MOFs
– a new family of materials with high potential!

At the CatMat opening
Oslo
December 3rd 2004

From the MOF community,
delivered by Richard Blom

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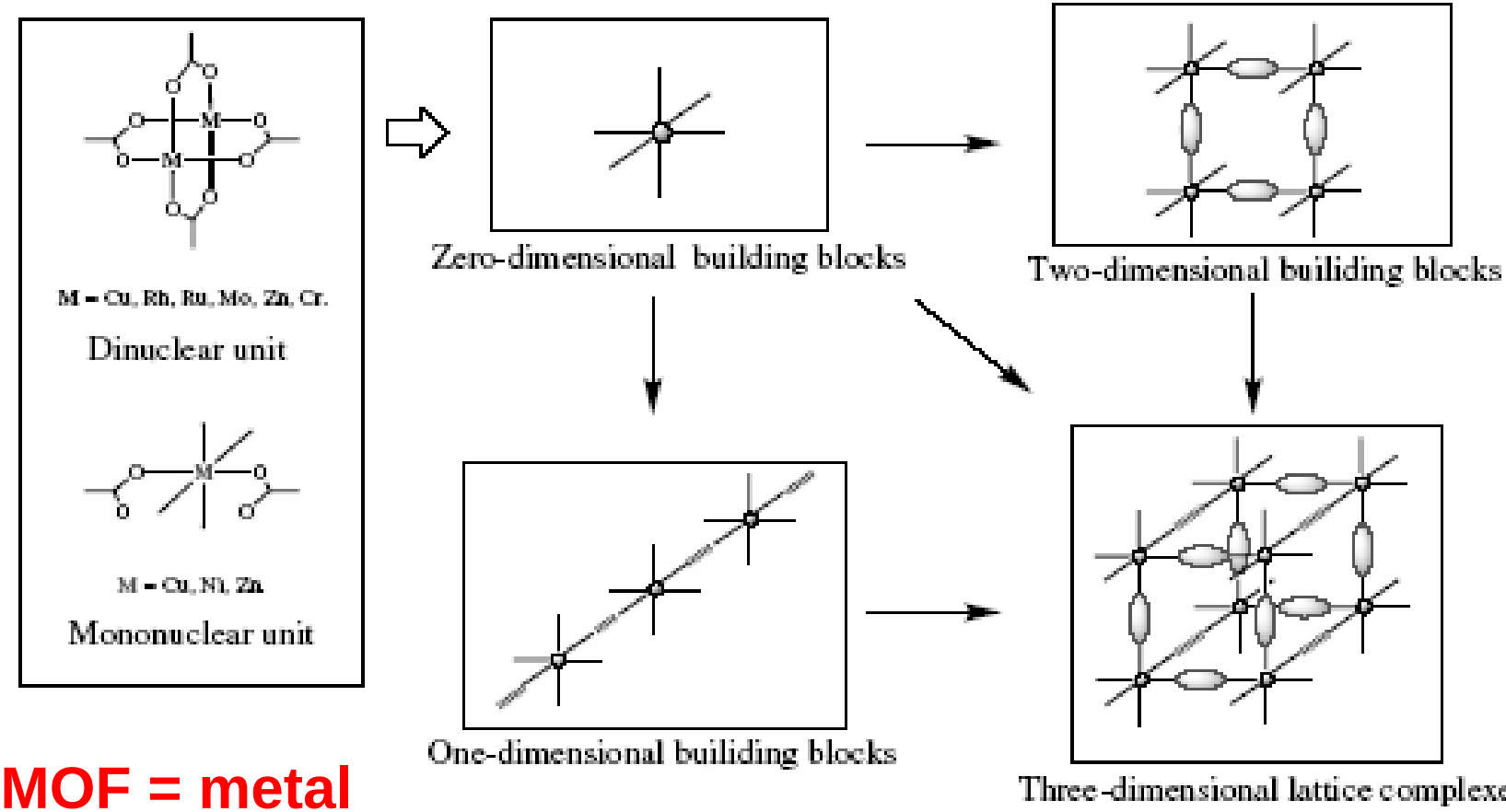
What is a MOF?



MOF = metal organic frameworks

Potential application areas:

- **Gas storage**
- **Gas separation**
- **Catalysis**
- **etc……**

Reso…m:

UiO
+ SINTEF
= SANT

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Dr. Ole Swang (2) …g
Dr. Rune Wendelbo (2… …inatorial methods
Dr. Ørnulf Vistad (2) …mbinatorial methods

(1) Dept. of Chemistry, Univers…
(2) SINTEF Materials and Chem…

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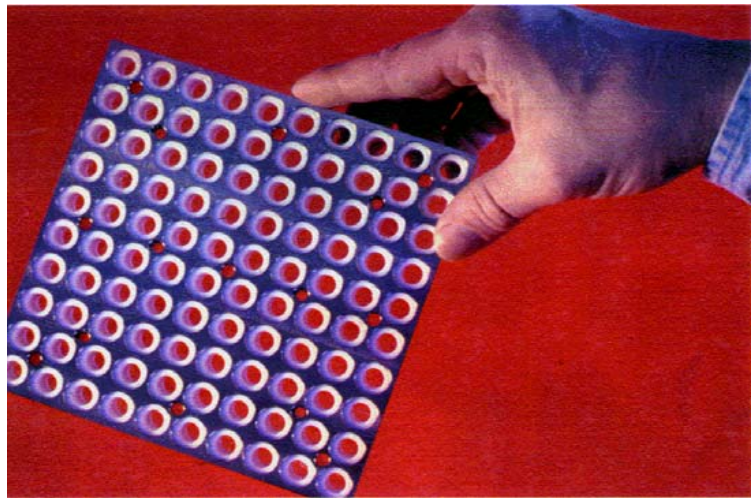
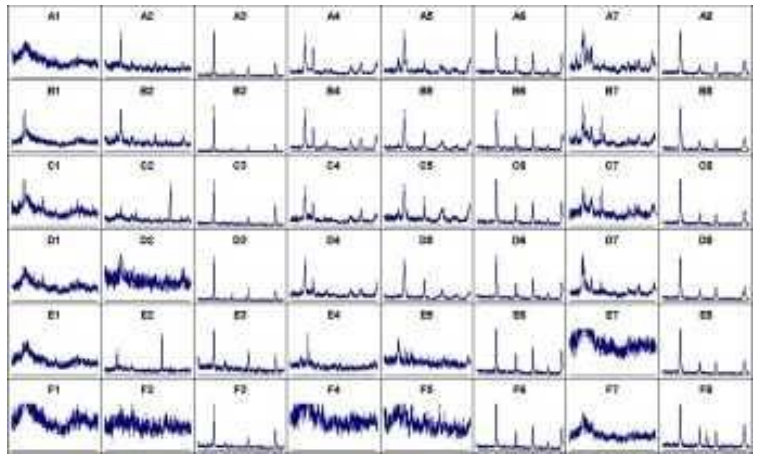
Combinatorial methods

