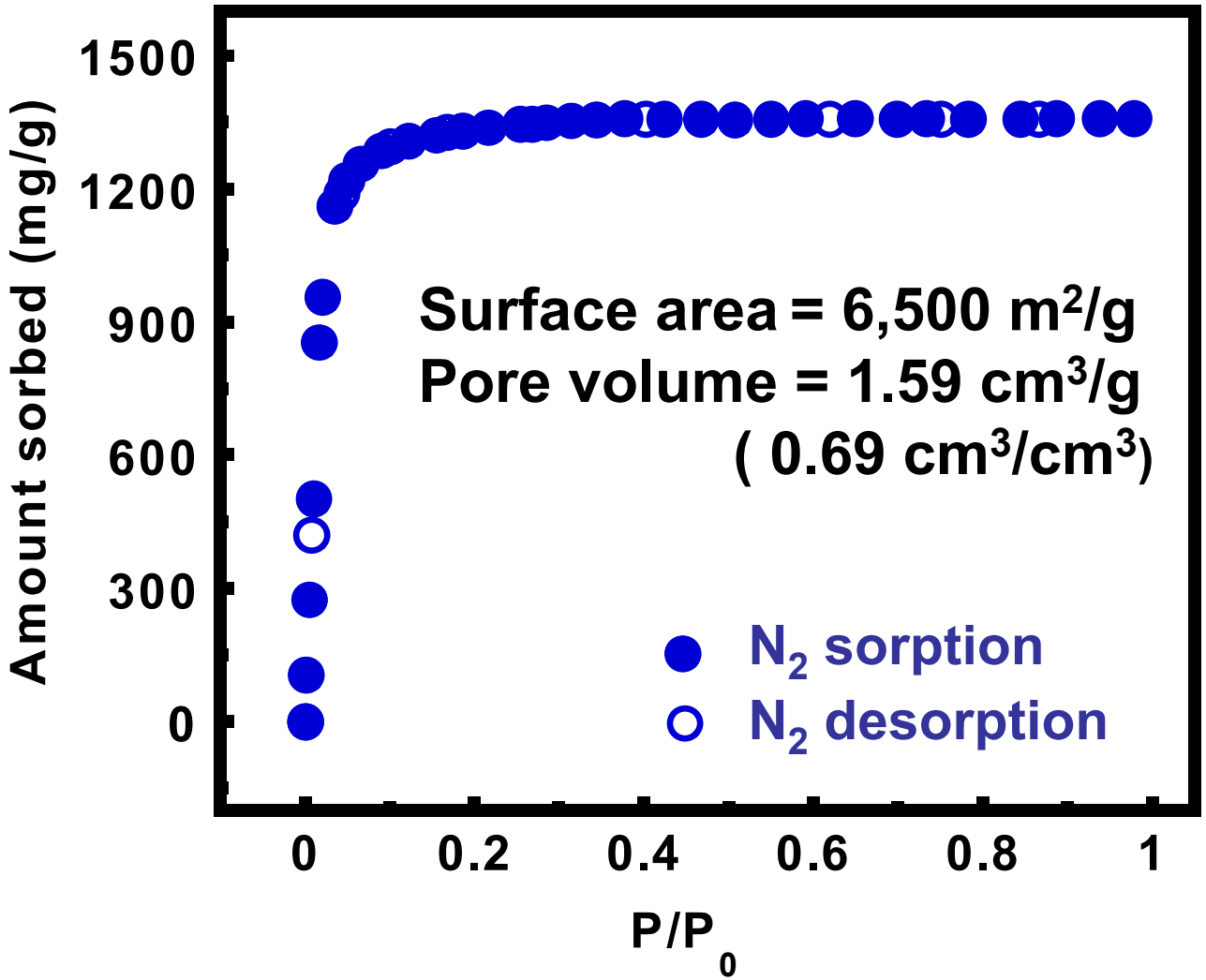


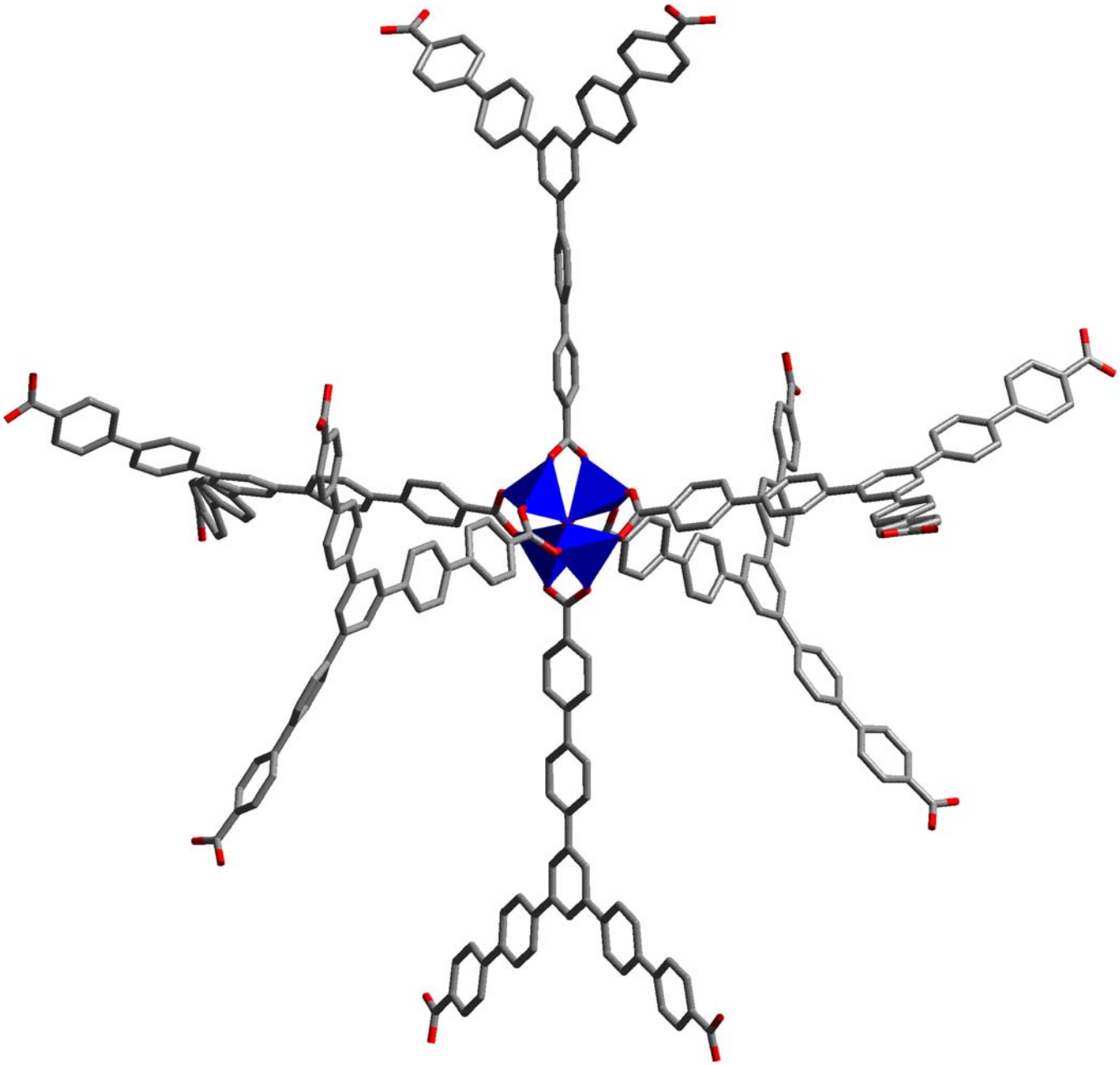


Nature 2004

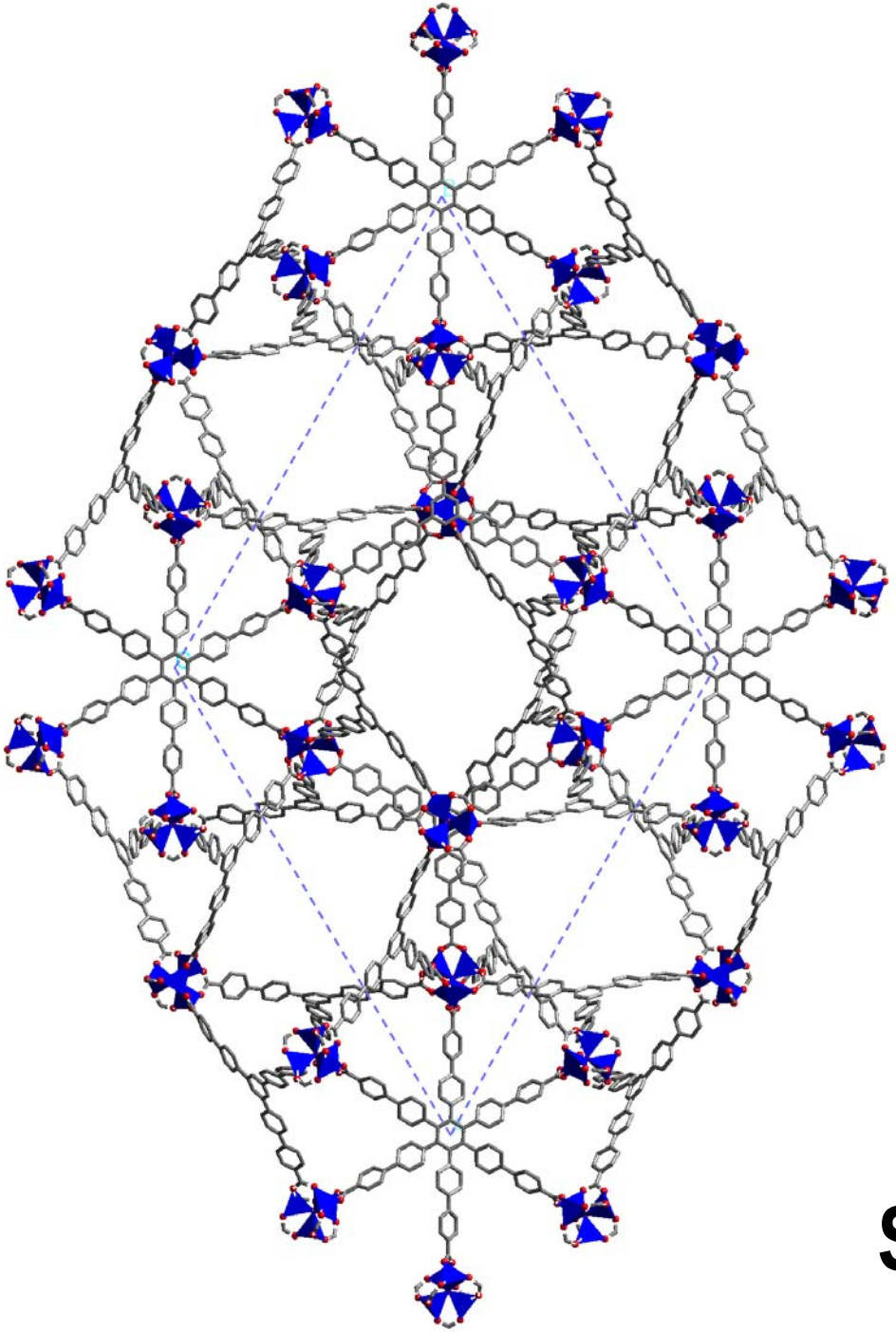

a
b
c

N_2 adsorption isotherm for $Zn_4O(BTB)_2$





$Zn_4O(BBC)_2$



MOF-200:

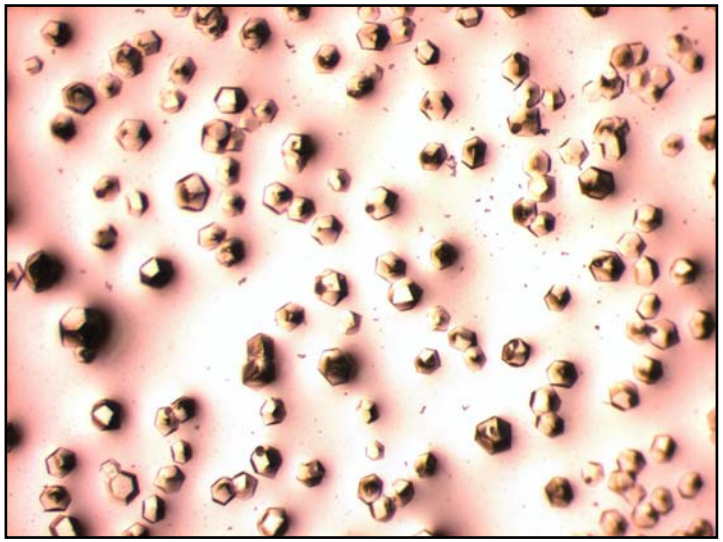
$Zn_4O(BBC)_2$

Trigonal, P-3

a = b = 51.45 Å

c = 41.80 Å

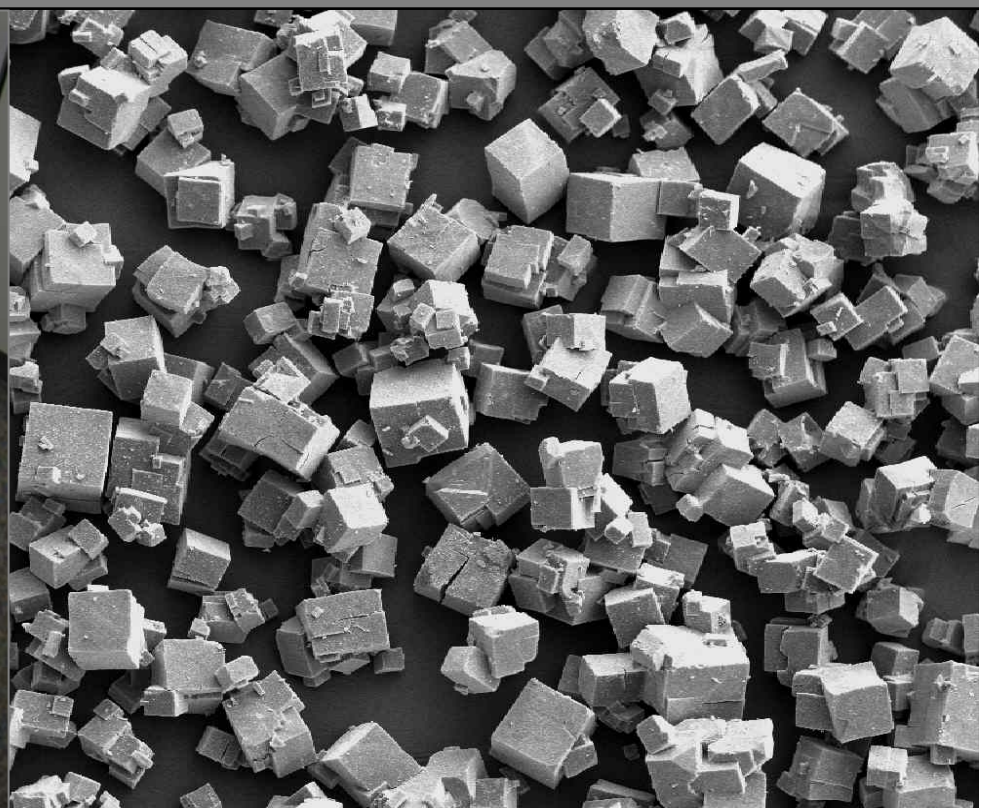
