Max-Planck-Institut für Metallforschung

# Physisorption of Hydrogen on Novel Porous Materials

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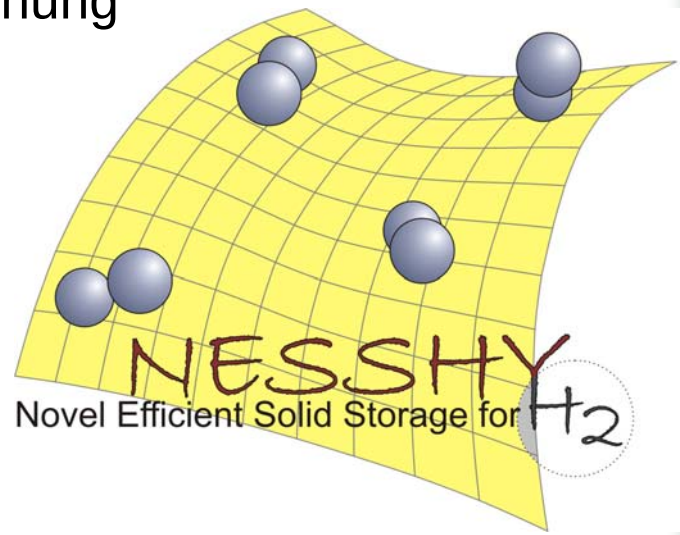
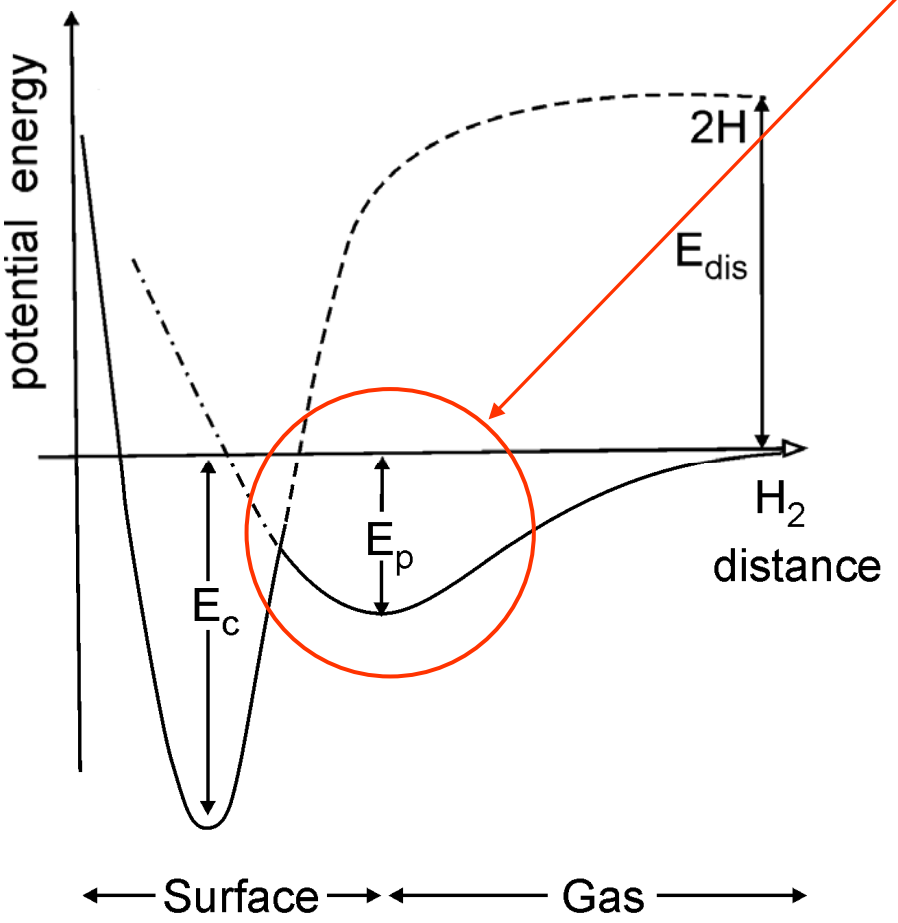


# Requirements for mobile application

- Low weight
- Small volume
- Driving range: 500 km
- Refueling time: < 3 min.
- No external cooling during refueling
- Lifetime: > 500 cycles
- Low material costs

# Mechanism of physisorption




- van der Waals forces
- small enthalpy of adsorption
- non activated process
- molecular adsorption

Advantages of physisorption:

- complete reversibility
- fast ad-/desorption kinetics

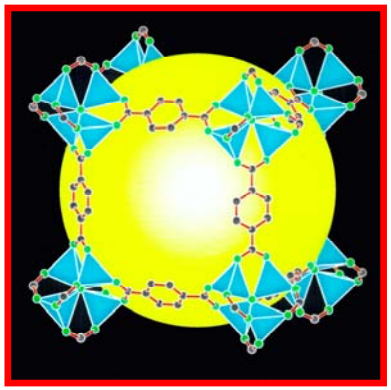
- but, low temperature adsorption and desorption

# High-surface-area materials

## Carbonaceous materials

► **talk at 8:40 by**
**Angel Linares-Solano**


## MOFs



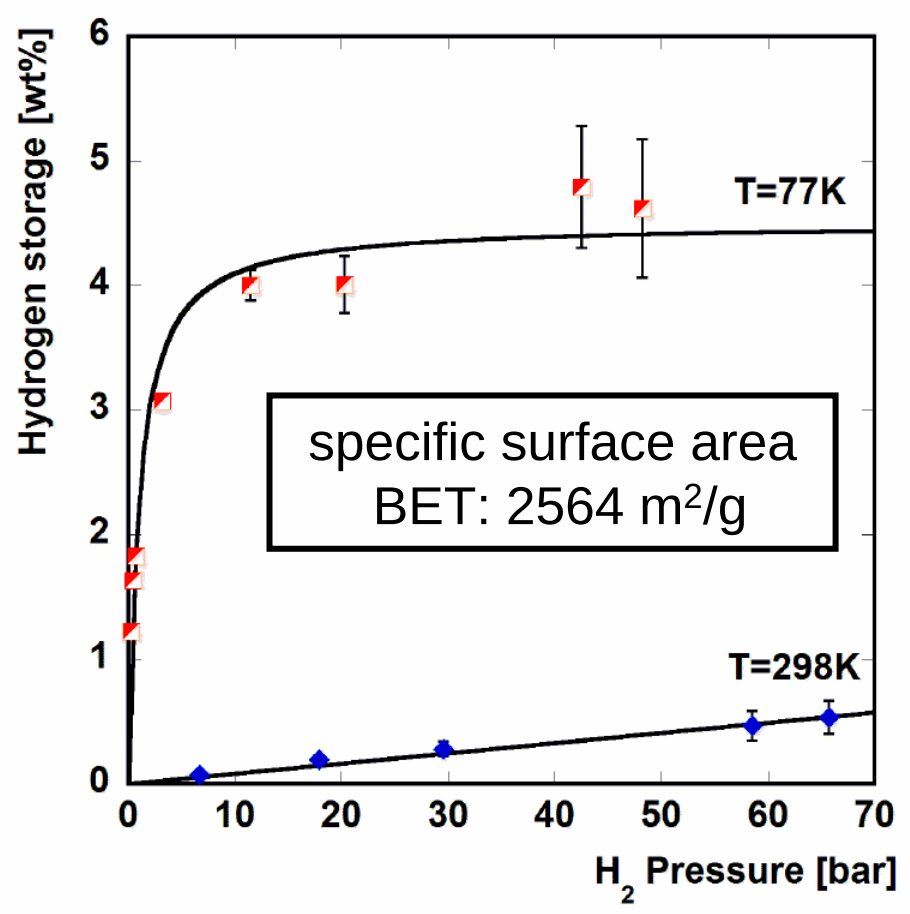
► **pore dimension**

► **metal, ligand**

- Over 2000 MOFs prepared
- Easy quality control (e.g. XRD)
- Non-toxic powder (> 1 μm)
- Large-scale synthesis is developed for some MOFs

