Max-Planck-Institut für Metallforschung

Physisorption of Hydrogen on Novel Porous Materials

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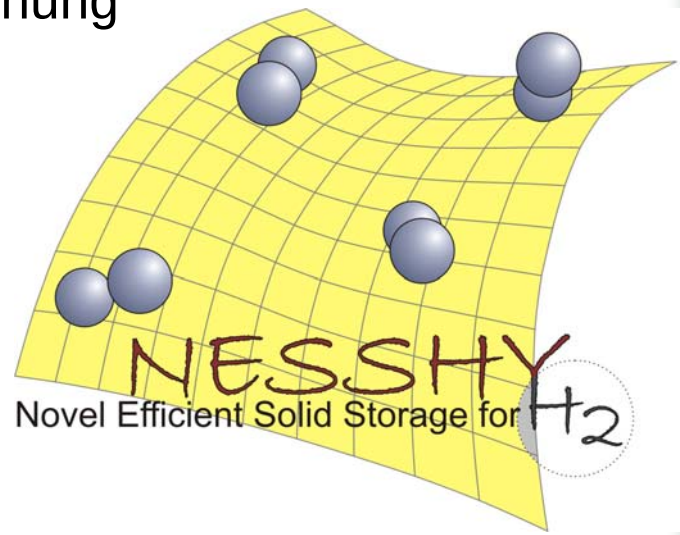
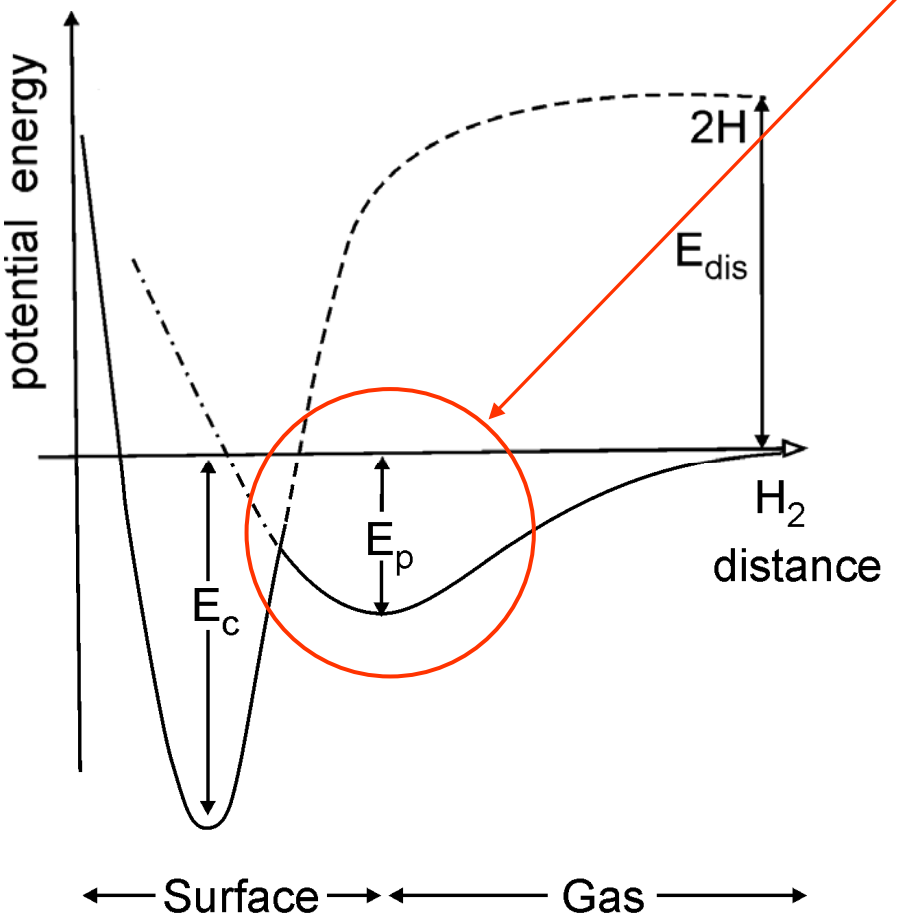


Requirements for mobile application

- 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

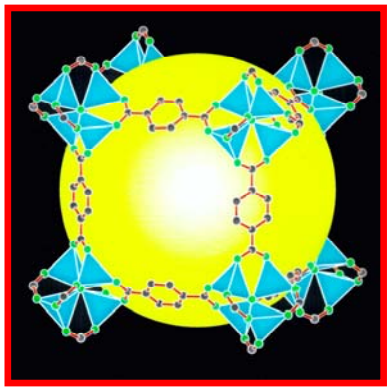
- but, low temperature adsorption and desorption