V = 95,822.1 $Å^3$



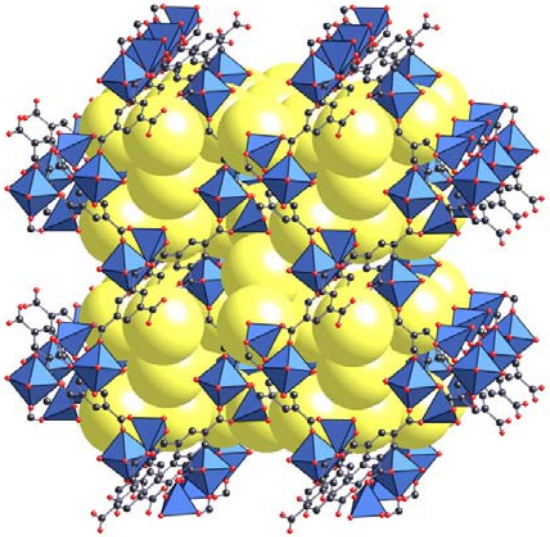
S.A. = ‘8,000’ m^2/g

Synthesis of Metal-Organic Frameworks (MOFs)

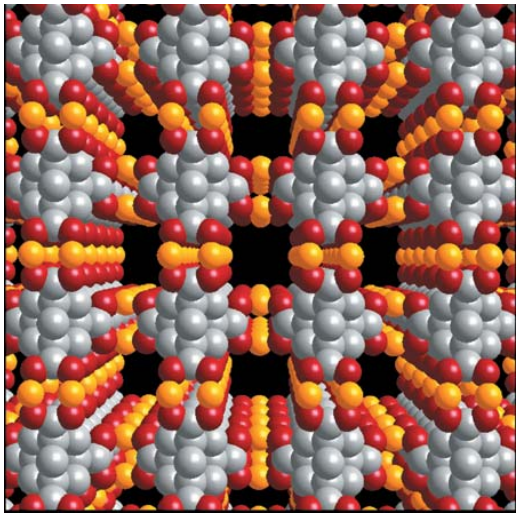
$$x\,Zn^{2+} + y\,H_2L + H_2O \xrightarrow[\text{amide and/or solvent}]{\Delta} Zn_x(L)_y\cdot(solv)_n$$



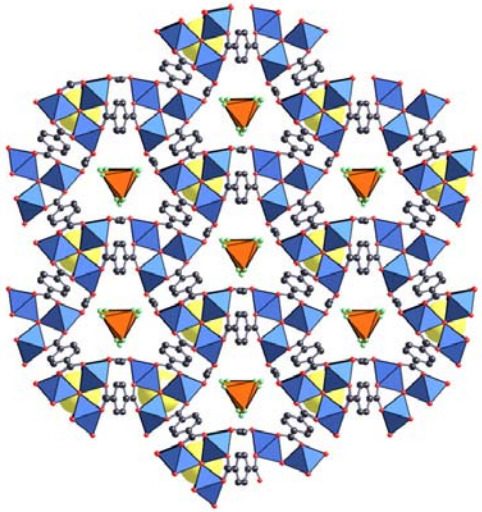
Dr. U. Müller, GCC/Z, BASF



triangles (srs)