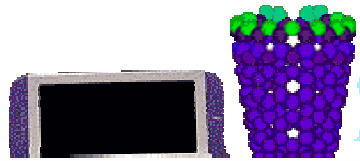
- Expertise:
  - development of equipment for combinatorial synthesis, characterization and testing
  - inorganic materials and coordination polymers
- Methodics:
  - A number of different automated rigs for combinatorial preparation, power XRD, SEM, and performance testing of solid materials





D.E. Akporiaye, A. Karlsson, R. Wendelbo and I.M. Dahl, *Angew. Chemie Int. Ed*., (**1998**), *37*, 608; D. Akporiaye, I. Dahl, A. Karlsson, M. Plassen, R. Wendelbo, D.S. Bem, R. W. Broach, G. J. Lewis, M. Miller, J. Moscoso, *Micro. Meso. Materials*, *48*, 367, (**2001**); Duncan Akporiaye, Rune Wendelbo, Ørnulv Vistad, Arne Karlsson, Martin Plassen, Karl Petter Lillerud, James McCoy, *Zeolite News Letters, Japan Association of Zeolite*, (**2003**), *20*, 18. + patents

H_2 Storage techniques:



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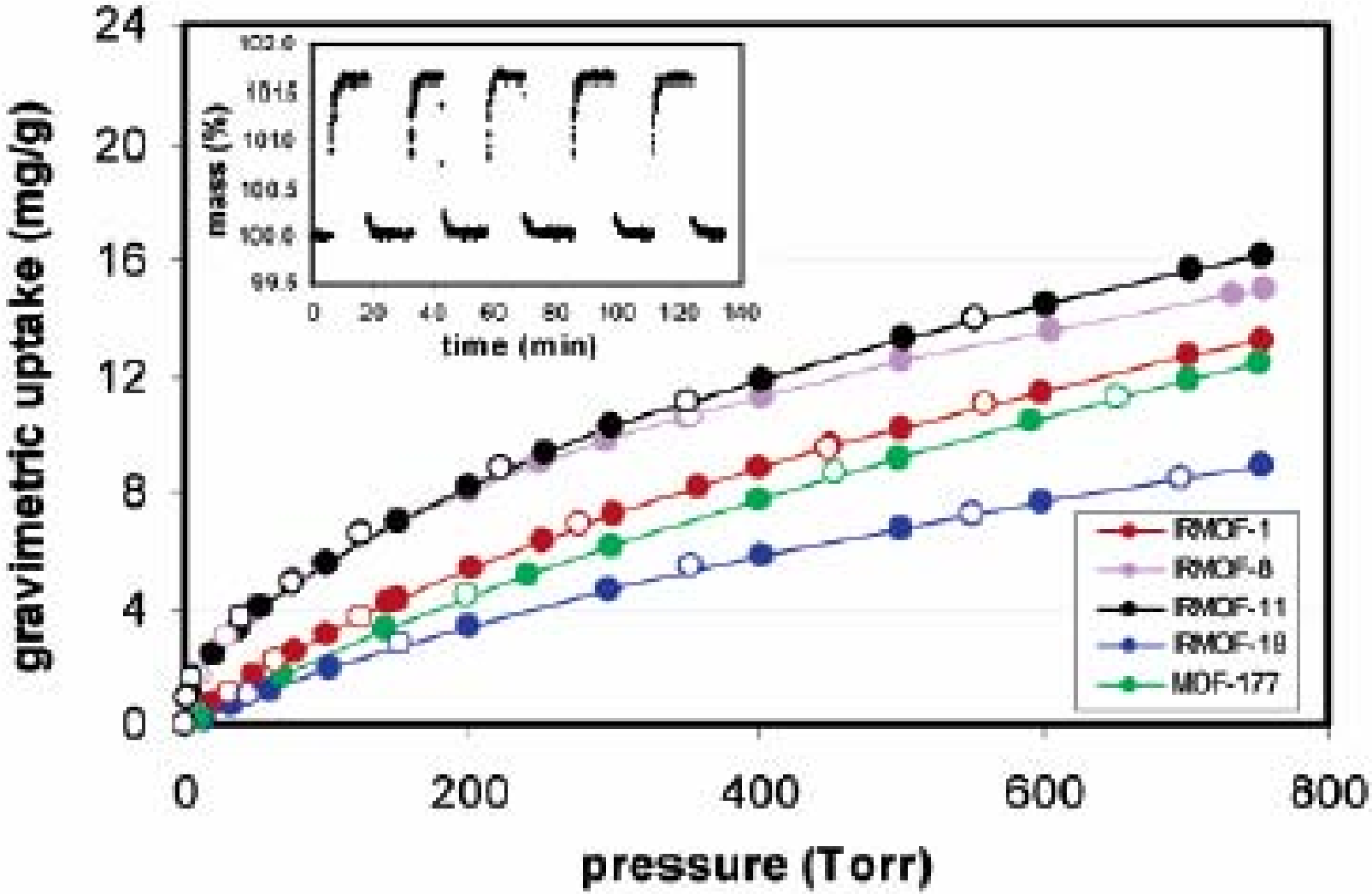