High-surface-area materials

Carbonaceous materials

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

MOFs



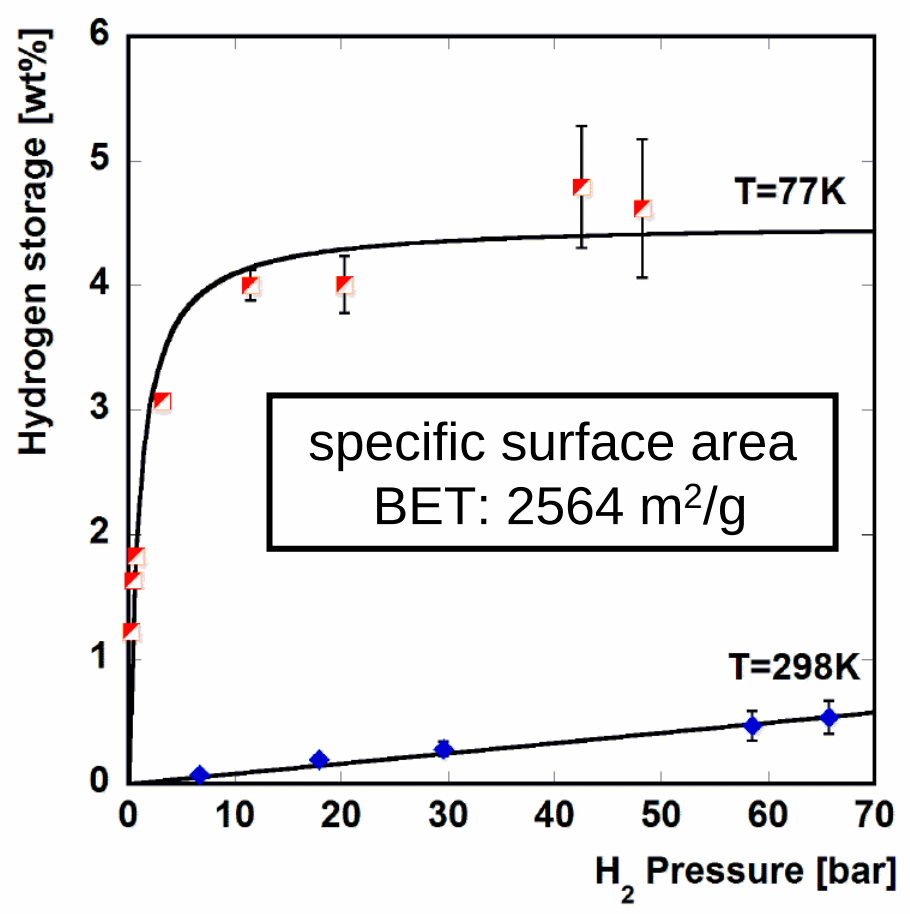
► **pore dimension**

► **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

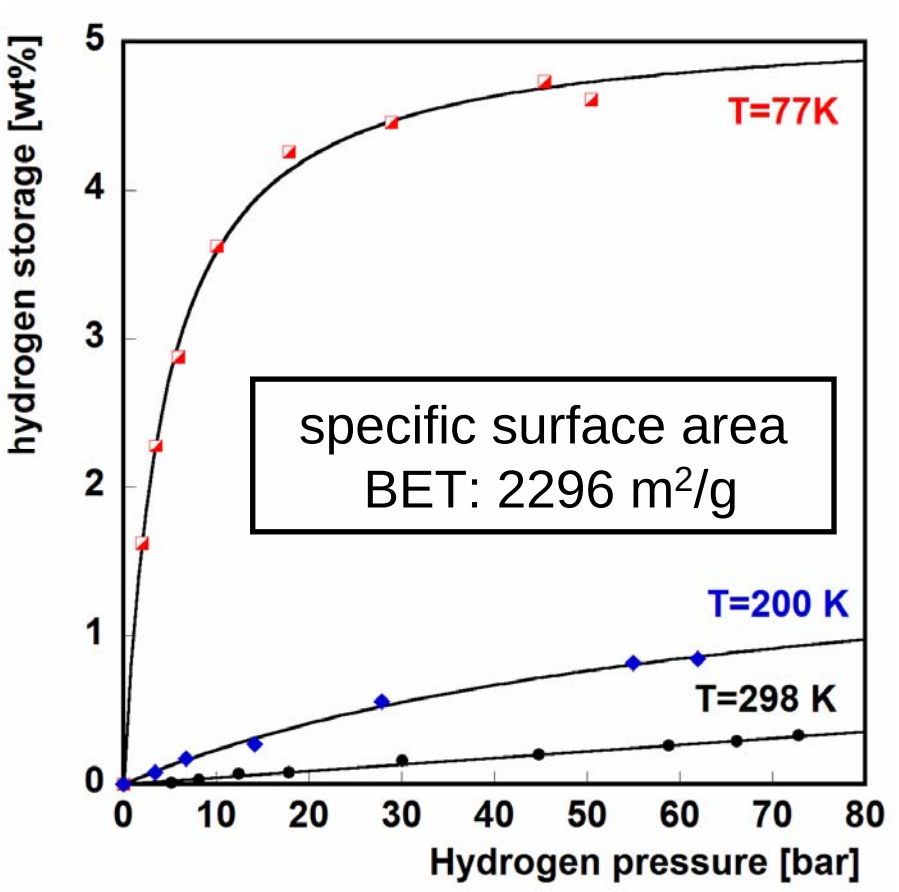