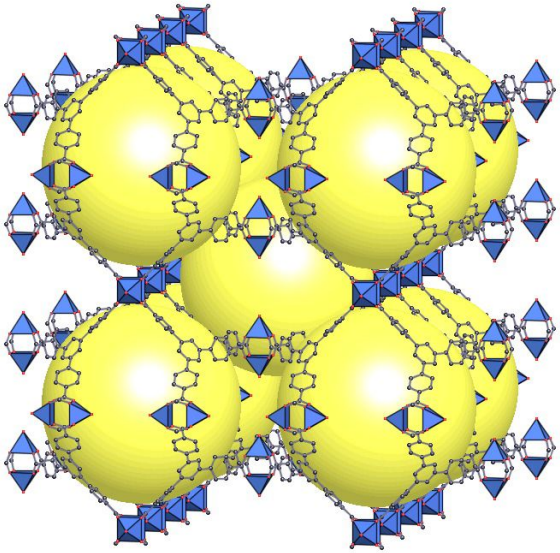


squares + tetrahedra (pts)

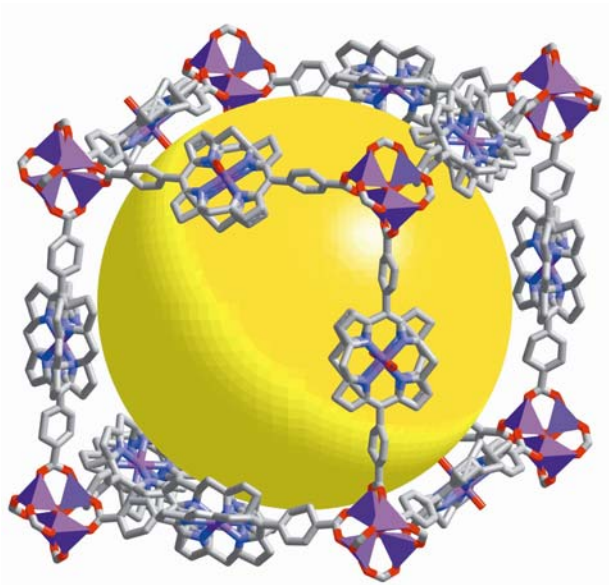


trigonal prisms (acs)

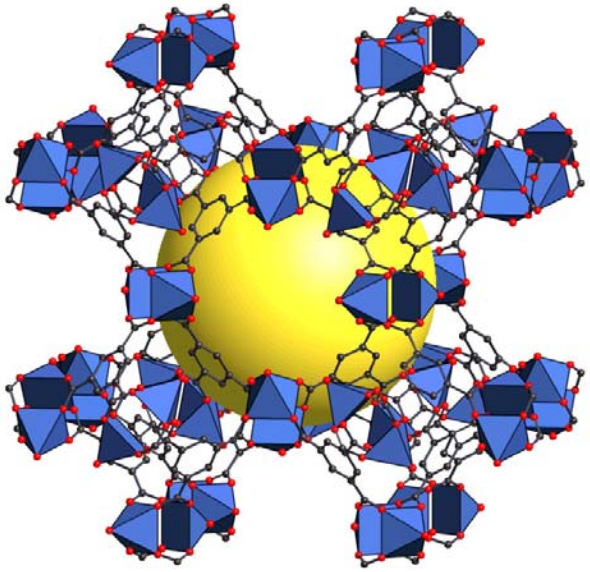
>500 MOFs PREPARED!



squares + triangles (pto)

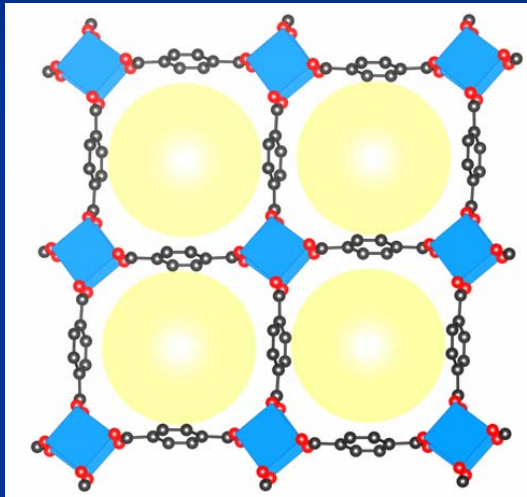


octahedra (pcu)



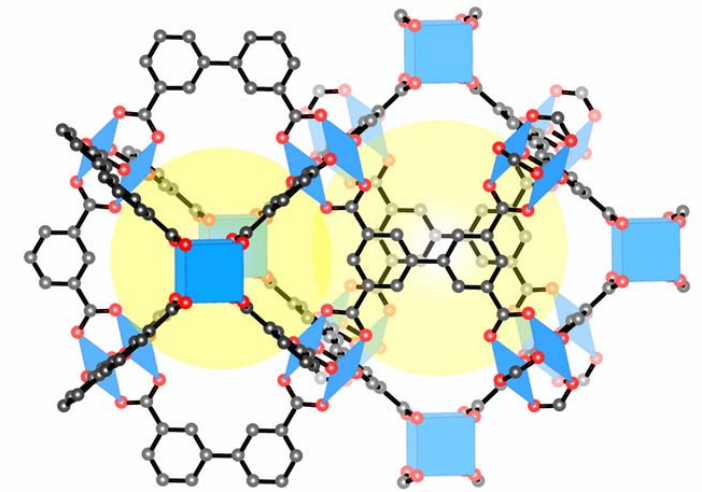
tetrahedra + triangles (bcu)