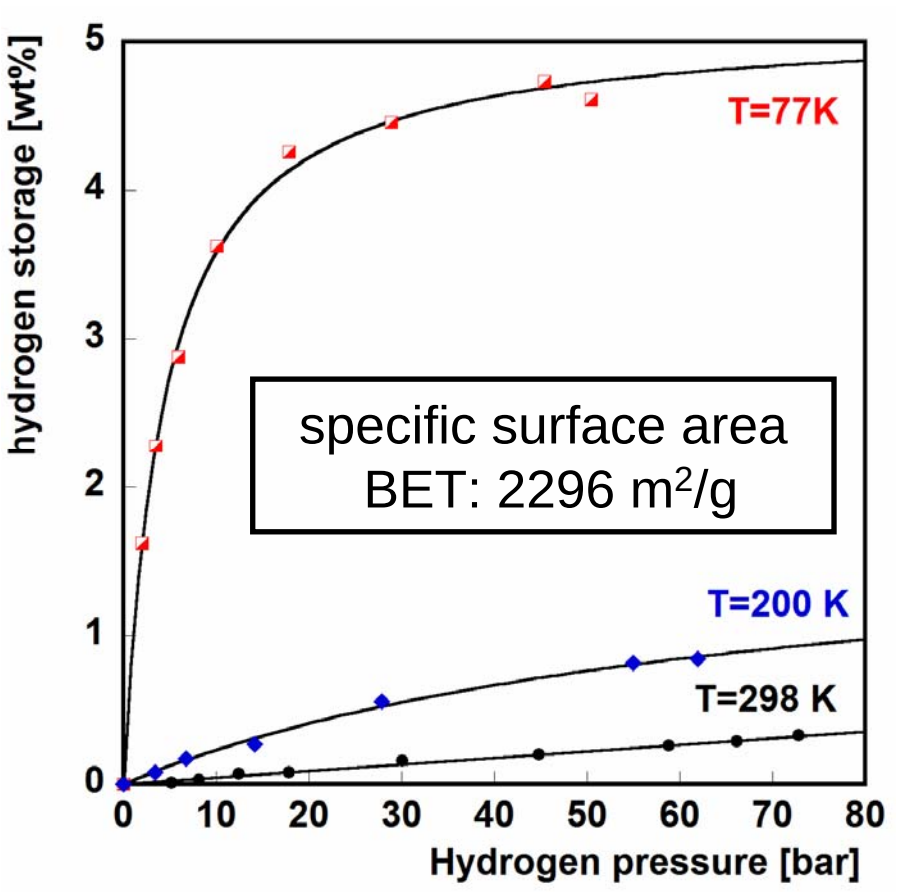
# Hydrogen adsorption

## Activated Carbon



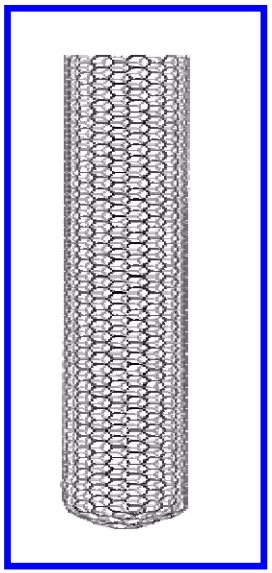

B. Panella et al. *Carbon* **43** (2005) 2209

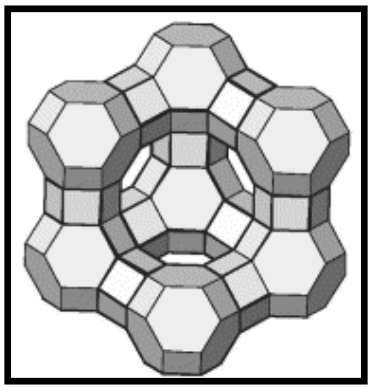
## MOF-5



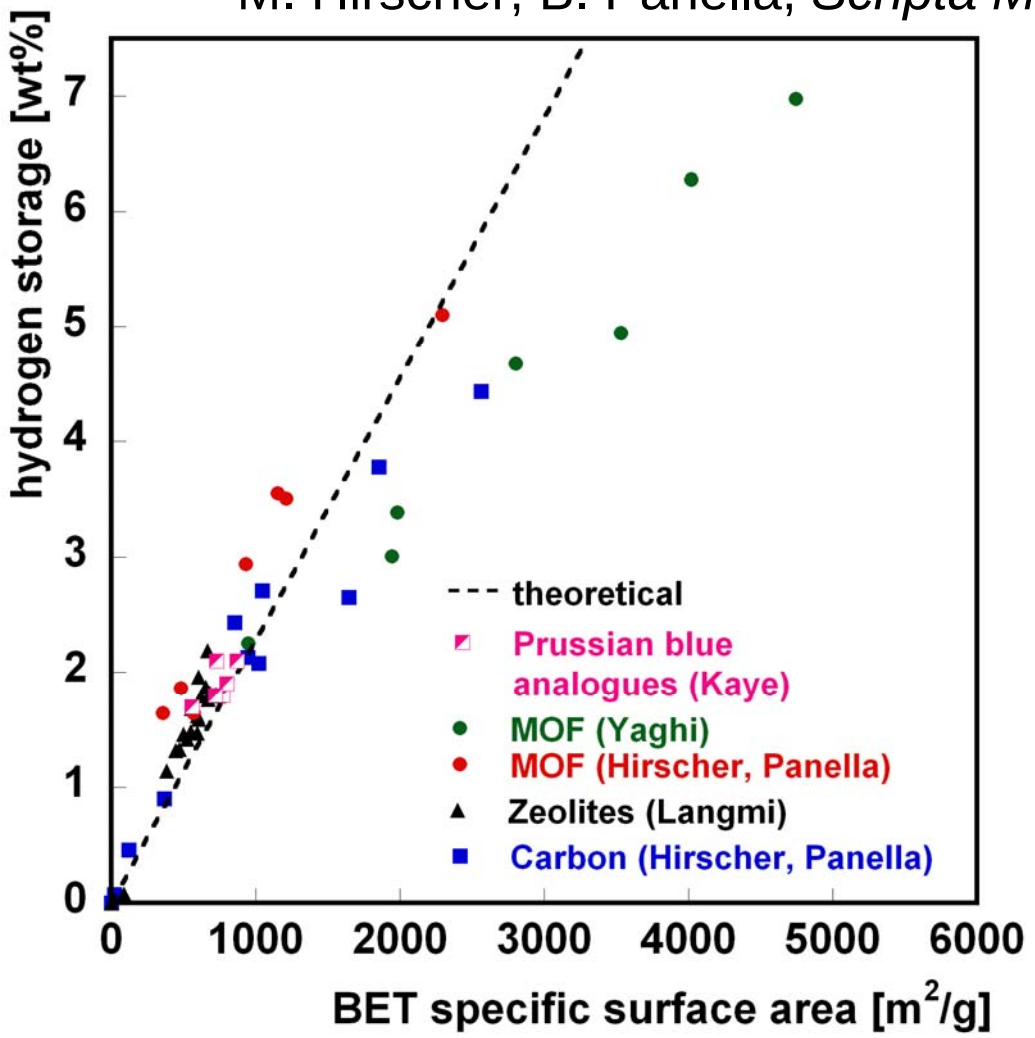

B. Panella et al., *Adv. Funct. Mater.* **16** (2006) 520

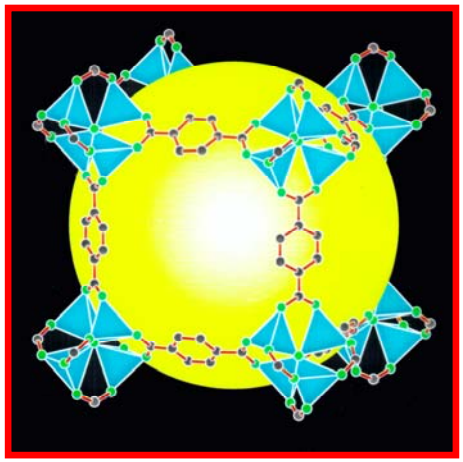
# Comparison of microporous materials





M. Hirscher, B. Panella, *Scripta Mater.* **56** (2007) 809