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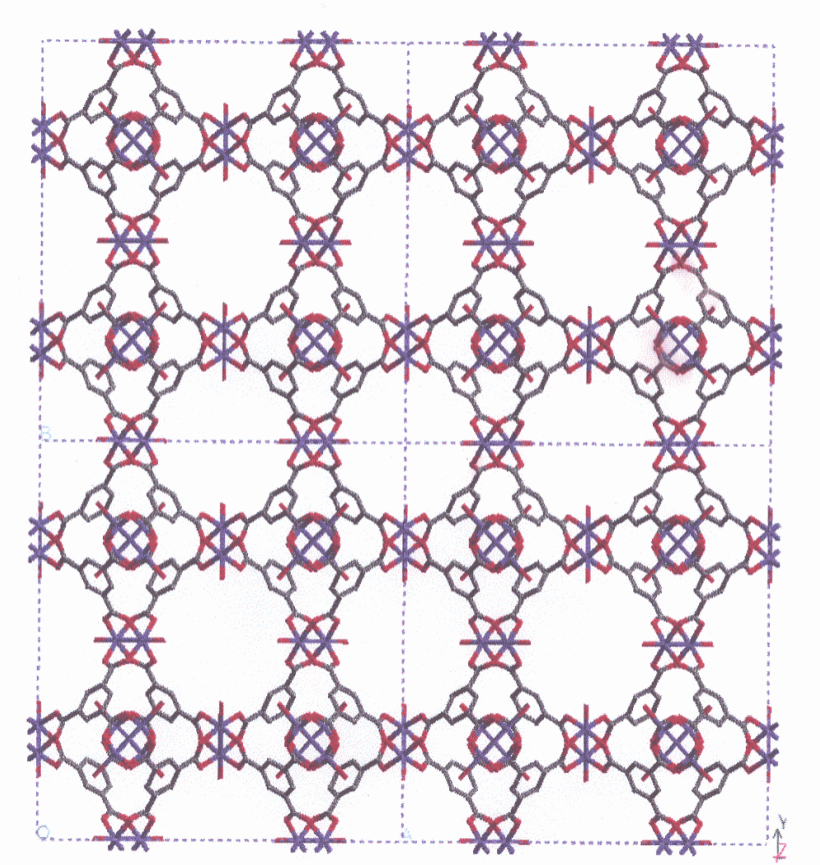
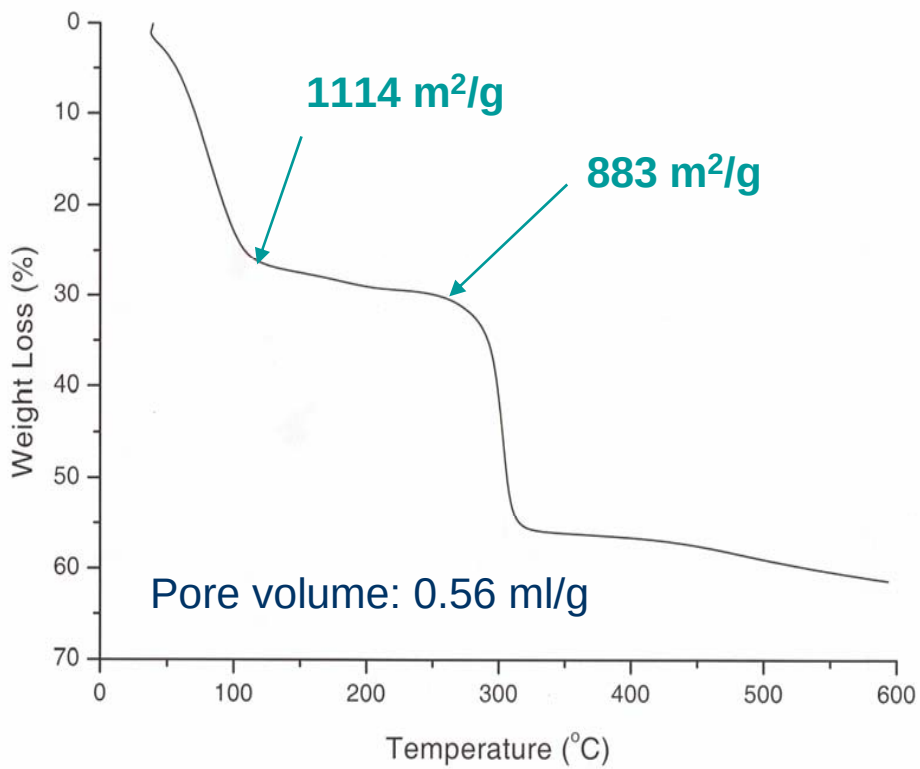
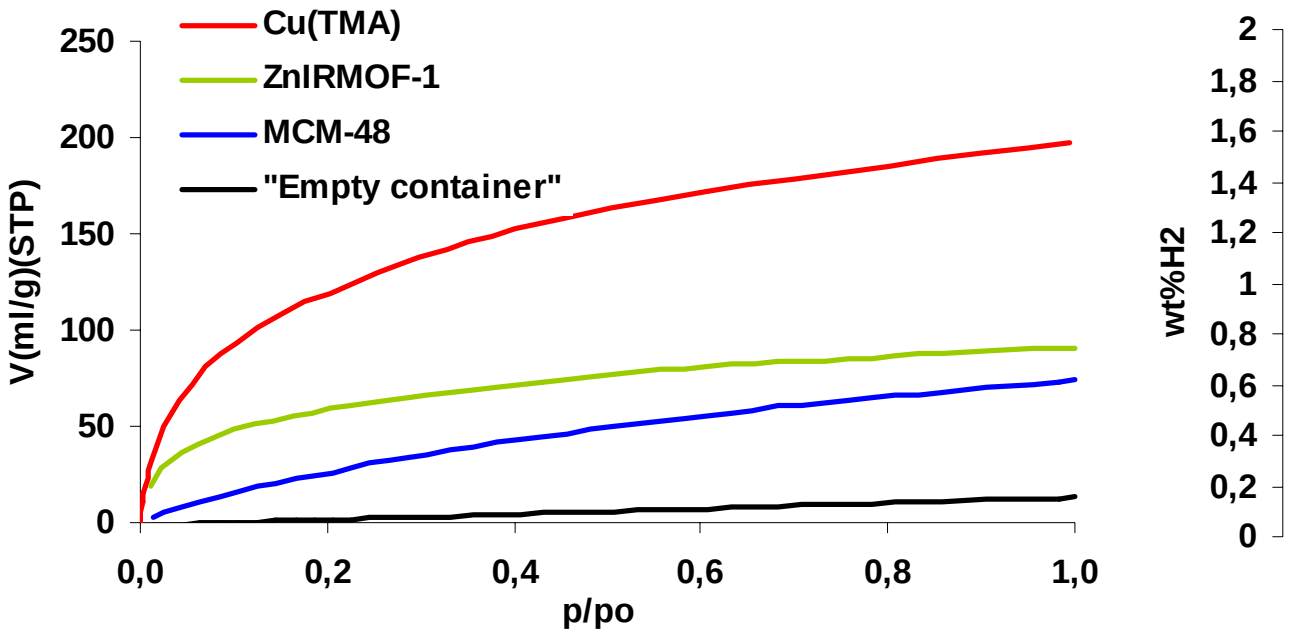
Hydrogen adsorption in coordination polymers: $[Cu_3(TMA)_3(H_2O)_3]_n$ * (Cu(TMA))