MOFs for CO_2 Adsorption



MOF-2: $Zn_2(BDC)_2$

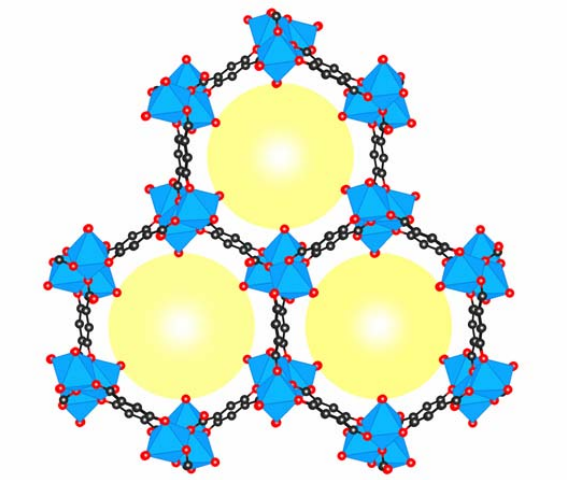
Layered



MOF-505: $Cu_2(BPTC)$

3-D open metal sites

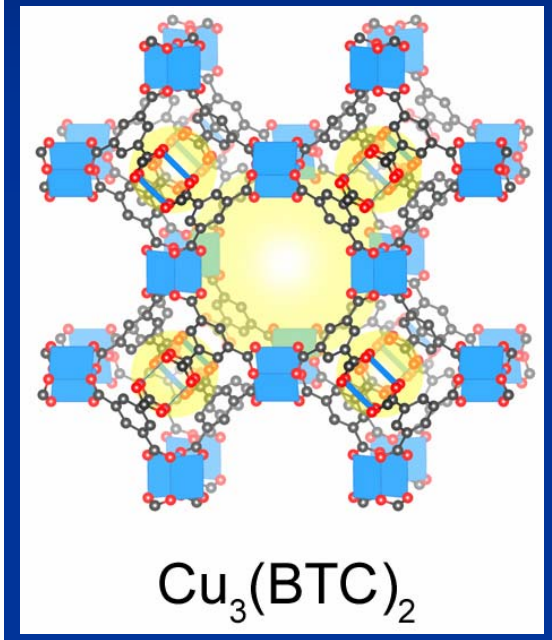
3-D channel system

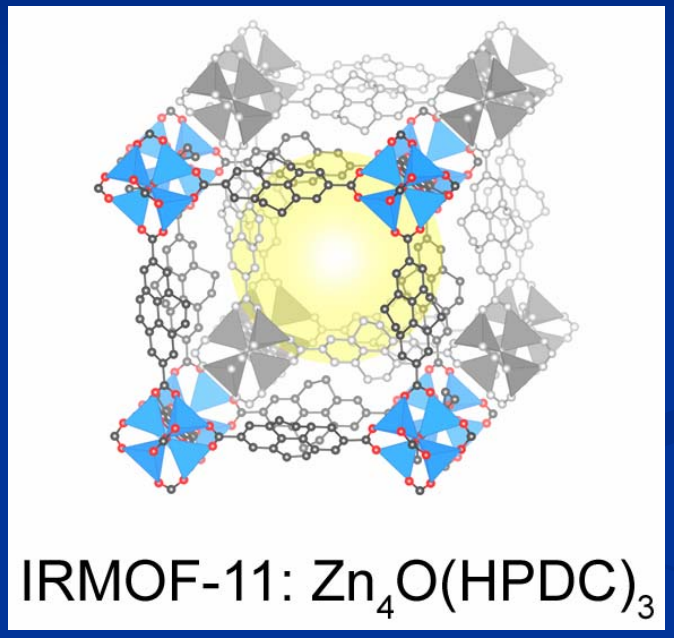


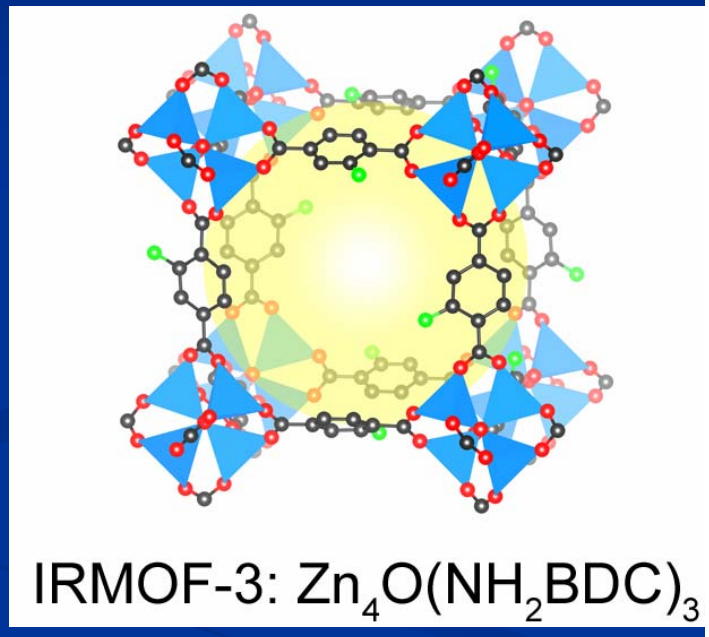
MOF-74: $Zn_2(DHBDC)$

3-D rod metal oxides

1-D channels







3-D framework

3-D channel system

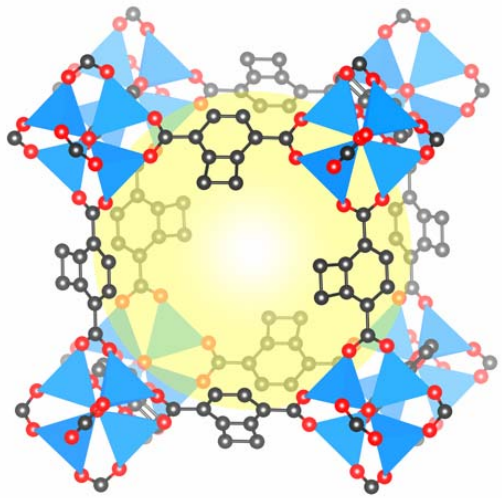
Open metal sites

3-D interpenetrated

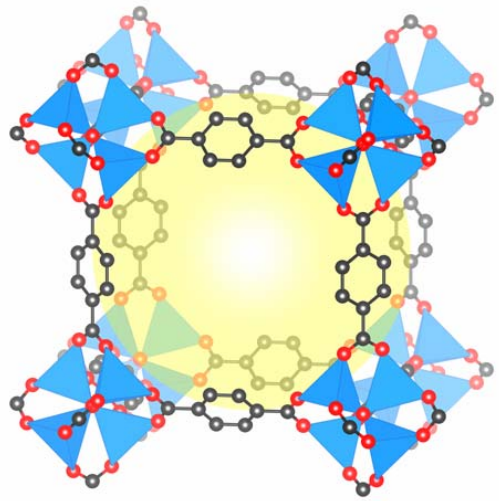
3-D channel system

3-D framework

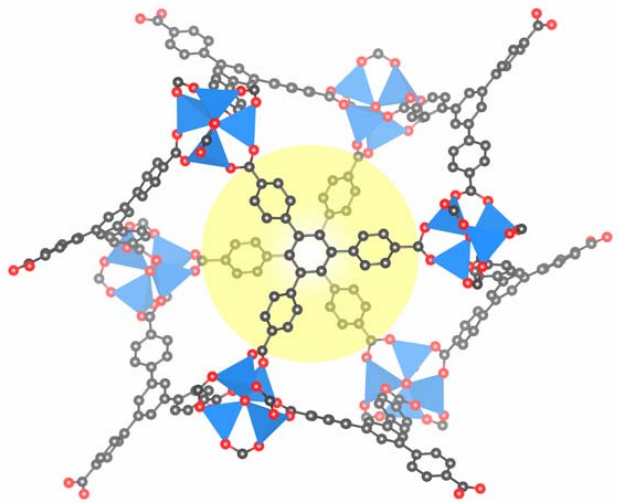
Amino functionalized



IRMOF-6: $Zn_4O(C_2H_4BDC)_3$



IRMOF-1: $Zn_4O(BDC)_3$



MOF-177: $Zn_4O(BTB)_2$

3-D framework

Constricted openings

High S.A.

3-D framework

3-D channel system

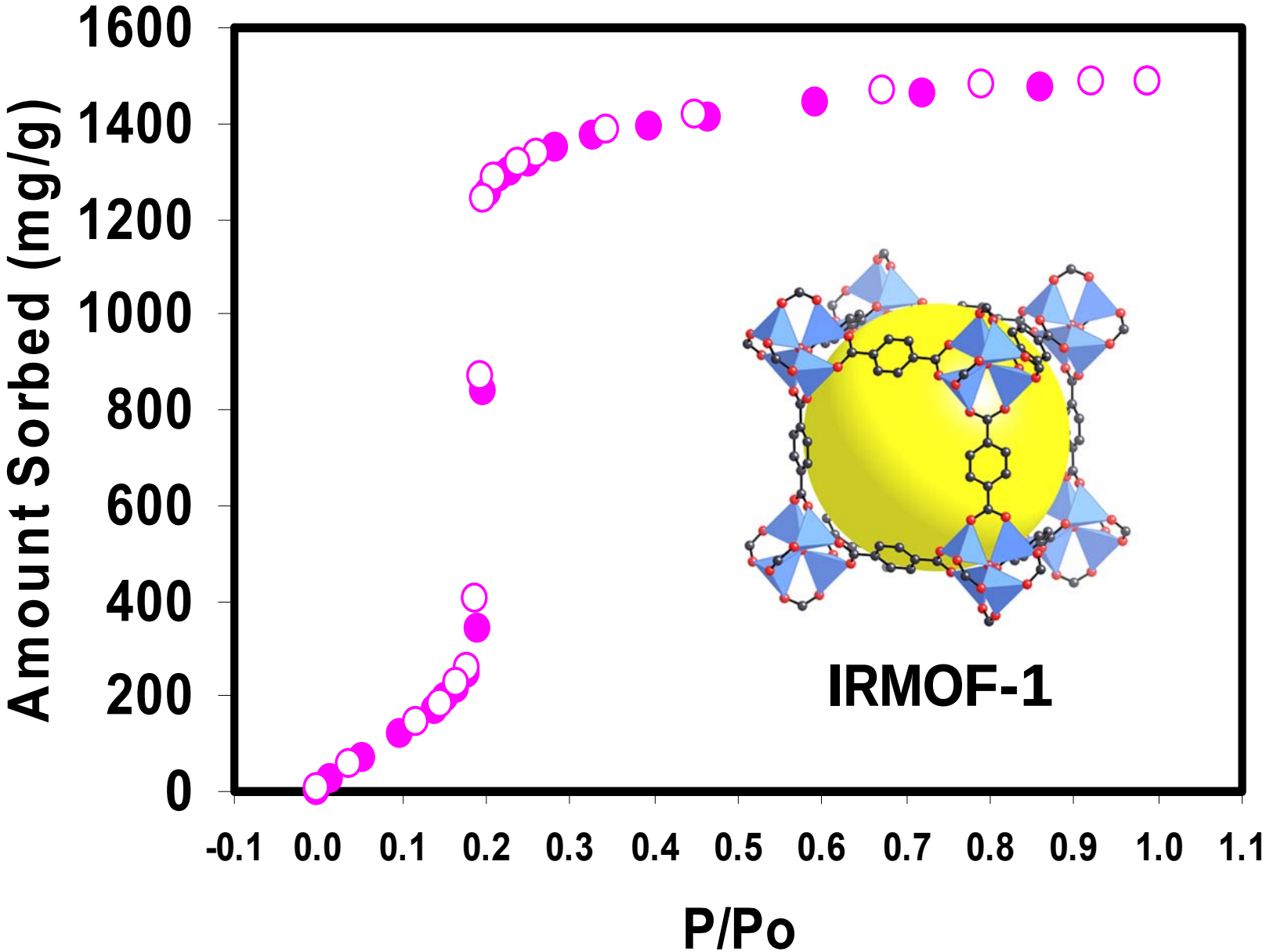
High S.A.