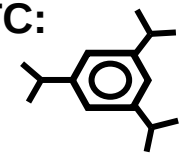



**Is surface area everything?**

# Zn-MOF and Cu-MOF compared

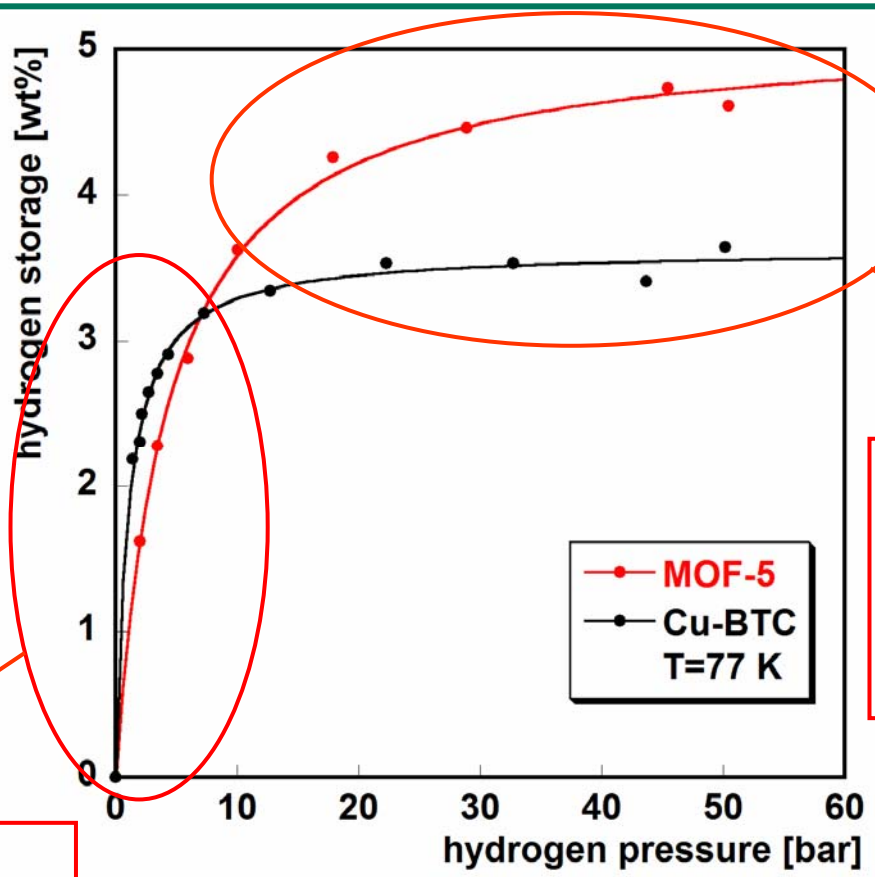
**Cu-BTC:**

**$Cu^{2+}$**



**BET SSA = 1154 $m^2/g$**

**$\Delta H_{ads}$ = - 4.5 kJ/mol**




**MOF-5:**

**$Zn^{2+}$**

**BET SSA = 2296 $m^2/g$**

**$\Delta H_{ads}$= - 3.8 kJ/mol**

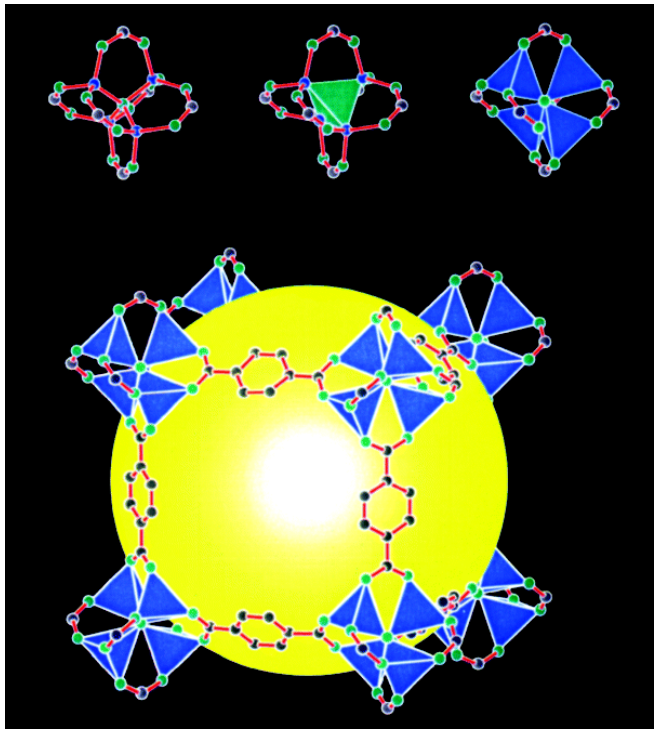
At high pressure MOF-5 stores more hydrogen due to higher SSA