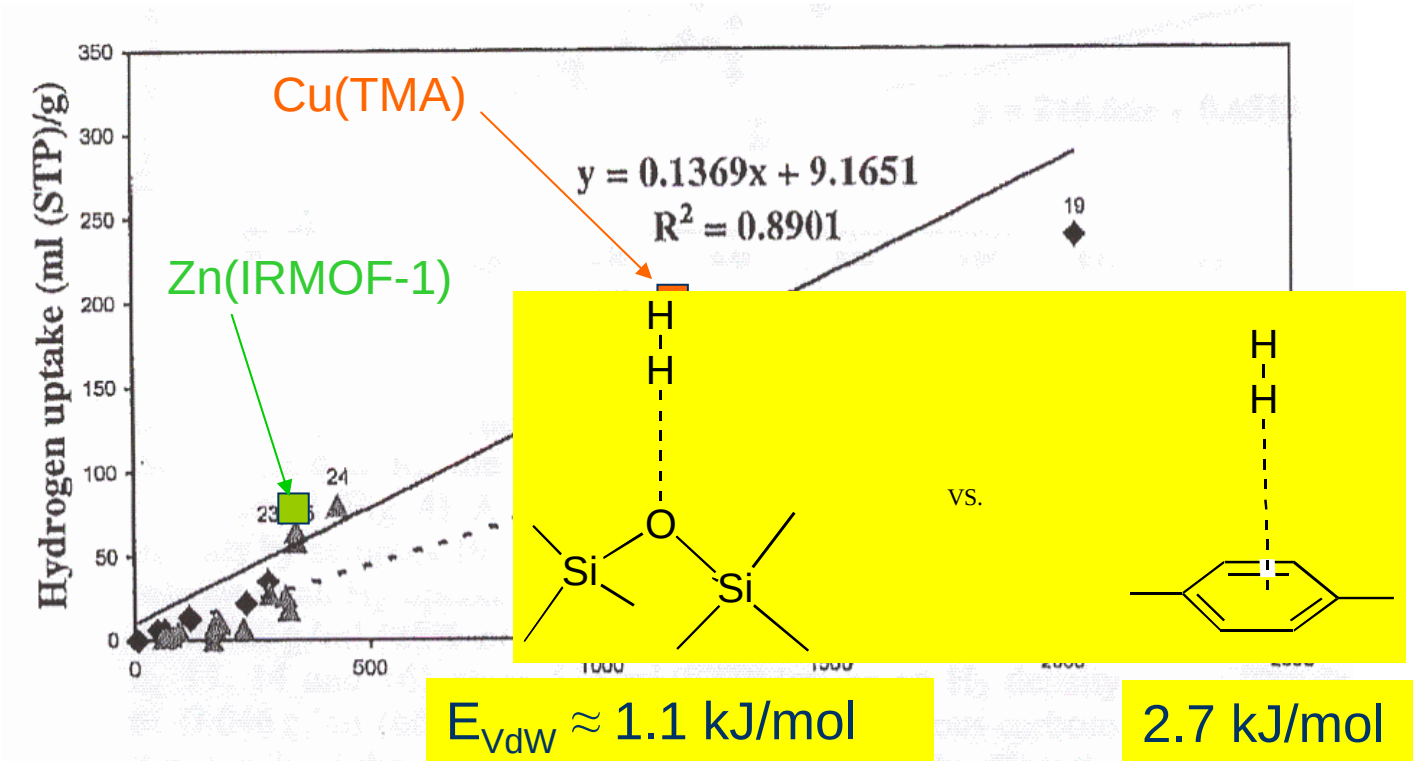
***** Williams *et al., Science*, **283** (1999) 1148; R. Blom, R. H. Heyn, O. Swang, H. Fjellvåg, K. O. Kongshaug and R. K. Birkedal Nielsen, *Chem. Eng. Trans*, **Vol. 4**, 2004, 325.

Hydrogen adsorption at 77 K - low pressures



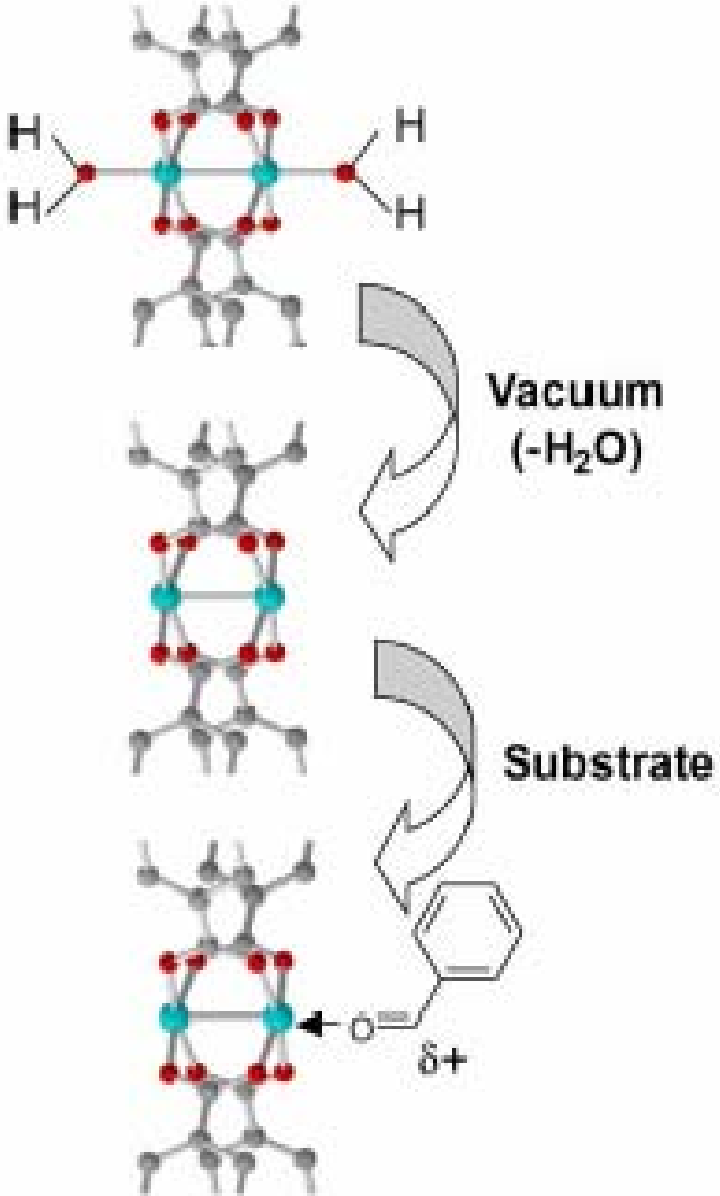
Cu(TMA):	Corresponds to:	0.038 kg H_2/l	26.4 l/kg H_2
	For comparison:		
	H_2 gas, 200 bar, RT:	0,018 kg H_2/l	56,3 l/kg H_2
	H_2 gas, 200 bar, 77K:	0,063 kg H_2/l	15,8 l/kg H_2
	LH_2:	0,071 kg H_2/l	14,1 l/kg H_2