Hydrogen adsorption

Activated Carbon



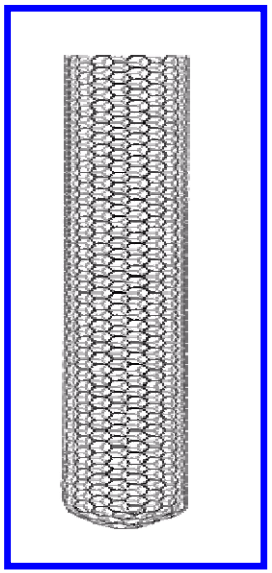
B. Panella et al. *Carbon* **43** (2005) 2209

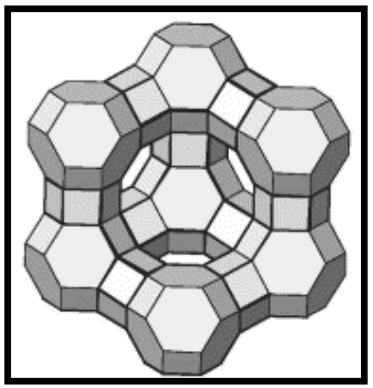
MOF-5



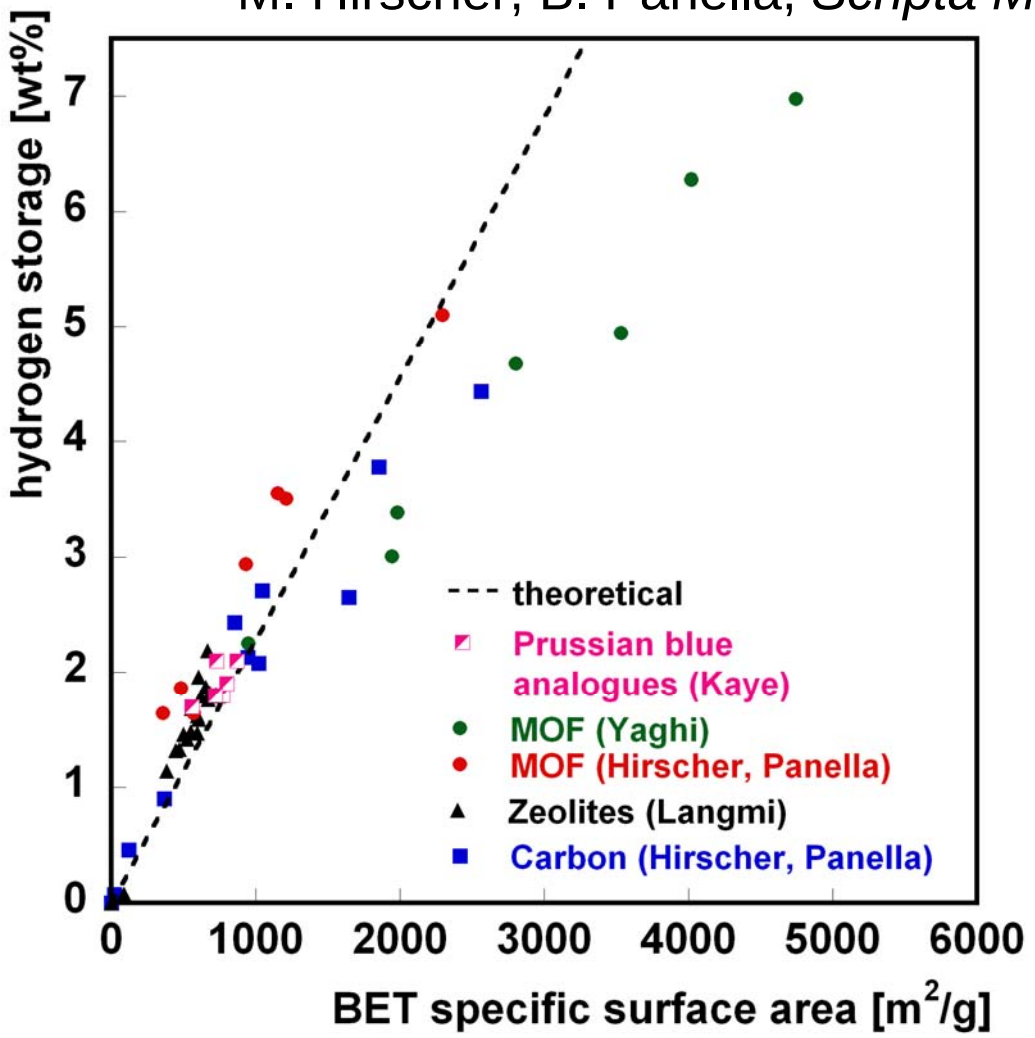
B. Panella et al., *Adv. Funct. Mater.* **16** (2006) 520