At low pressure Cu-BTC stores more hydrogen due to stronger interaction

B. Panella et al., *Adv. Funct. Mater.* **16** (2006) 520

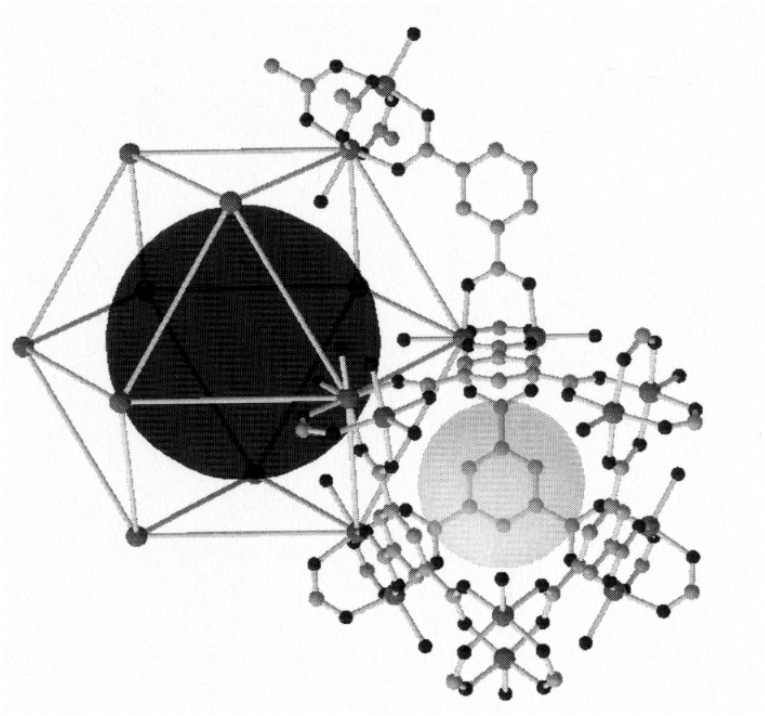
# Pores and pore size

## MOF-5



H. Li et al., *Nature* **402** (1999) 276

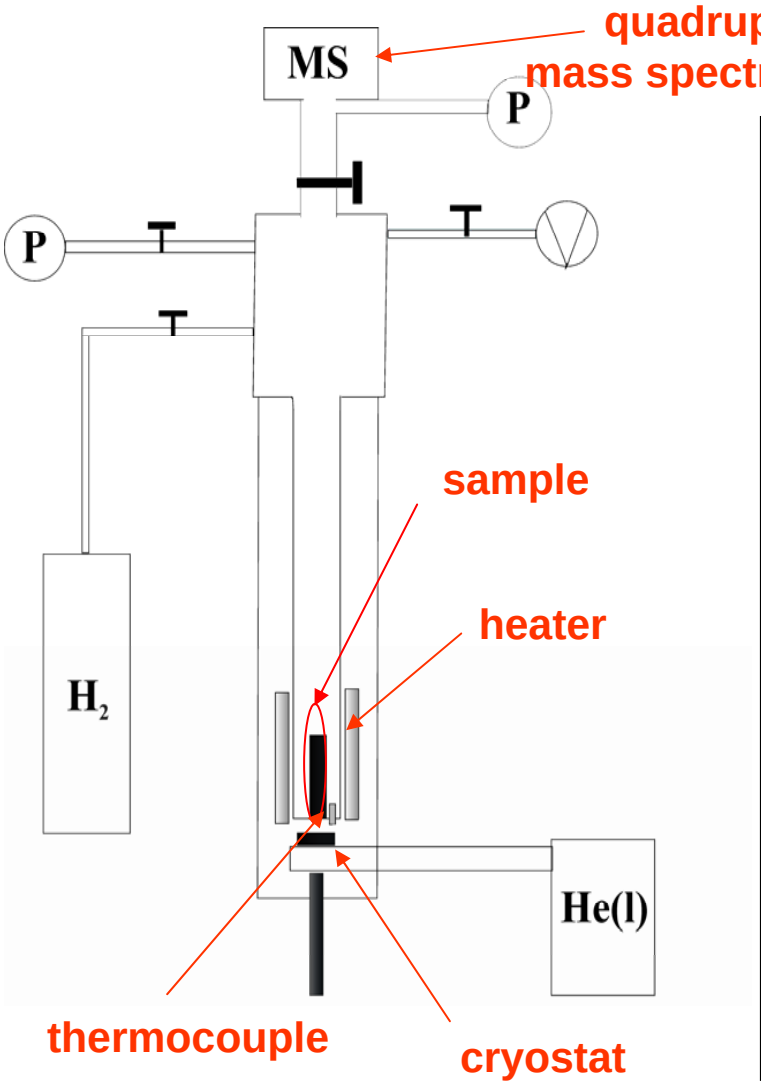
## Cu-BTC

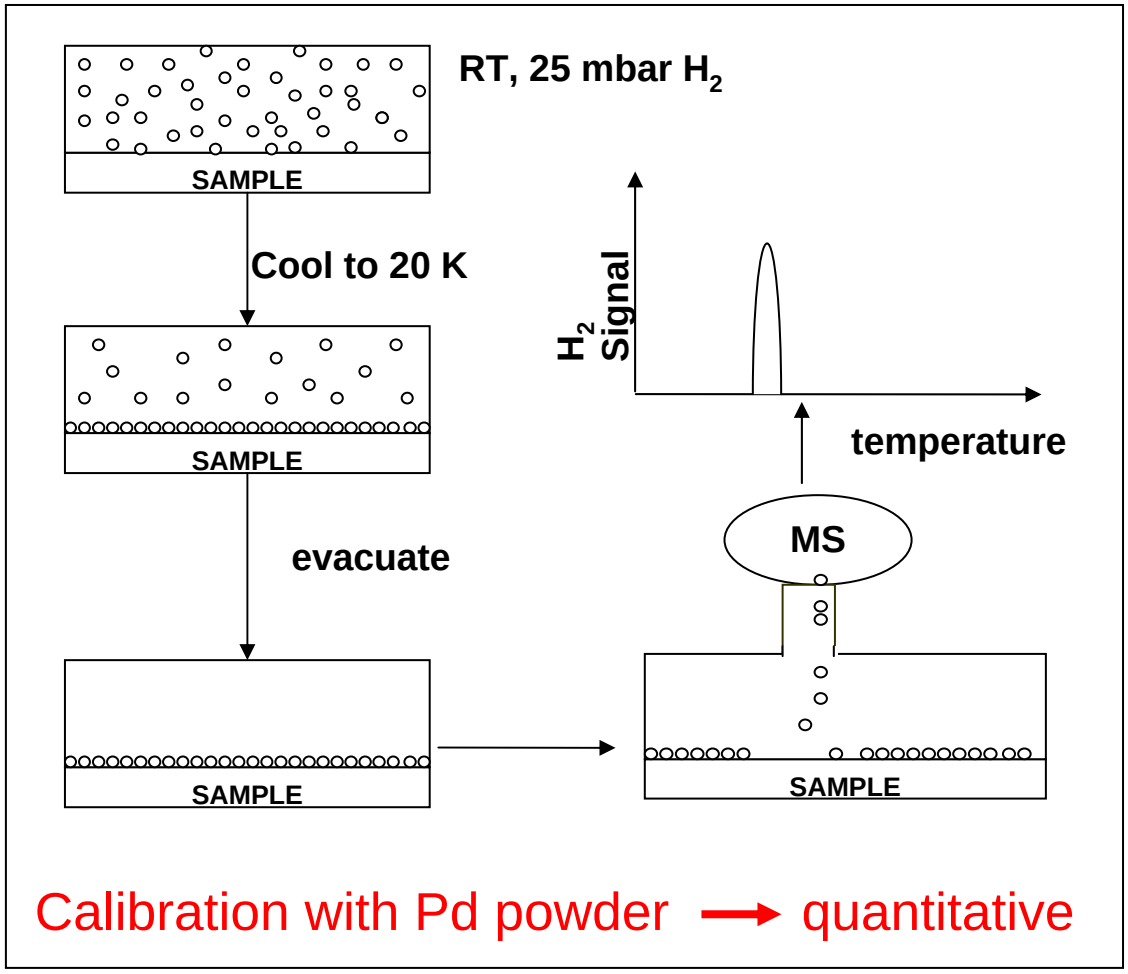


P. Krawiec et al., *Adv. Eng. Mater.* **8** (2006) 294

**How to get any microscopic information?**

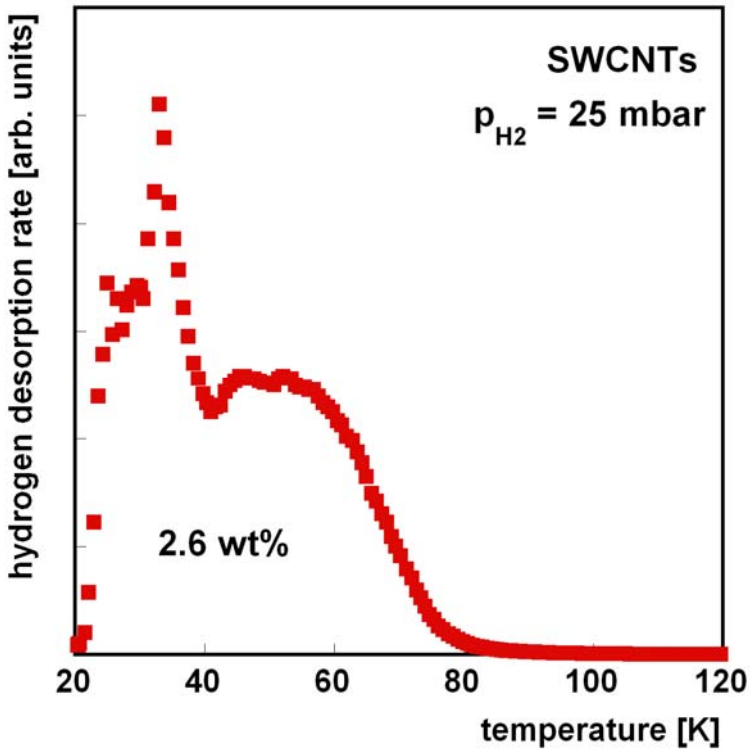
# Low-temp. thermal desorption spectroscopy