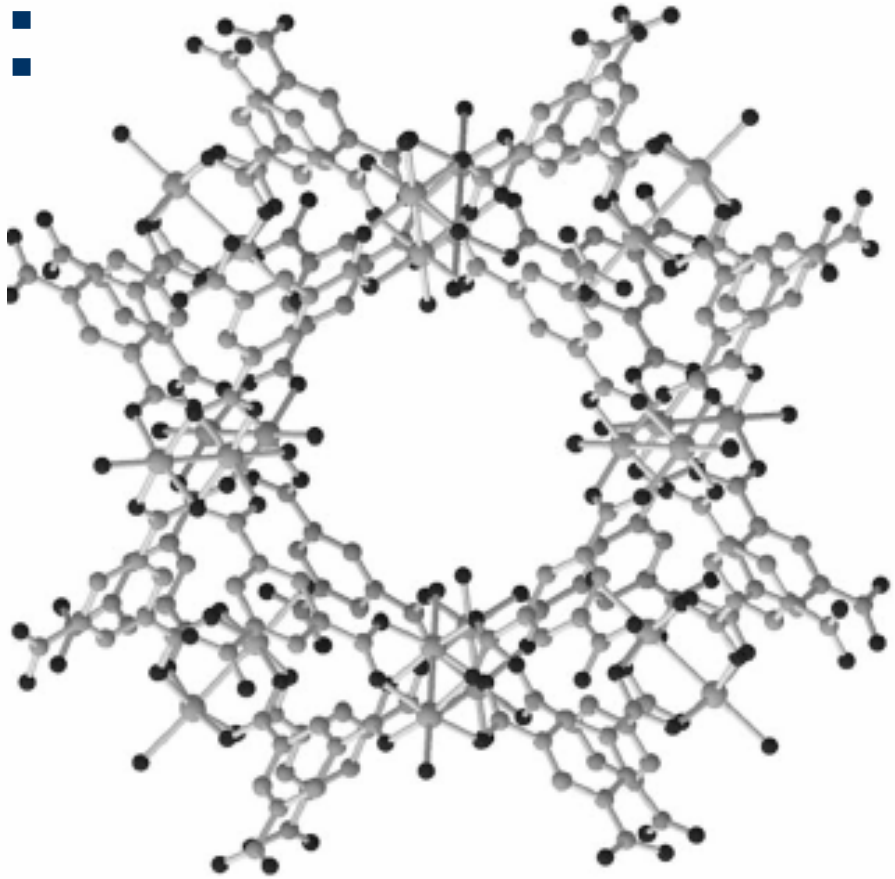
Hydrogen uptake at 1 atm vs. BET Surface area:



Coordination polymers (Cu(TMA) and Zn(IRMOF-1)) similar to carbon materials, MCM-48 falls within group of oxide materials

* de Jong *et al., Appl. Phys.* , A72 (2000) 619-623





$Cu_3(BTC)_2(H_2O)_3$

K. Schlichte et al., *Micropor. Mesopor. Mat*. *73* (**2004**) 81

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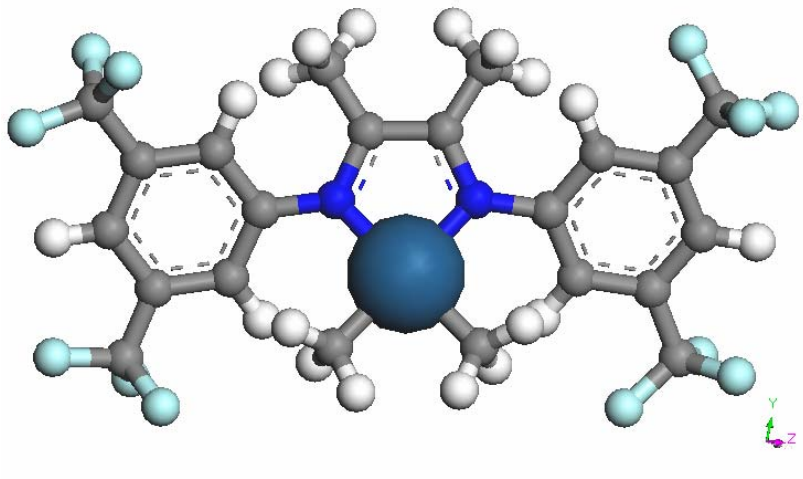
Hydrocarbon Activation

Pt-Complexes for Hydrocarbon Activation



Lars Johansson, Olav B. Ryan, and ***Mats Tilset*** *J. Am. Chem. Soc.* **1999,** *121,* 1974-1975

Heiberg, H.; Johansson, L. G.; Ryan, O. B.; Swang, O.; Tilset, M.; Gropen, O. *J. Am. Chem. Soc.* 2000, *122*, 10831.

Homogenous systems presently show the highest activity towards methane activation.

The Tilset group (UiO) and SINTEF Oslo have developed platinum complexes that show extremely high activity for activating alkanes.

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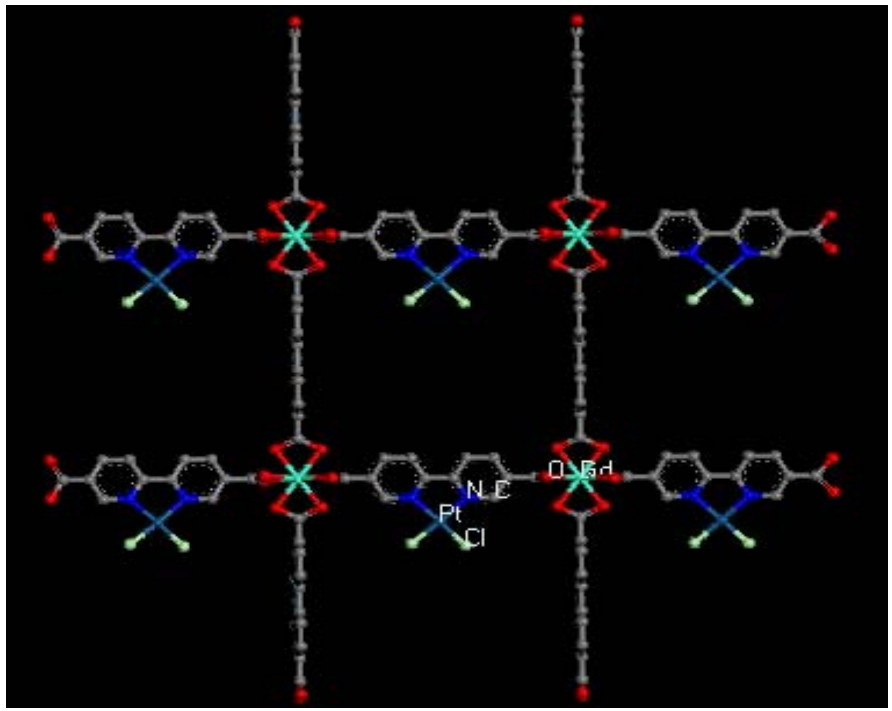
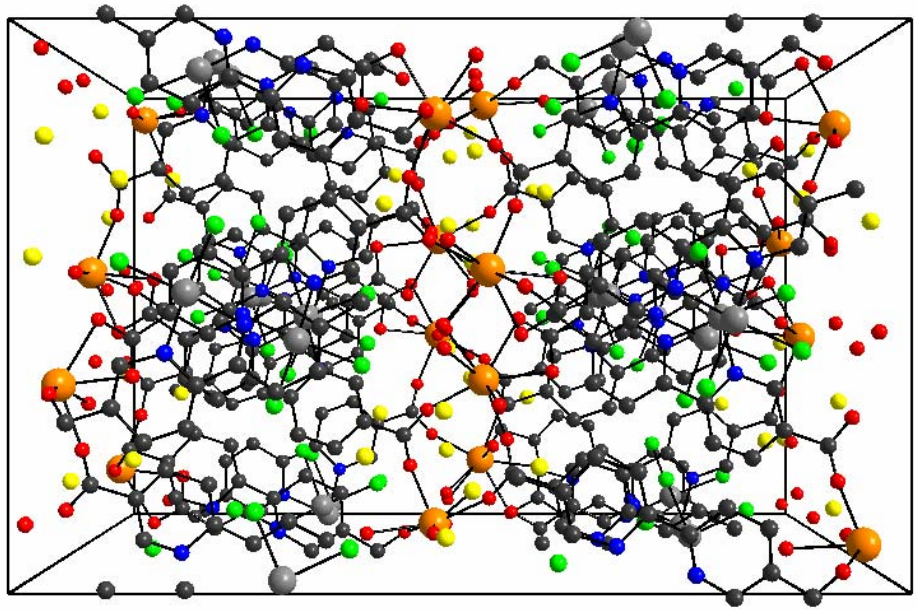
Design of the 3rd generation platinum-organic compound