3-D framework

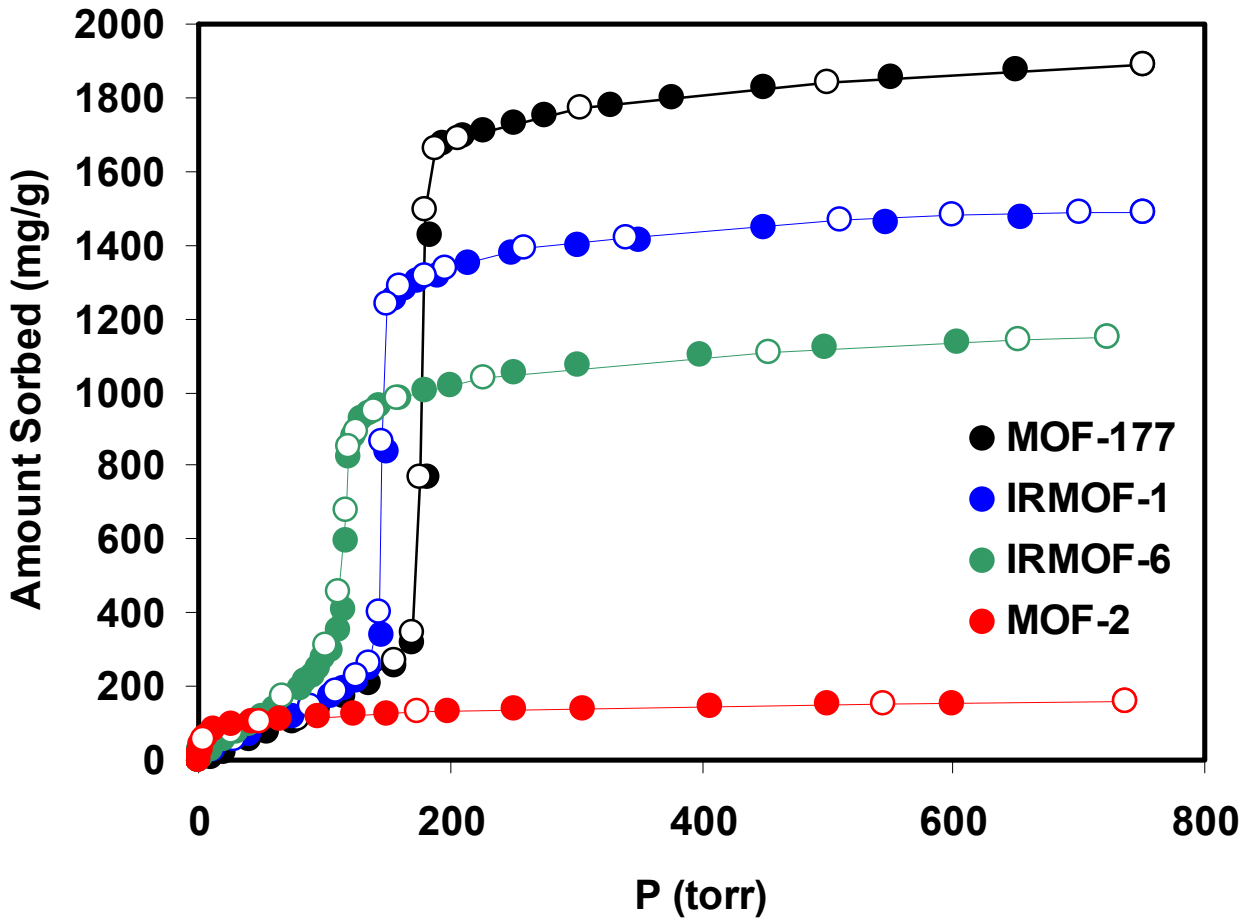
3-D channel system

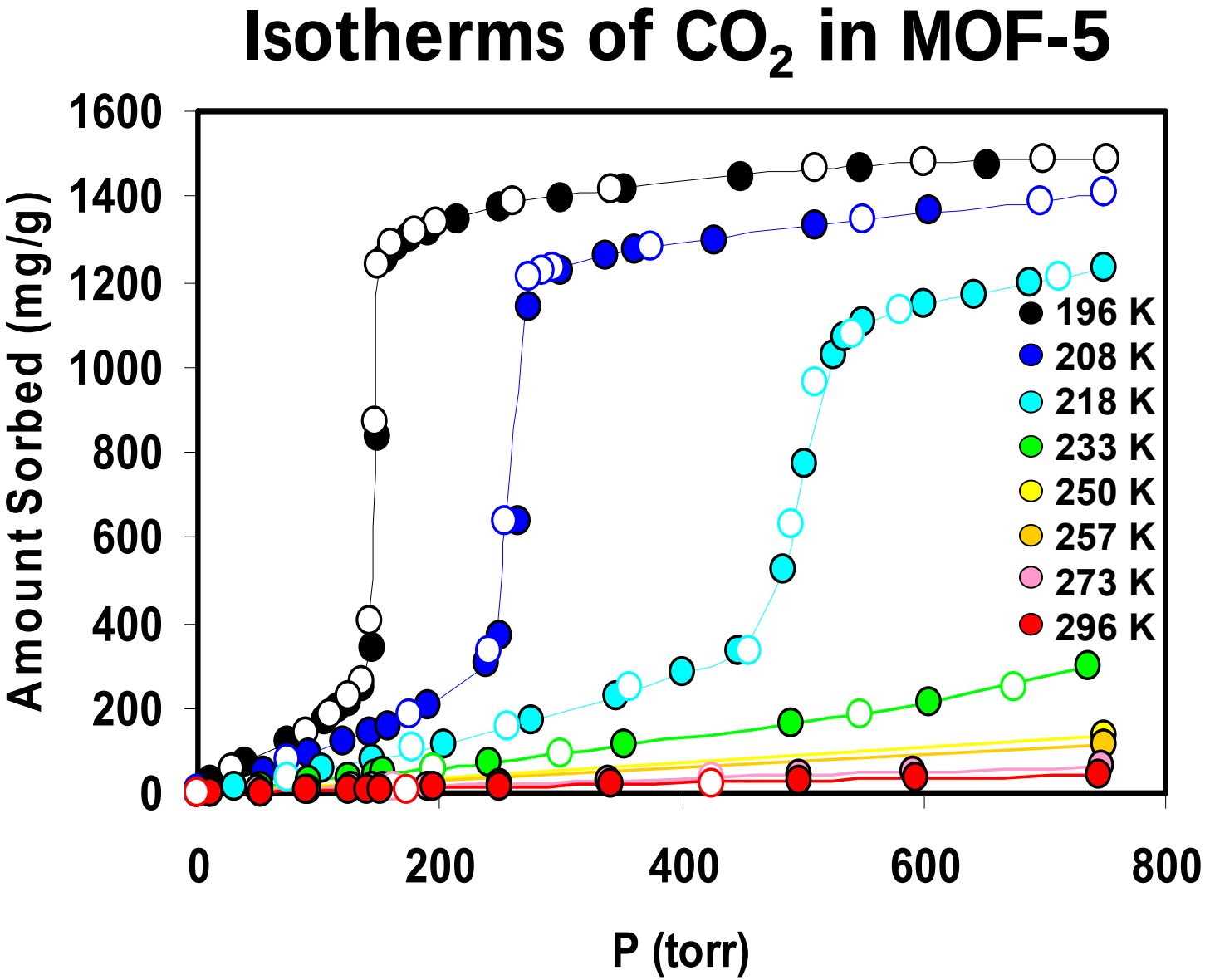
Ultra high S.A.