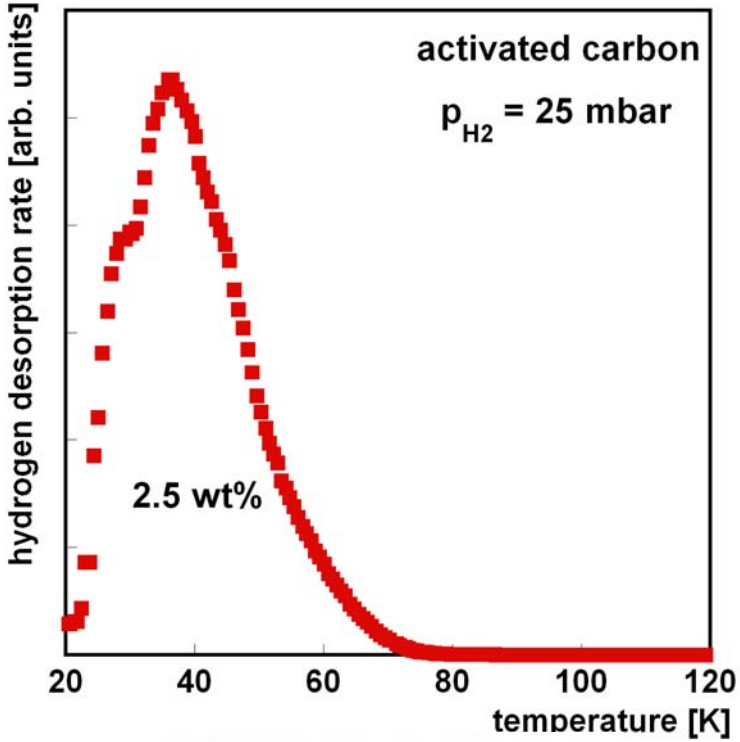


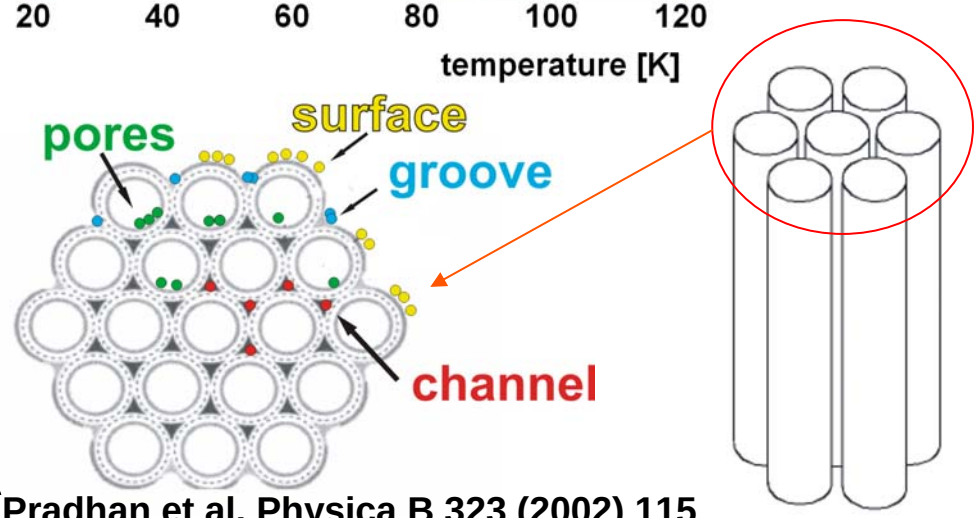



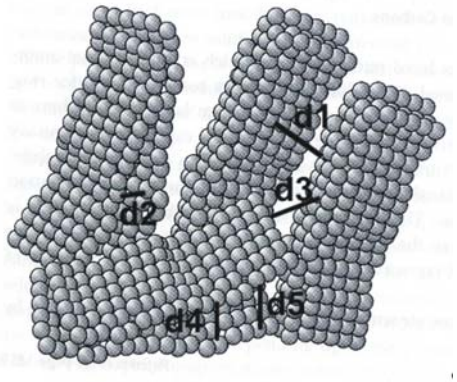

B. Panella et al. *Micropor. Mesopor. Mater.* **103** (2007) 230

# TDS of $H_2$ on carbon materials



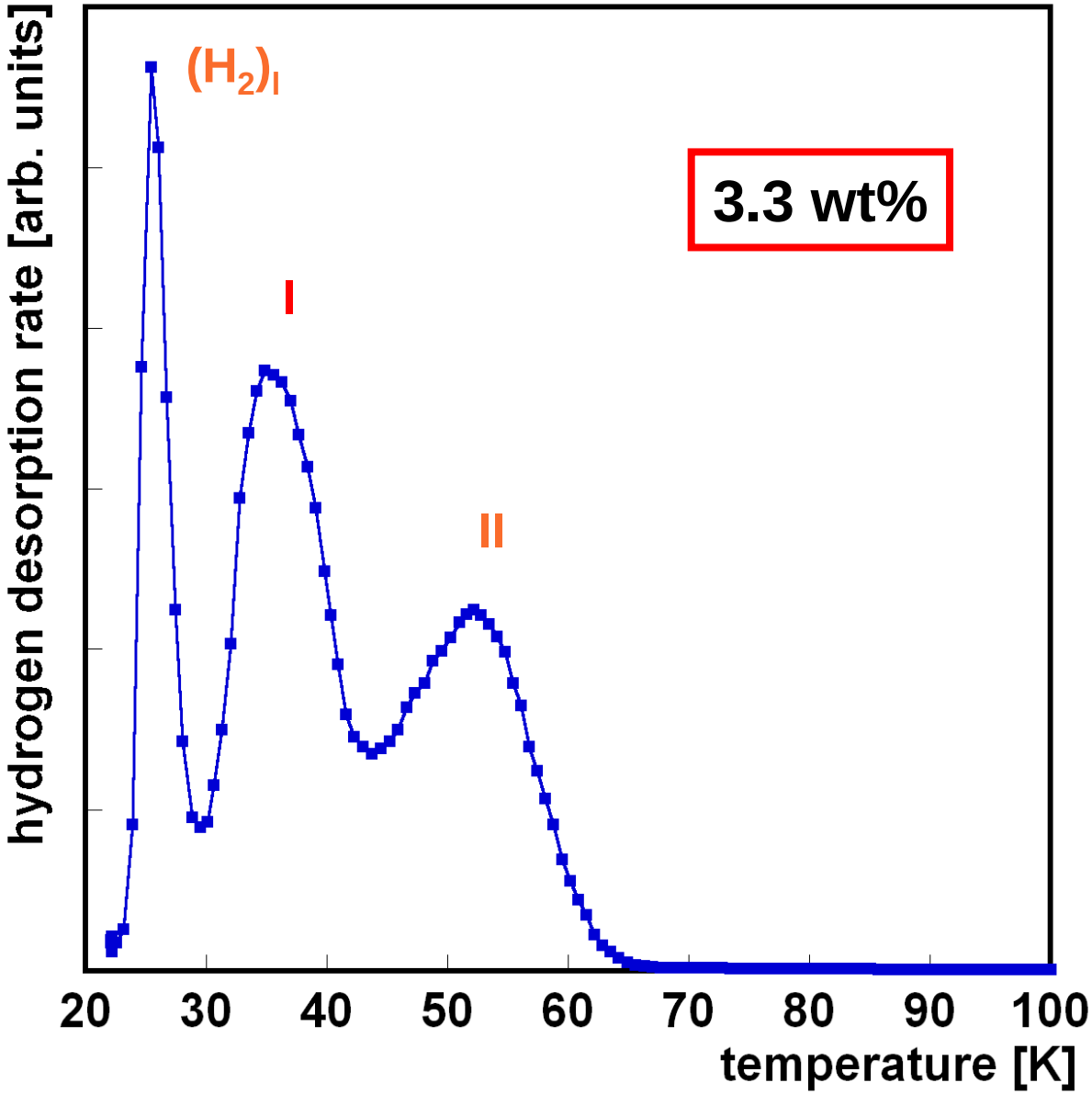



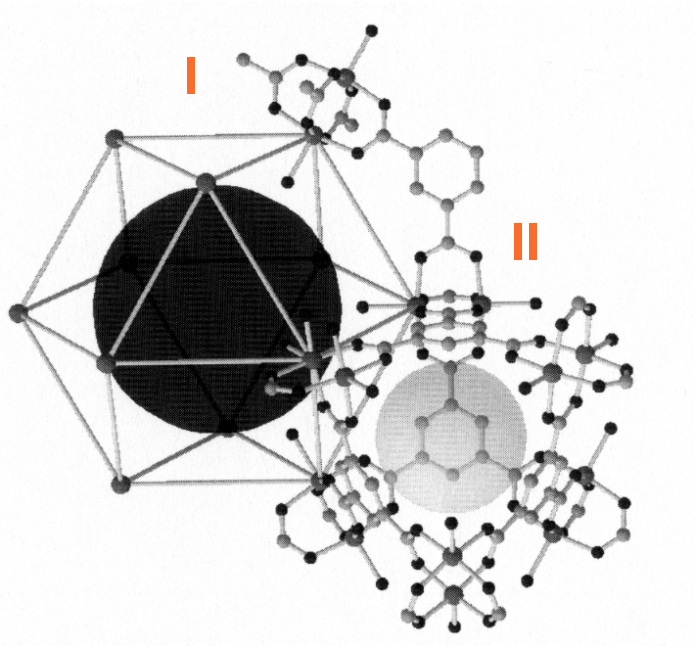

*Pradhan et al. Physica B 323 (2002) 115

* Handbook of porous solids, Wiley-VCH

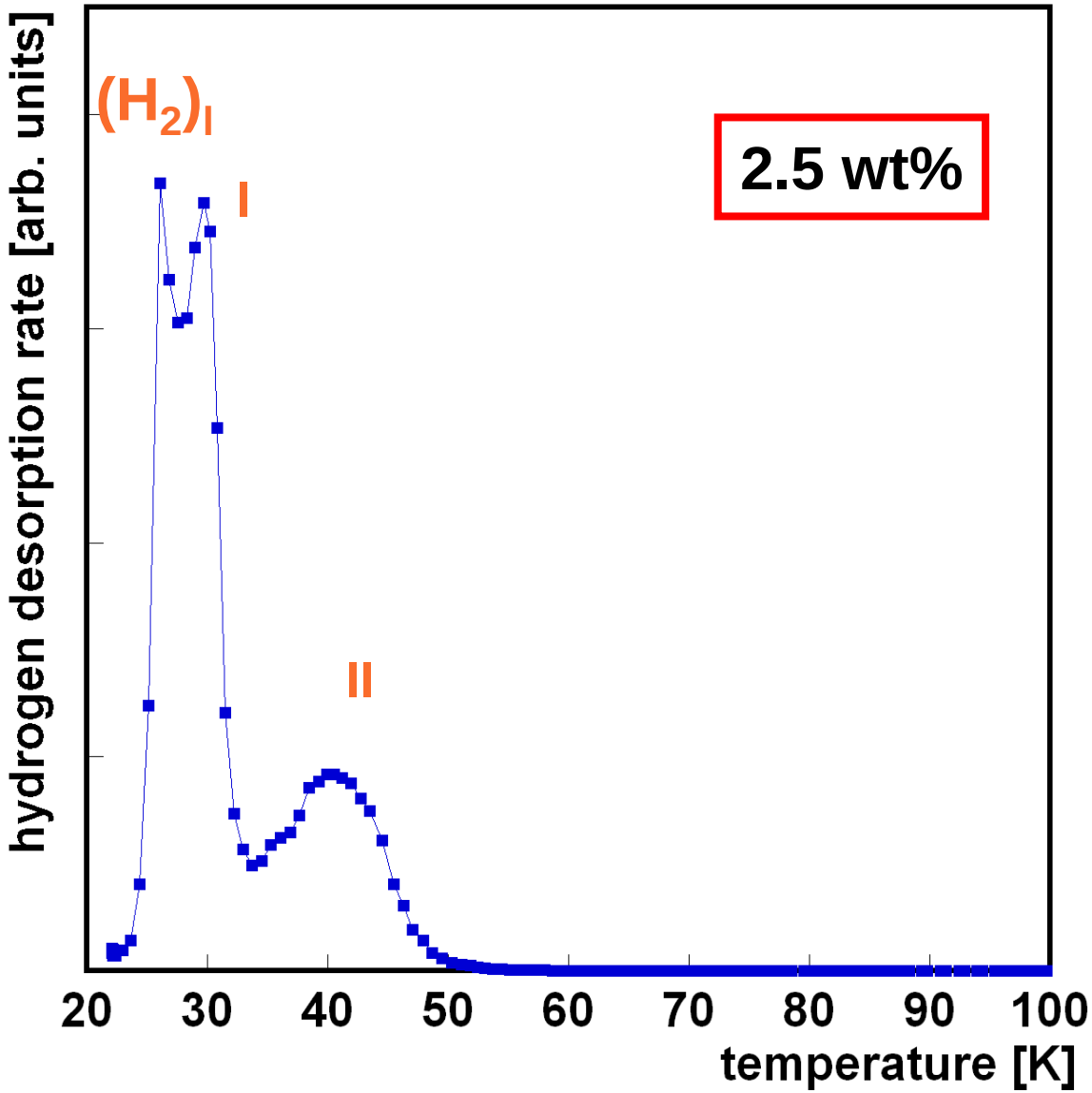
# Cu-BTC

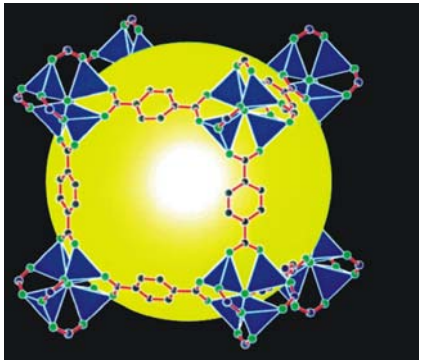