- Introduce an other metal to build up the 3D framework
- Use 2,2-bipyridine-5,5-dicarboxylic acid as the ligand
- Gadolinium has been chosen to be the new metal



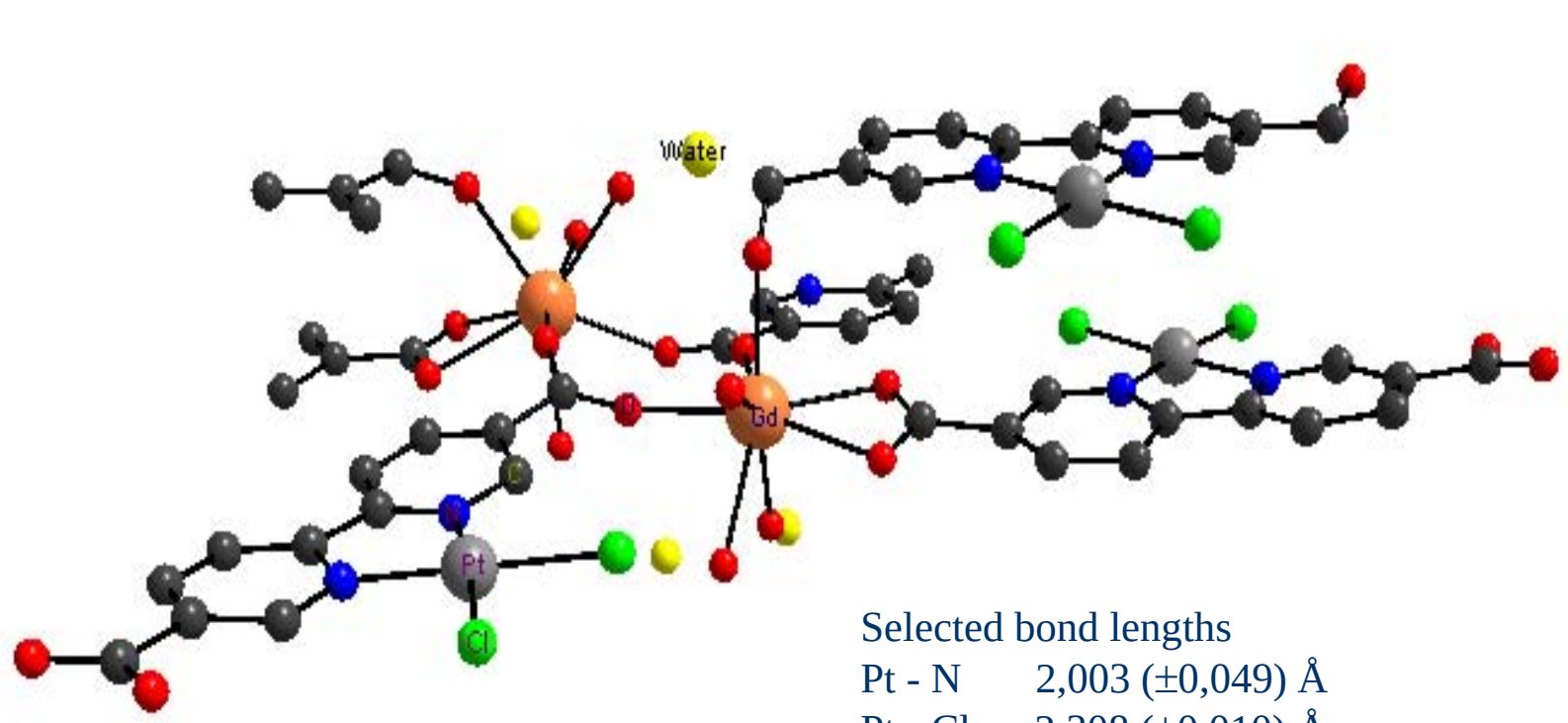
Lattice of the 3rd generation platinum-organic compound



- Lattice parameter:
  a = 28,2274 Å, α = 90°
  b = 17,9877 Å, β = 90°
  c = 19,8177 Å, γ = 90°
- R = 0,2062 (all data)
- Space group: Pbca

The structure is solved by K.C. Szeto and K.O. Kongshaug from single crystal X-ray diffraction

Structure description



Selected bond lengths

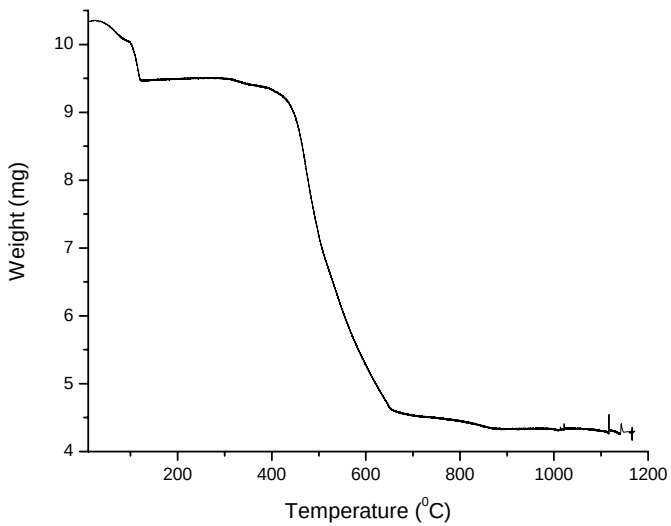
Pt - N	2,003 (±0,049) Å	
Pt - Cl	2,308 (±0,010) Å	
Gd - O	2,350 (±0,039) Å	[μ^1-carboxylate]
Gd - O	2,298 (±0,040) Å	[μ^2-carboxylate]
Gd - O	2,486 (±0,034) Å	[η^2-carboxylate]
Gd - O	2,422 (±0,058) Å	[water]