CO_2 Uptake at 196 K

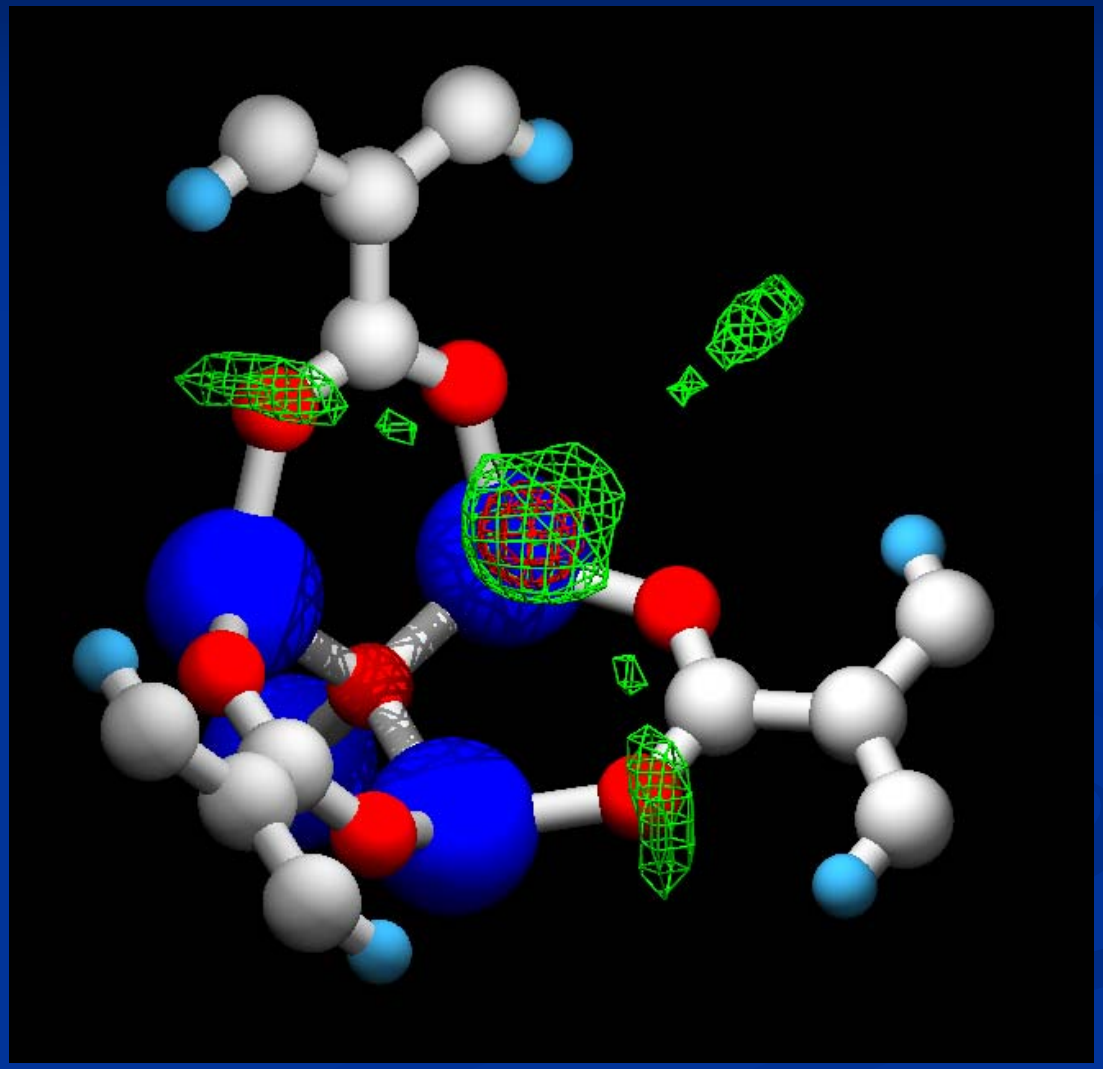


CO_2 Uptake at 196 K

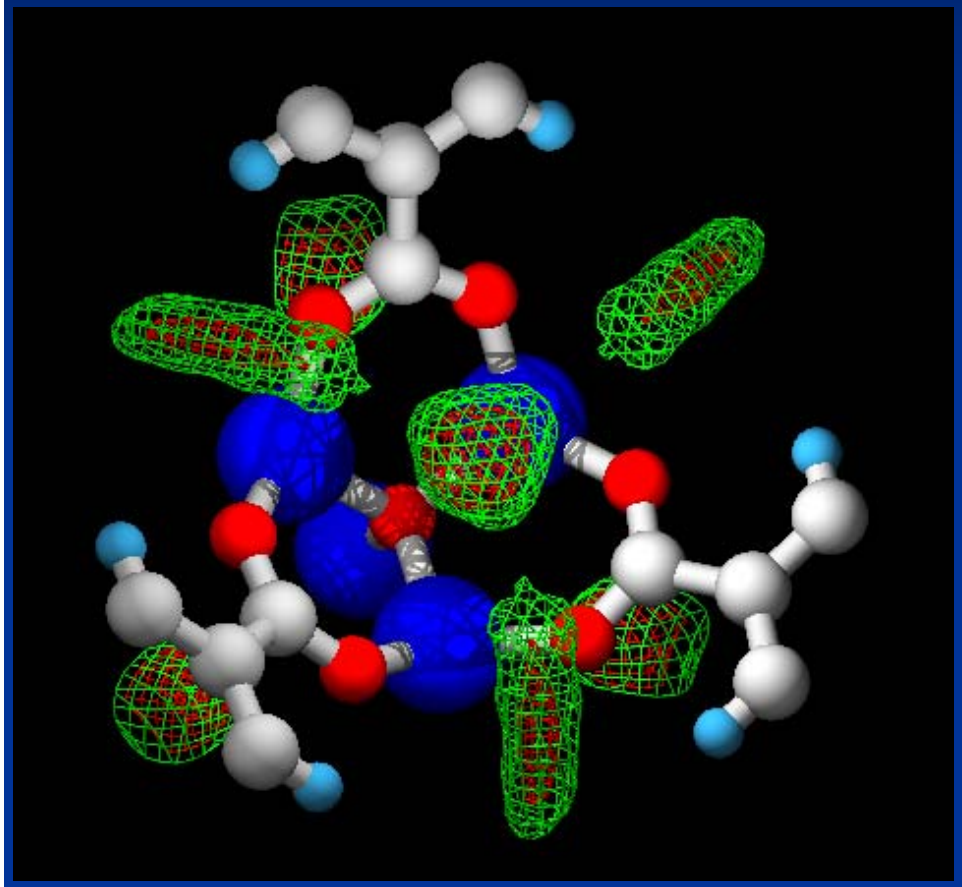


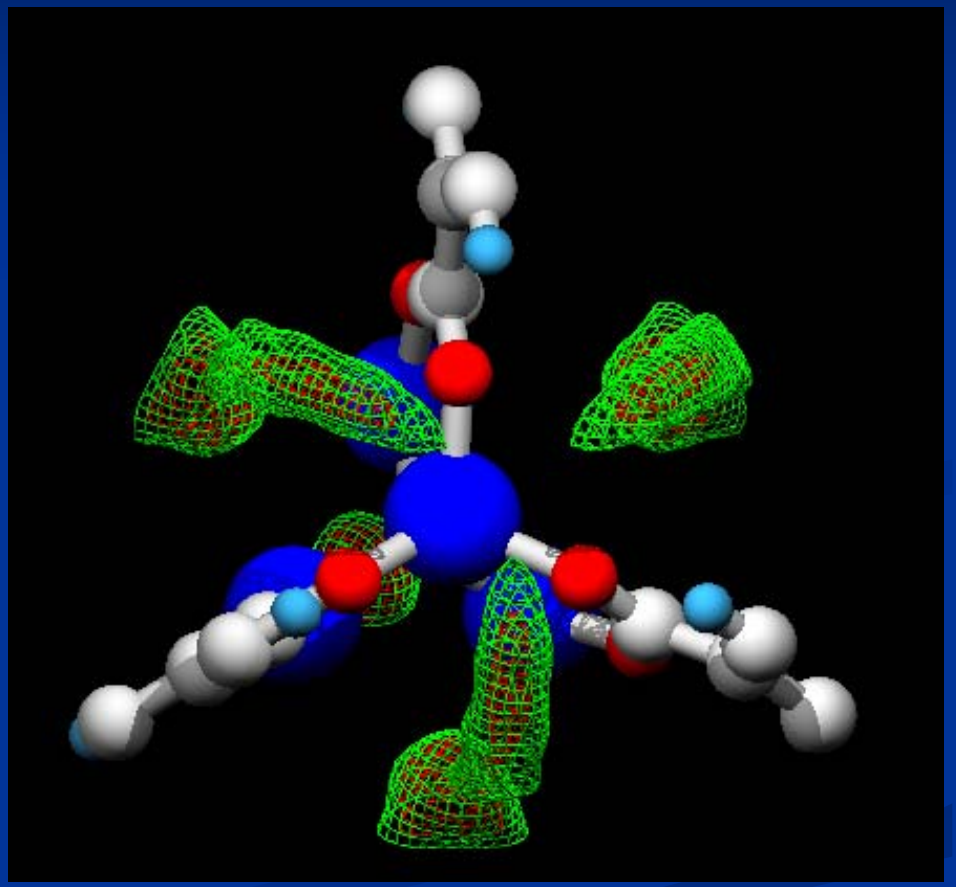

Isotherms of CO_2 in MOF-5
Amount Sorbed (mg/g)
1600
1400
1200
1000
800
600
400
200
0
0
200
400
600
800
P (torr)
196 K
208 K
218 K
233 K
250 K
257 K
273 K
296 K