*** Krawiec et al. Adv. Eng. Mater. 8 (2006) 293**

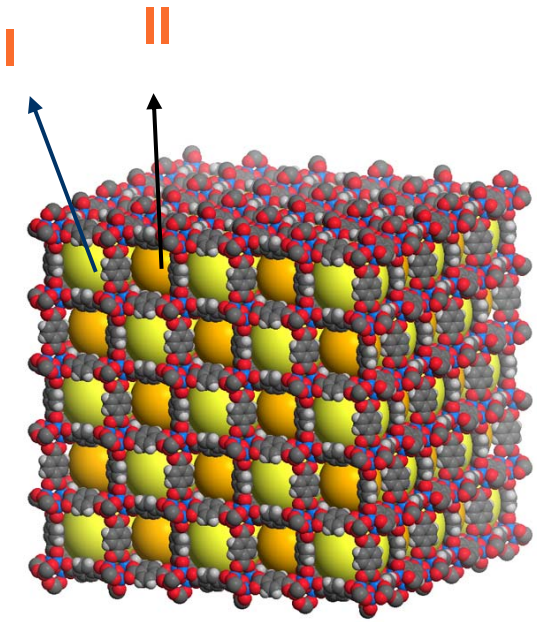


# MOF-5



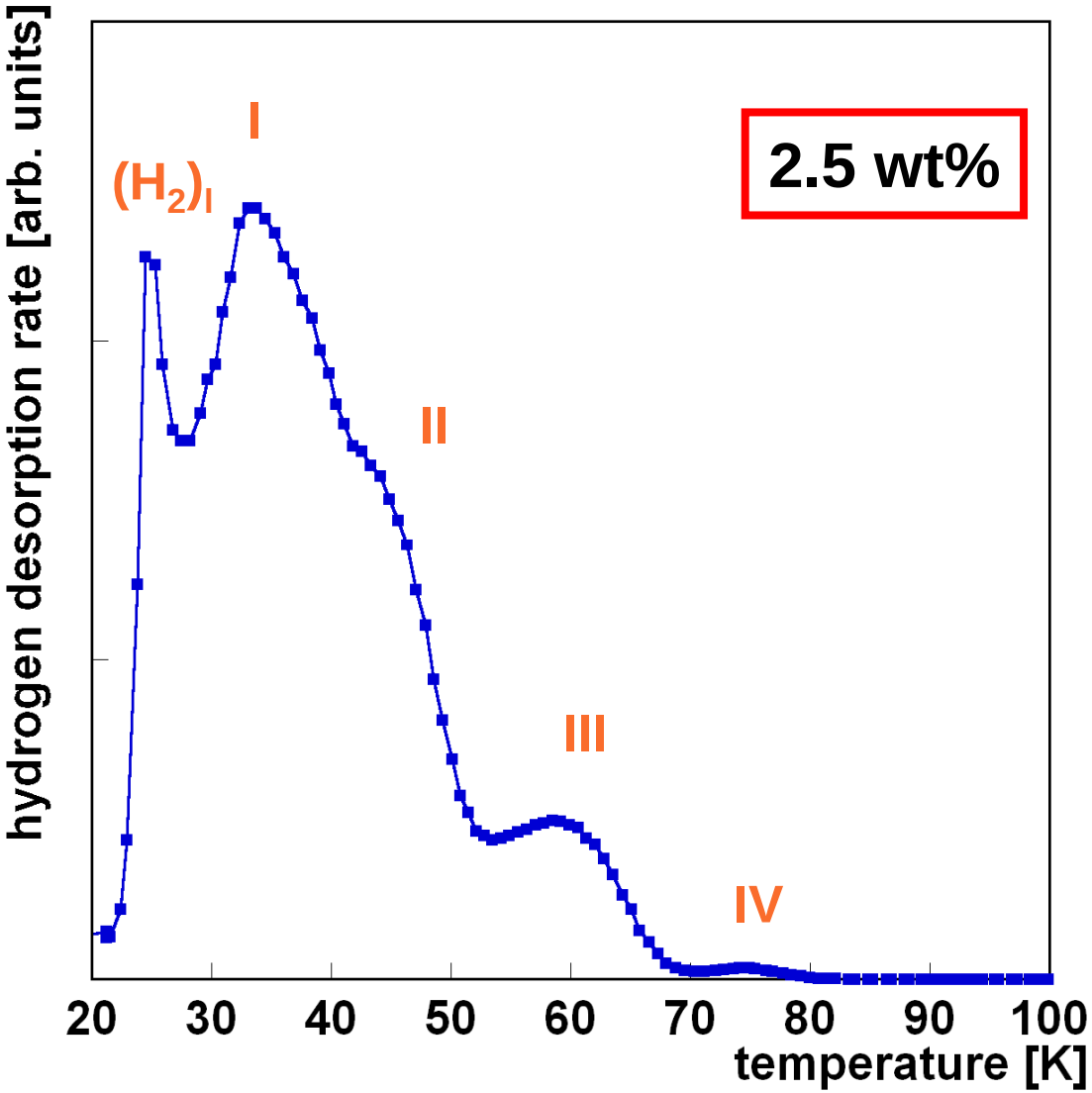



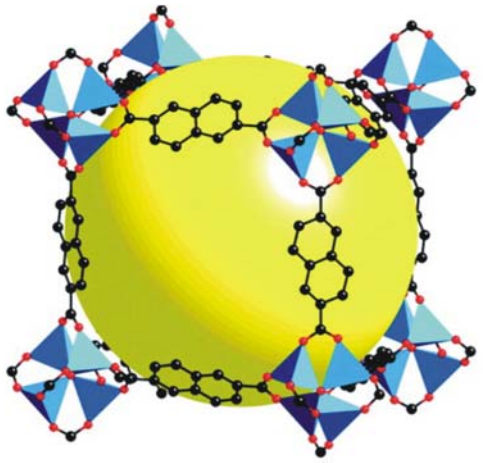
Li et al. Science 402 (1999) 276



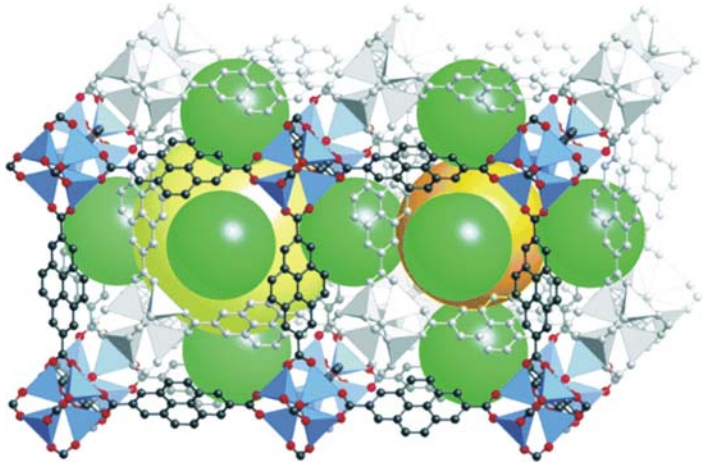

*Picture kindly provided by J. Rowsell

# IRMOF-8



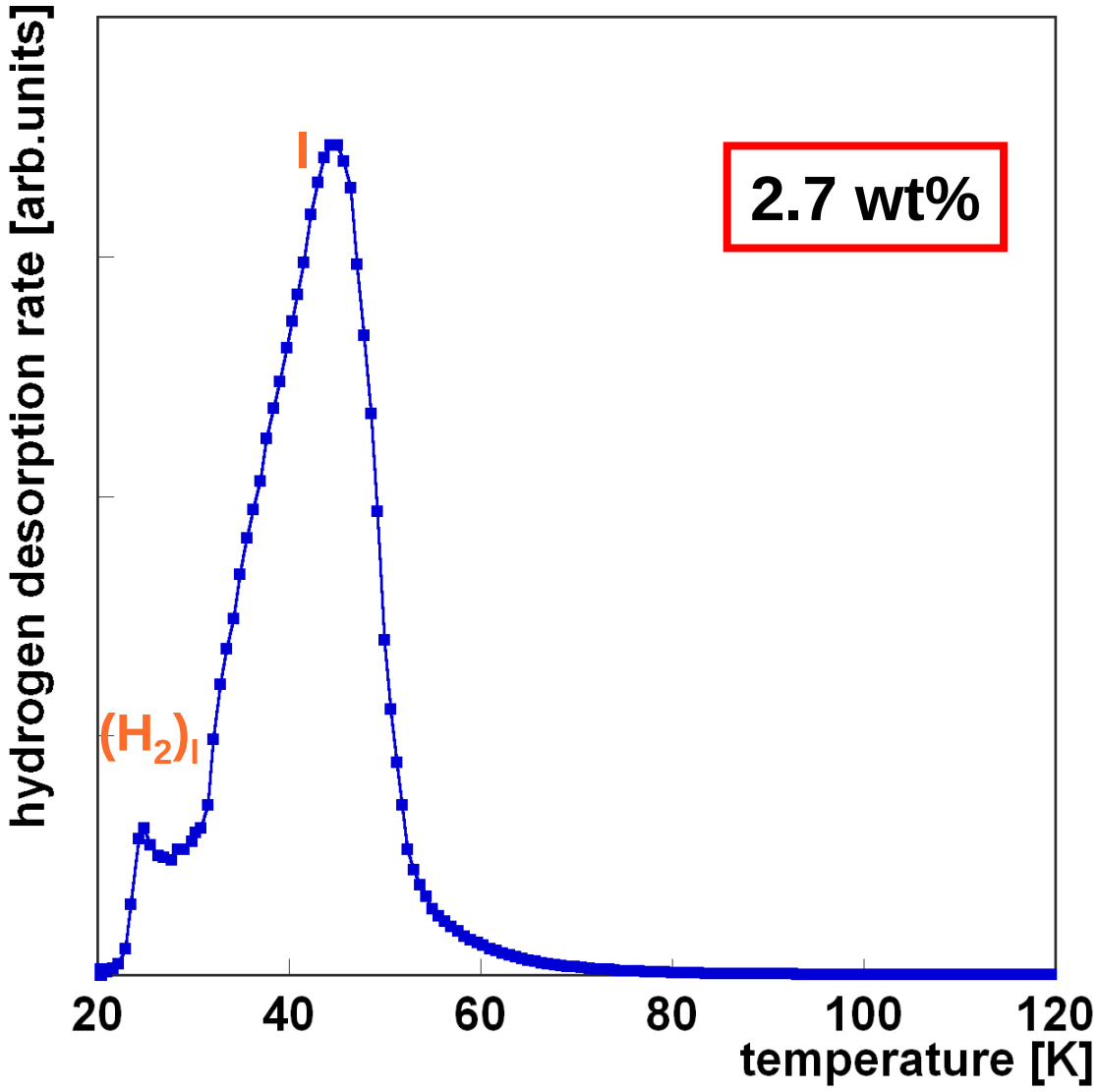



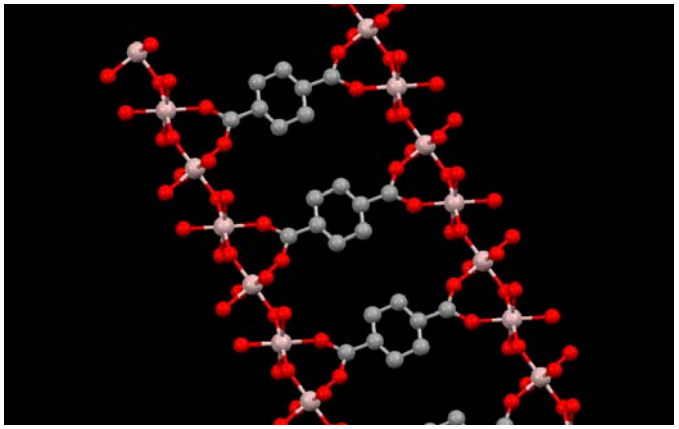
Rosi et al. Science, 300 (2003) 1127

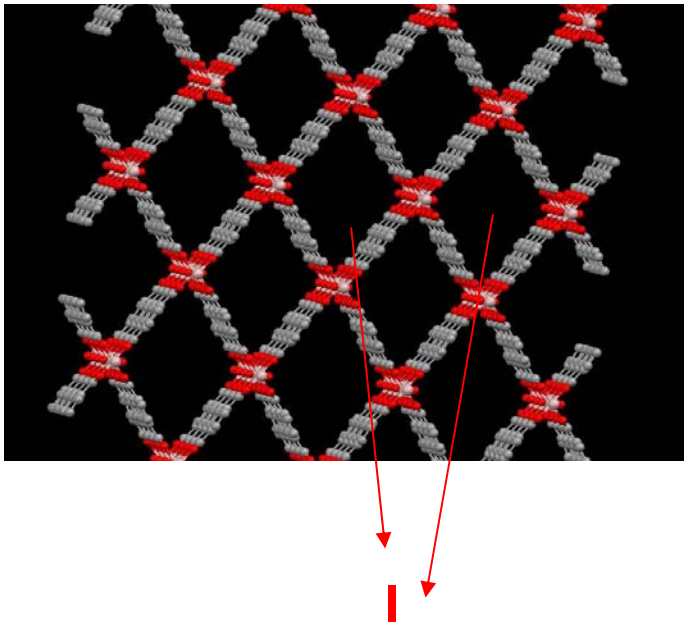