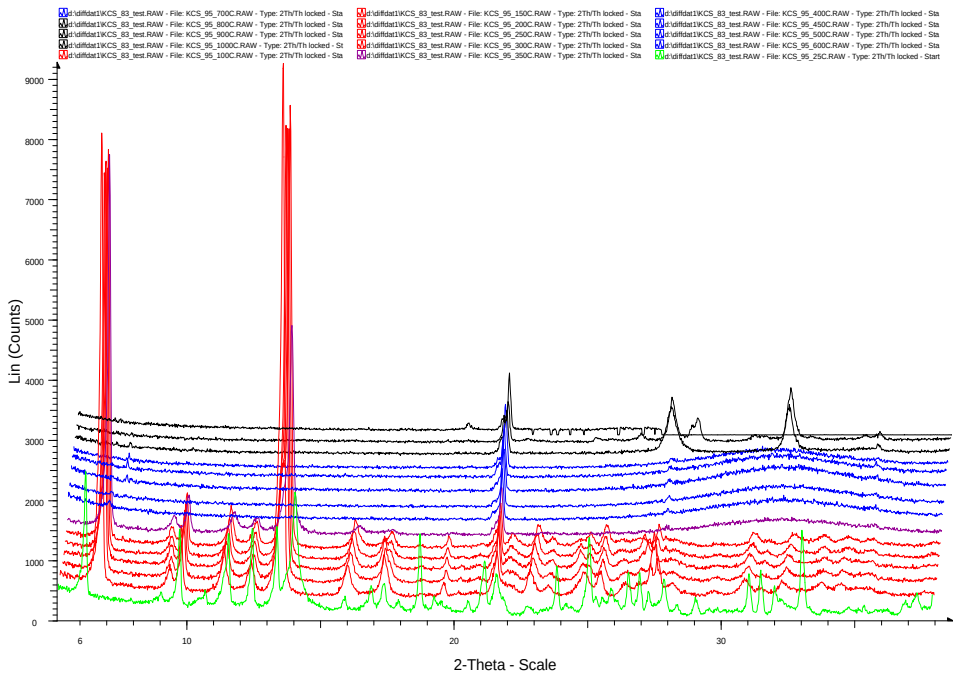
Selected angle

N - Pt - N	80,42° (±0,57°)
Cl - Pt - Cl	87,91° (±0,16°)

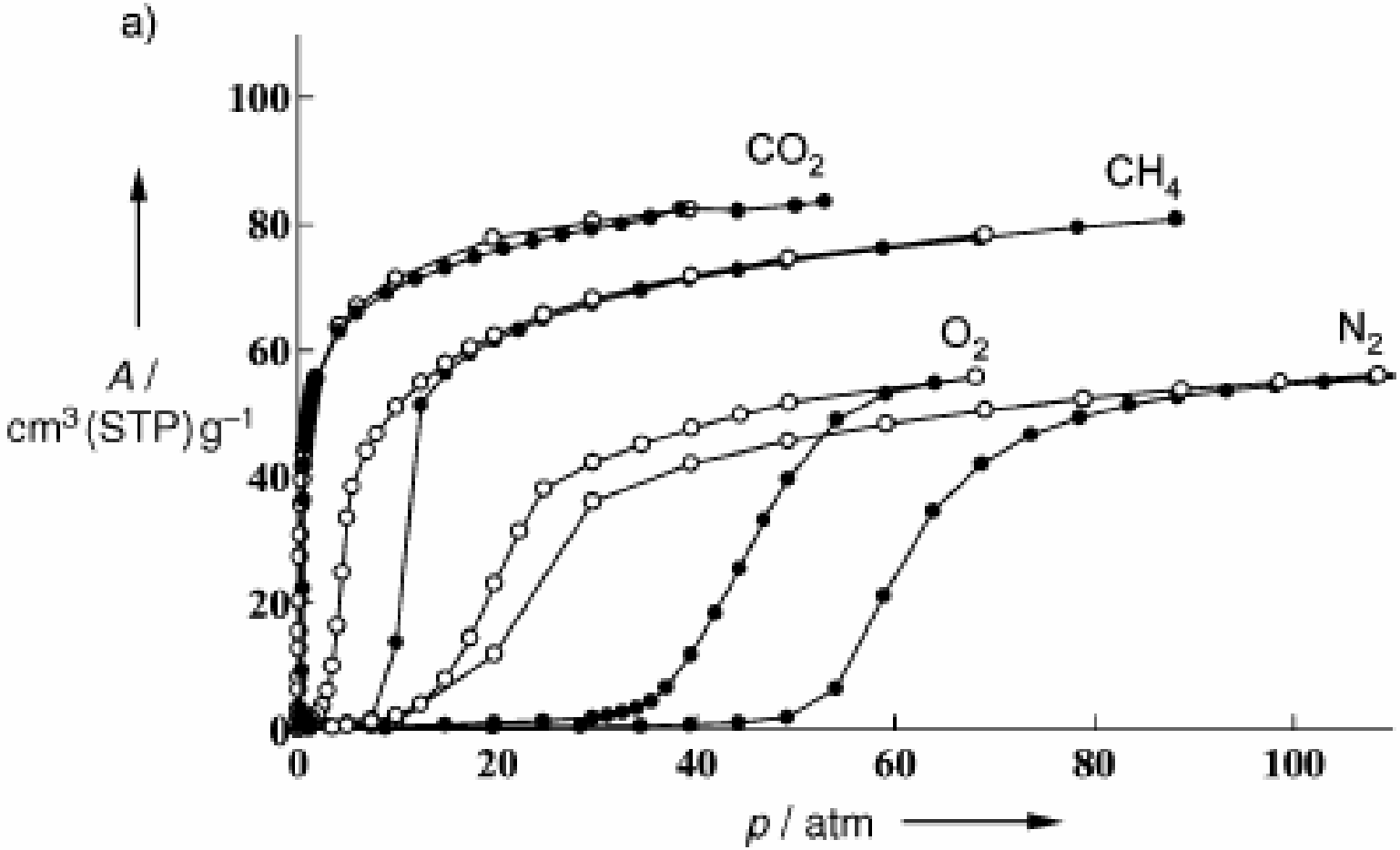
Thermal property

- Reconstruction of the structure at 100°C
- The high temperature modification is thermal stable up to 350°C
- The sample contains metallic platinum and Gd_2O_3 after heating