MOF-5/CO_2 200 K SXRD

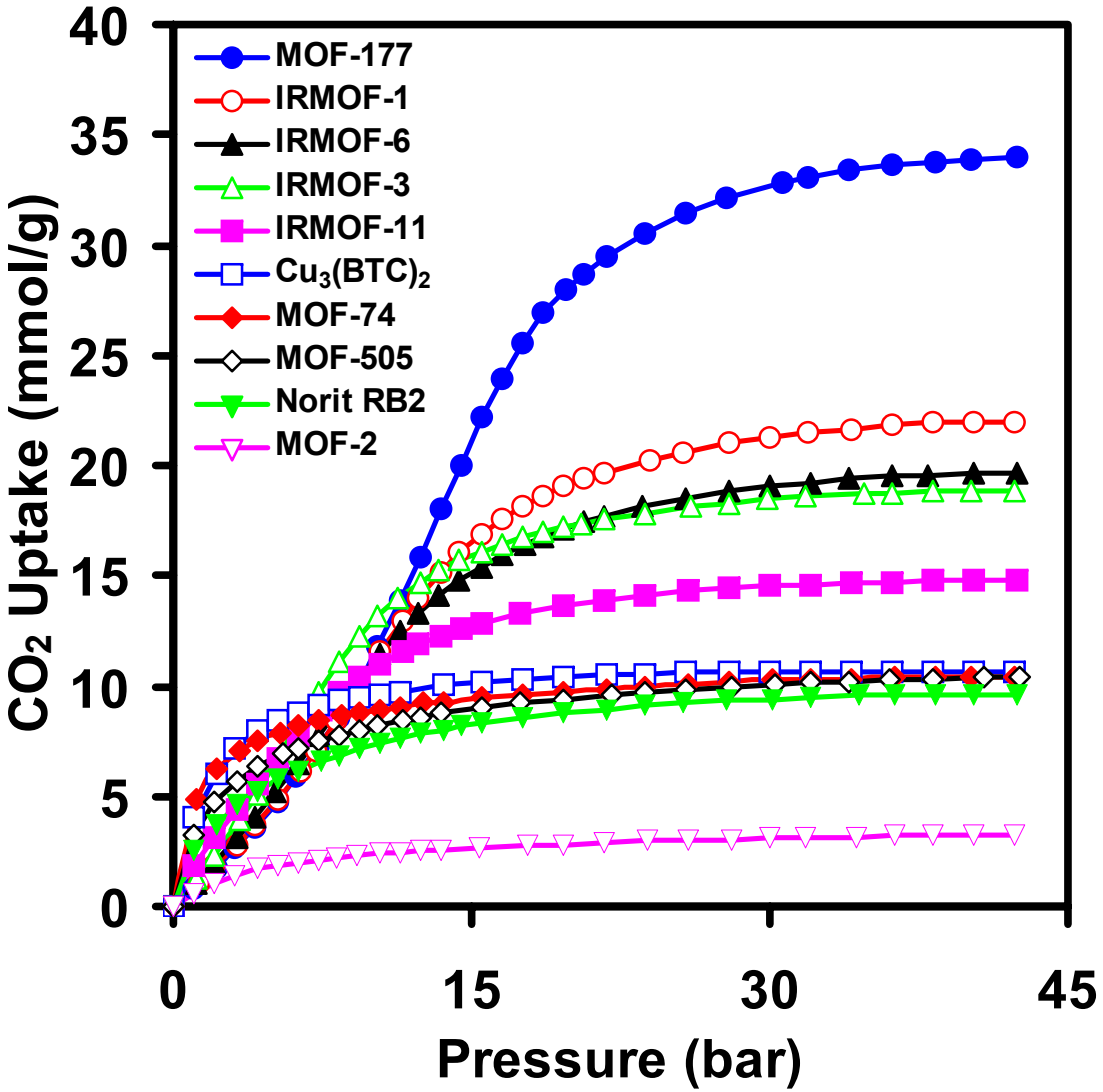


MOF-5/CO_2 150 K SXRD

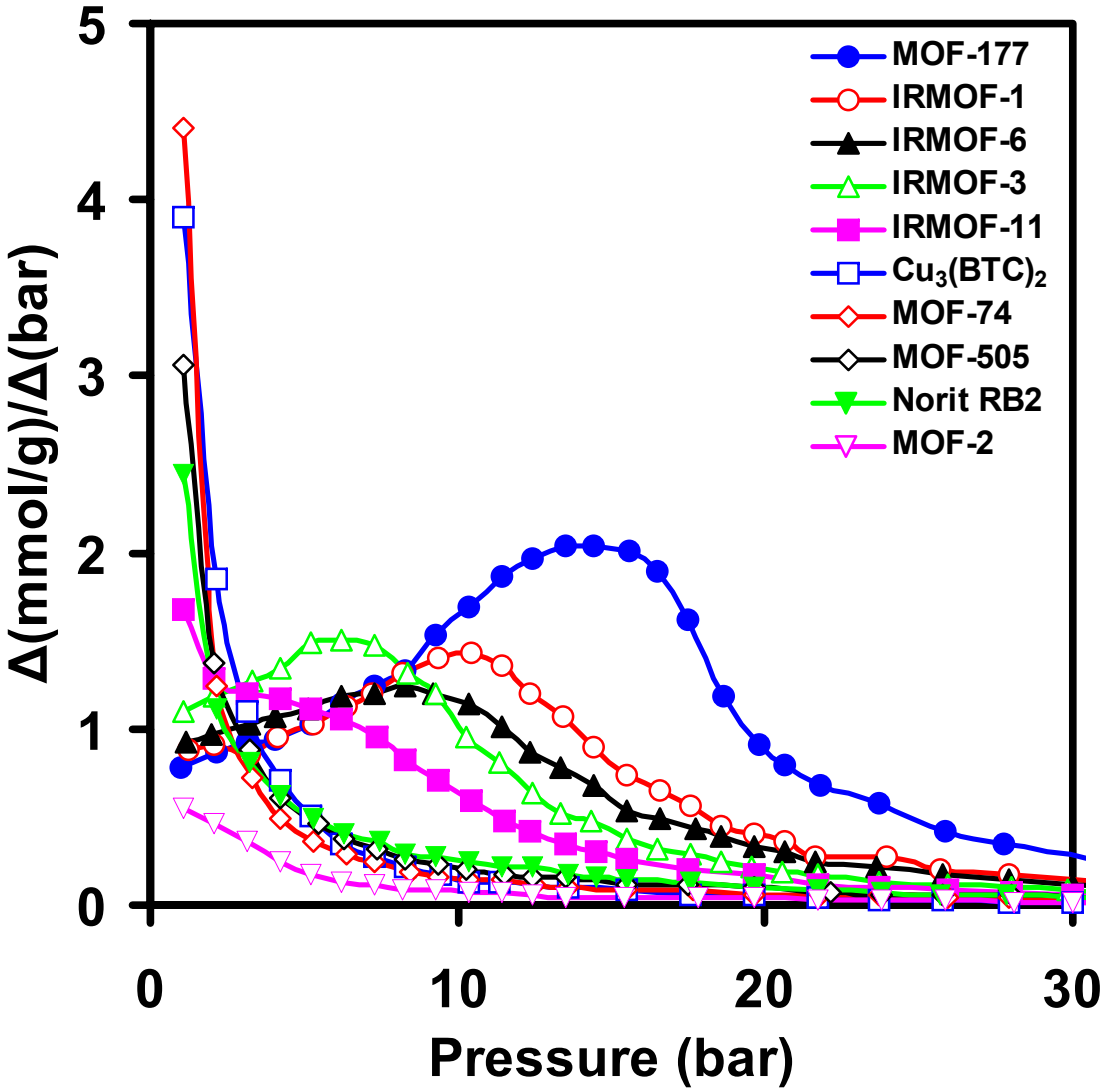




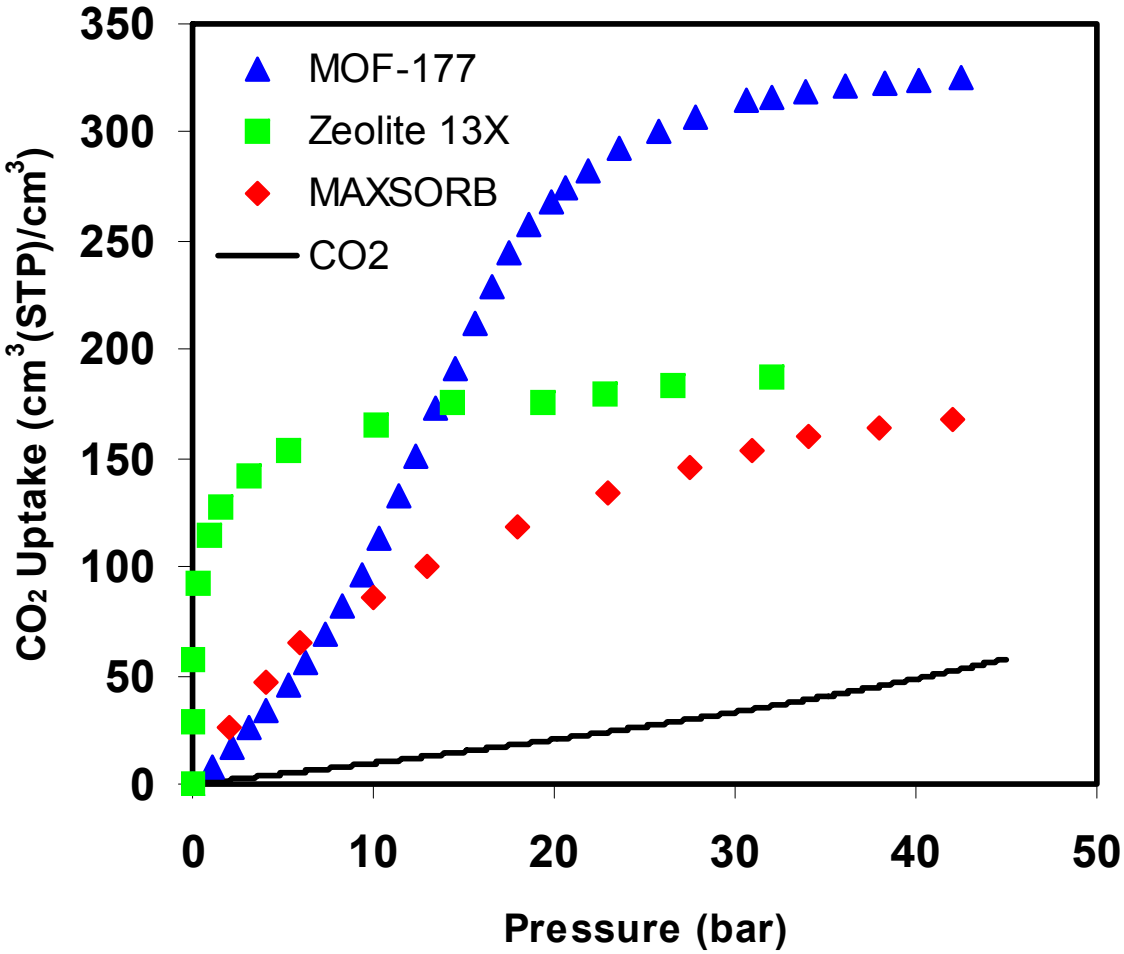
RT CO_2 Adsorption on MOFs



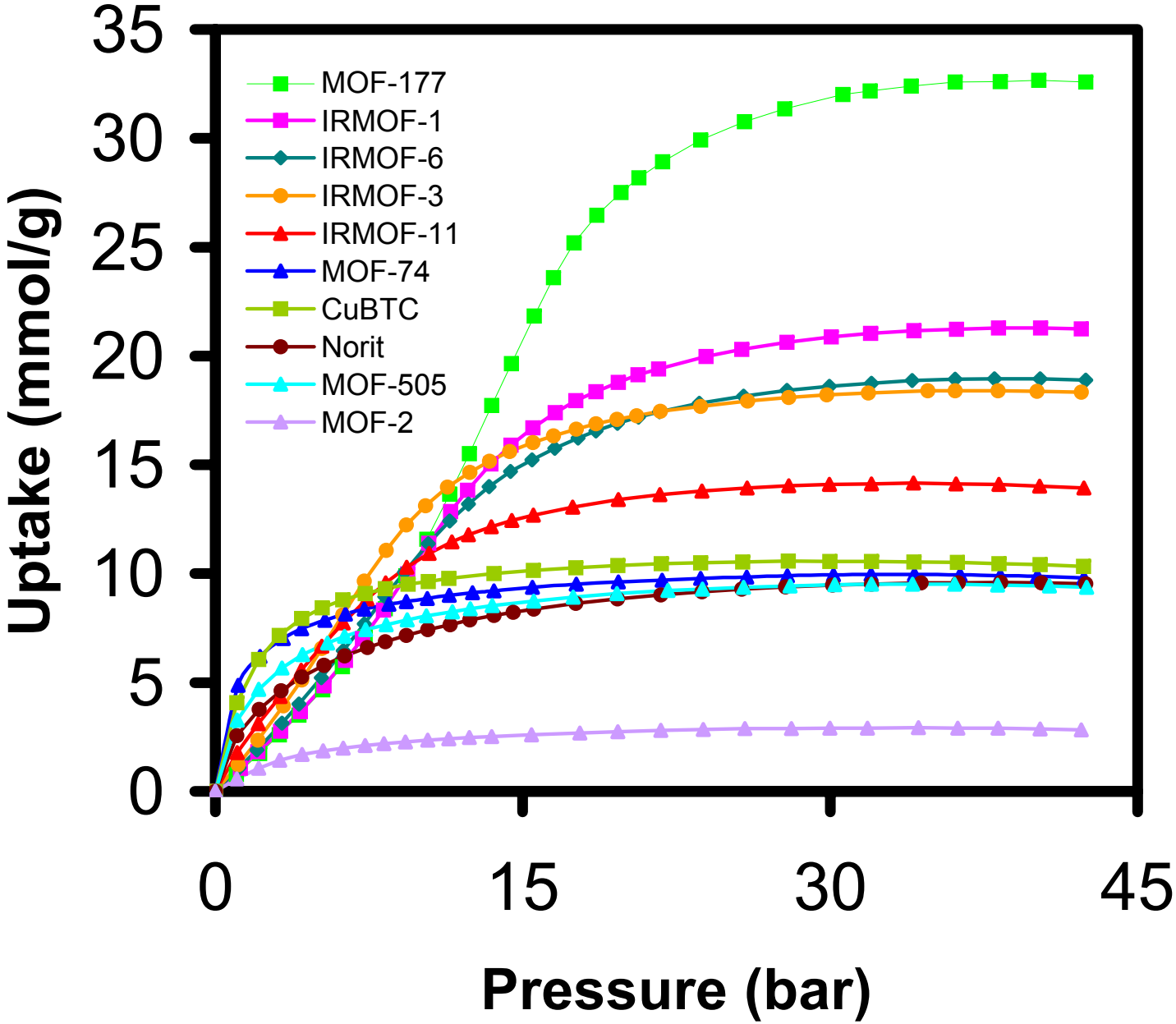
Derivative plots of isotherms



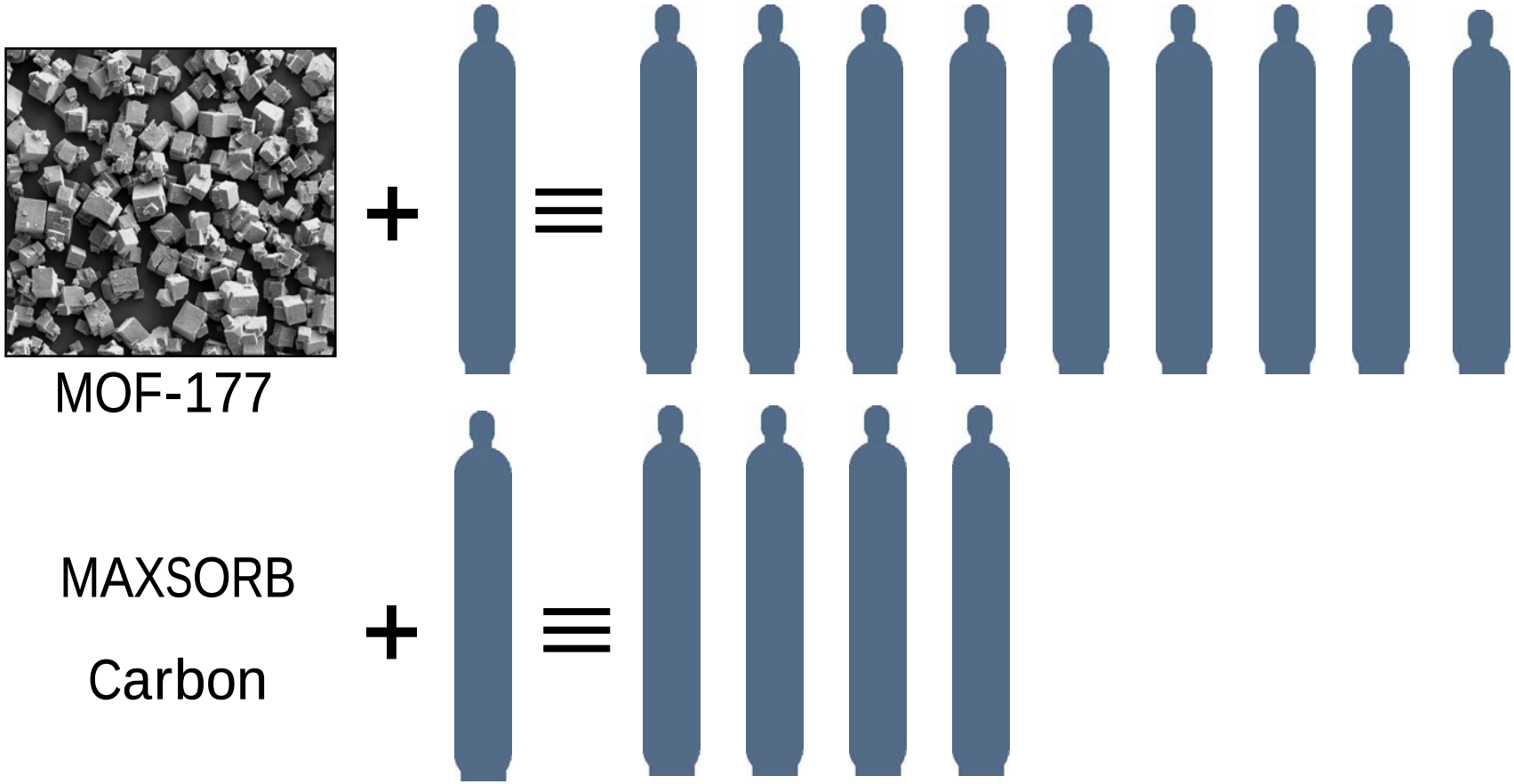
Exceptional CO_2 Capacity of MOF-177 at Room Temperature



Carbon Dioxide Storage at Room Temperature



Carbon dioxide storage at 32 bar and 298K (140 % wt of MOF-177)



CENTER FOR RETICULAR MATERIALS RESEARCH

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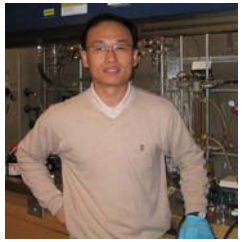
Acknowledgments to Group Members

Dr. Hiroyasu Furukawa



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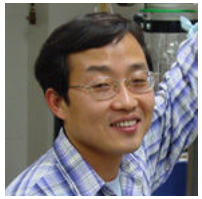

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