Rowsell et al. J. Am. Chem. Soc. 128 (2006) 1304

# Mil-53


hydrogen desorption rate [arb.units]
I
2.7 wt%
(H2)I
20
40
60
80
100
120
temperature [K]

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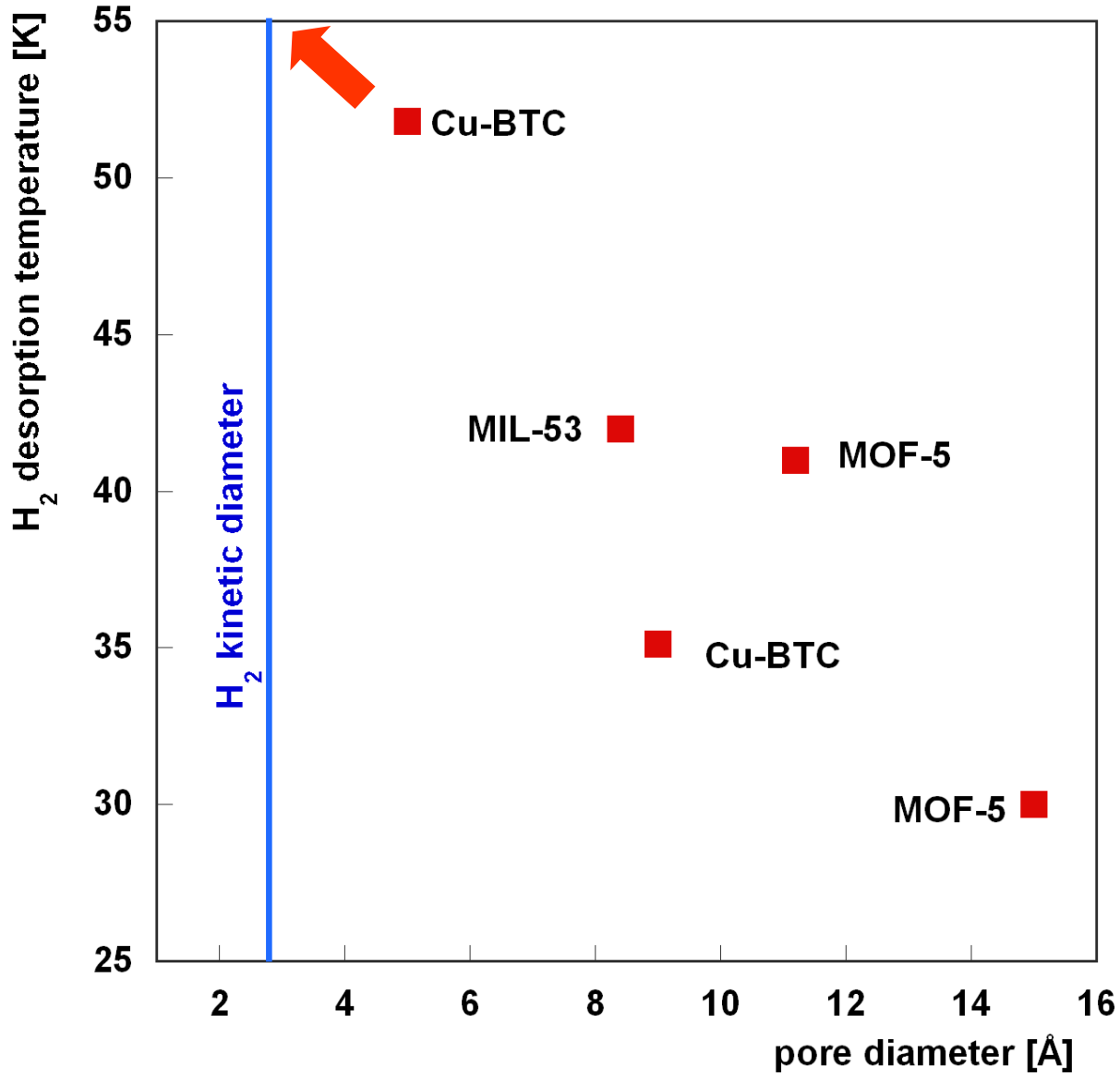
# Effect of pore size




B. Panella et al. *Angew. Chem. Int. Ed.* in press, DOI: 10.1002/anie.200704053

# Conclusion and outlook

| | | |
|---|---|---|
| Physisorption or adsorption of $H_2$ on porous materials | → | Fast kinetics and reversibility<br>short refueling time<br>low heat evolution |
| Large specific surface area | → | High storage capacity at low temperatures (77 K) |
| New technique | → | Low-temperature TDS |
| Heat of adsorption depends on material | → | Pore size?<br>Metal, ligand? |

Synthesis of novel materials with **large surface area**

Find **optimal pore size** or composition

**Cryo-adsorption tank < 2 MPa** → **free tank shape**

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