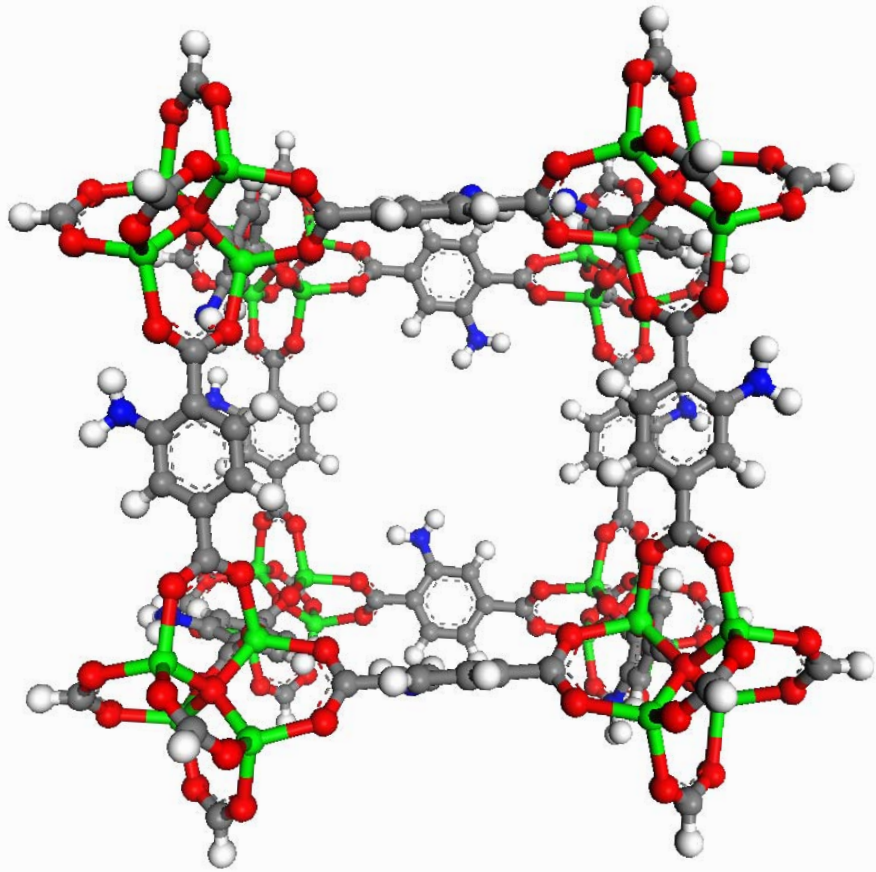
Selective adsorption



CO_2 adsorption: Project motivation and goal:

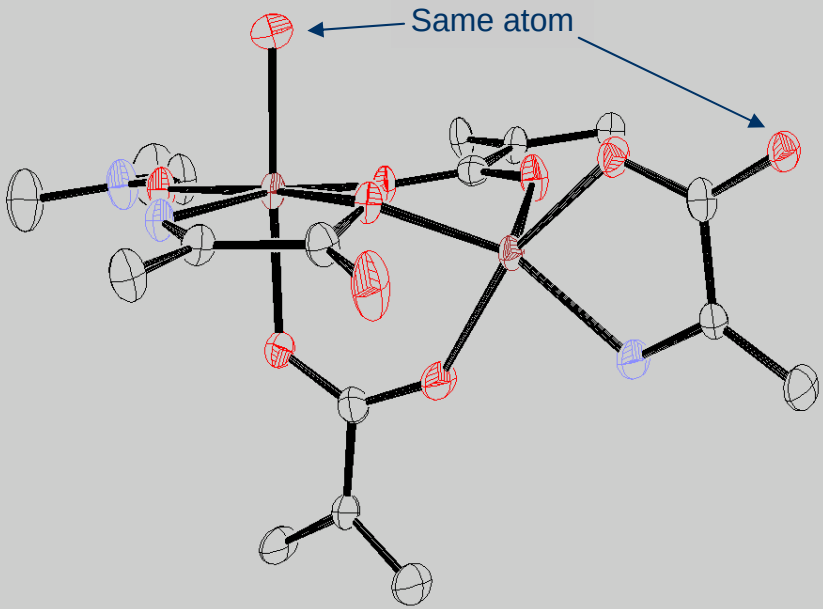
- **Motivation**:
  Might be more favorable than solution based amine processes due to:
  - no solvent (water cycling….)
  - higher stability
  - lower desorption temp.

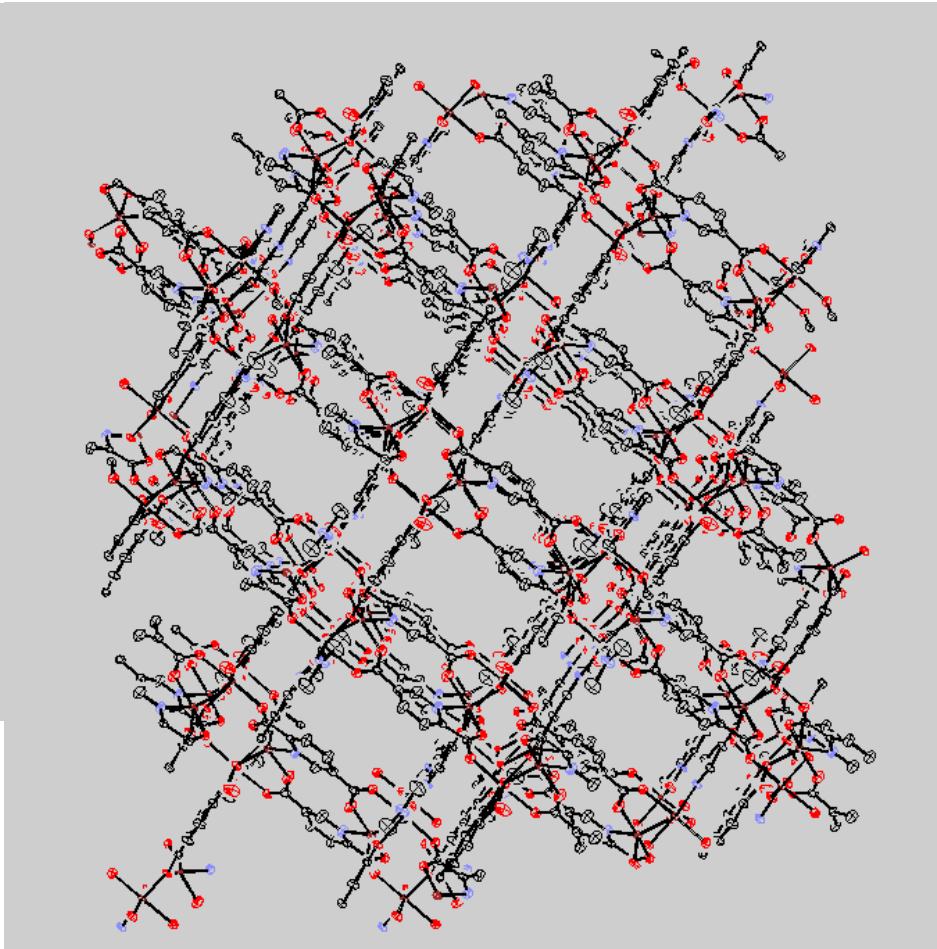
- **Goal**:
  To make new solid adsorbents for CO_2 removal from flue gases (and other gas mixes of interest…)



Eddaoudi, M.; Kim, J.; Rosi, N.; Vodak, D.; Wachter, J.; O'Keefe, M.; Yaghi, O. M. *Science* **2002,** *295,* 469

Some Pretty Pictures…..





- 6- and 5-coordinate Zn centers
- 2-Dimensional structure
- 0.5 DMF and 4 H_2O molecules in lattice
- Bond distances, angles normal

R. Heyn, unpublished results

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