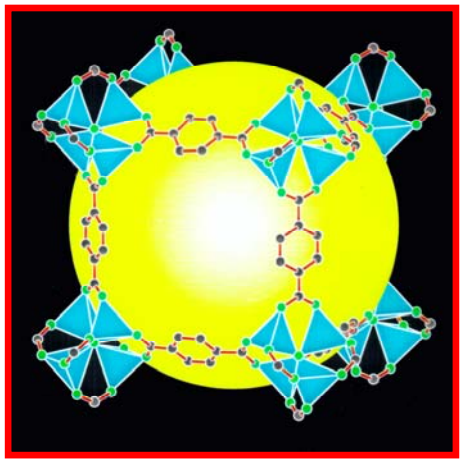
Comparison of microporous materials





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



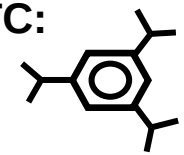


Is surface area everything?

Zn-MOF and Cu-MOF compared

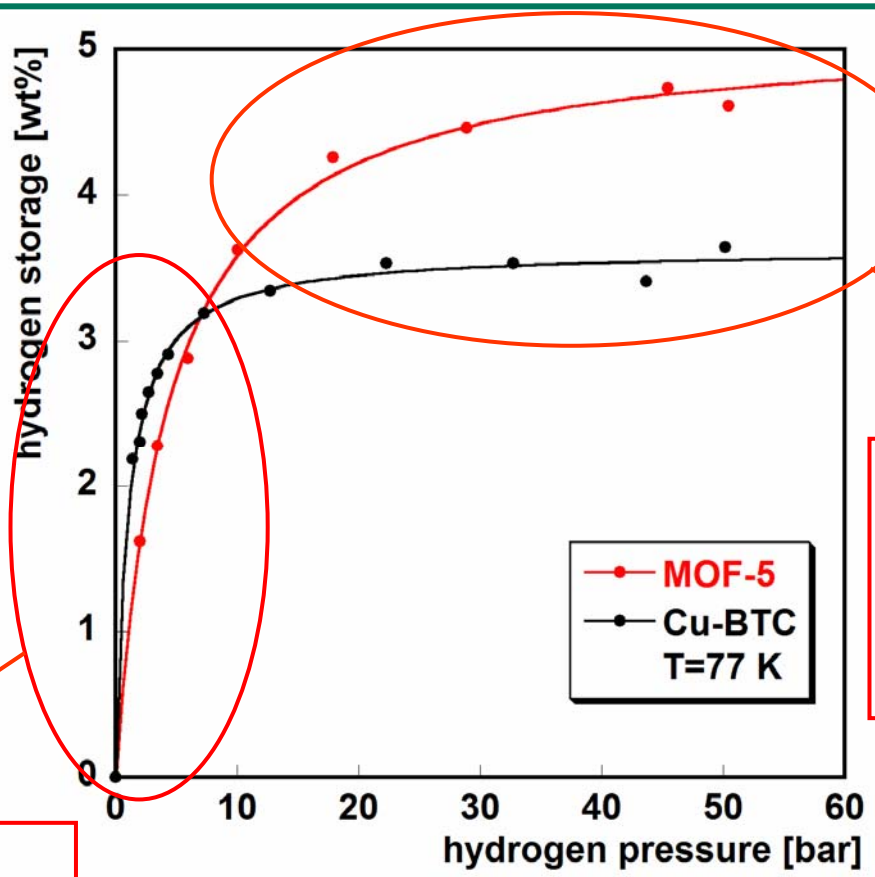
Cu-BTC:

Cu^{2+}



BET SSA = 1154 m^2/g

ΔH_{ads} = - 4.5 kJ/mol



MOF-5:

Zn^{2+}

BET SSA = 2296 m^2/g

ΔH_{ads}= - 3.8 kJ/mol

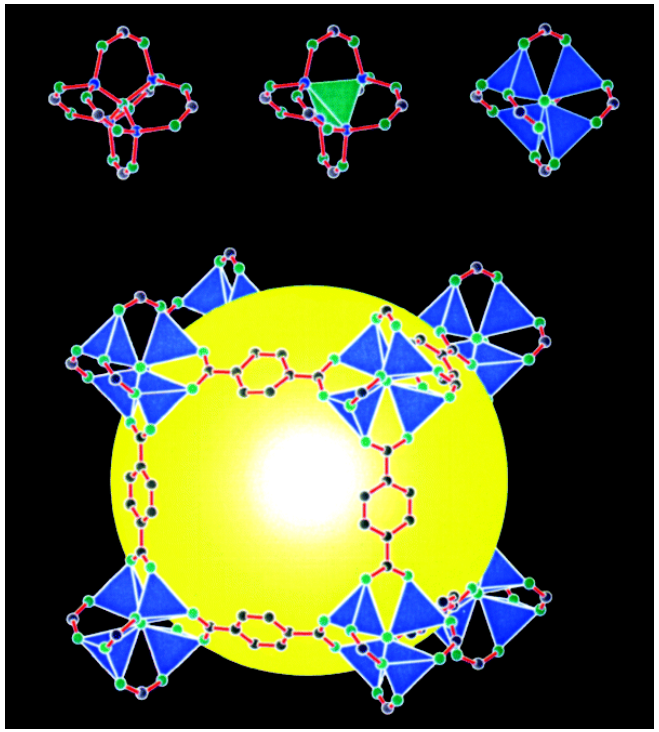
At high pressure MOF-5 stores more hydrogen due to higher SSA

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

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

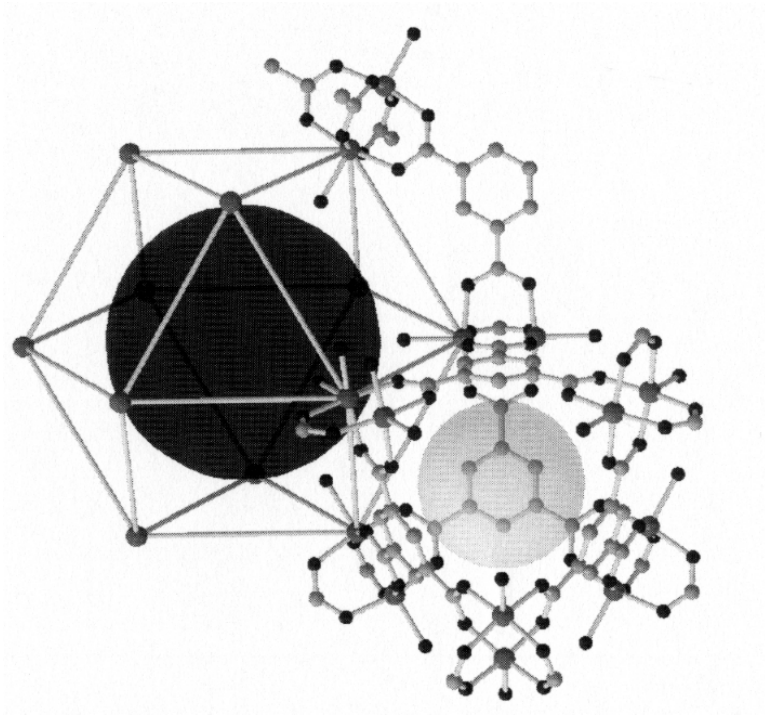
Pores and pore size

MOF-5



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

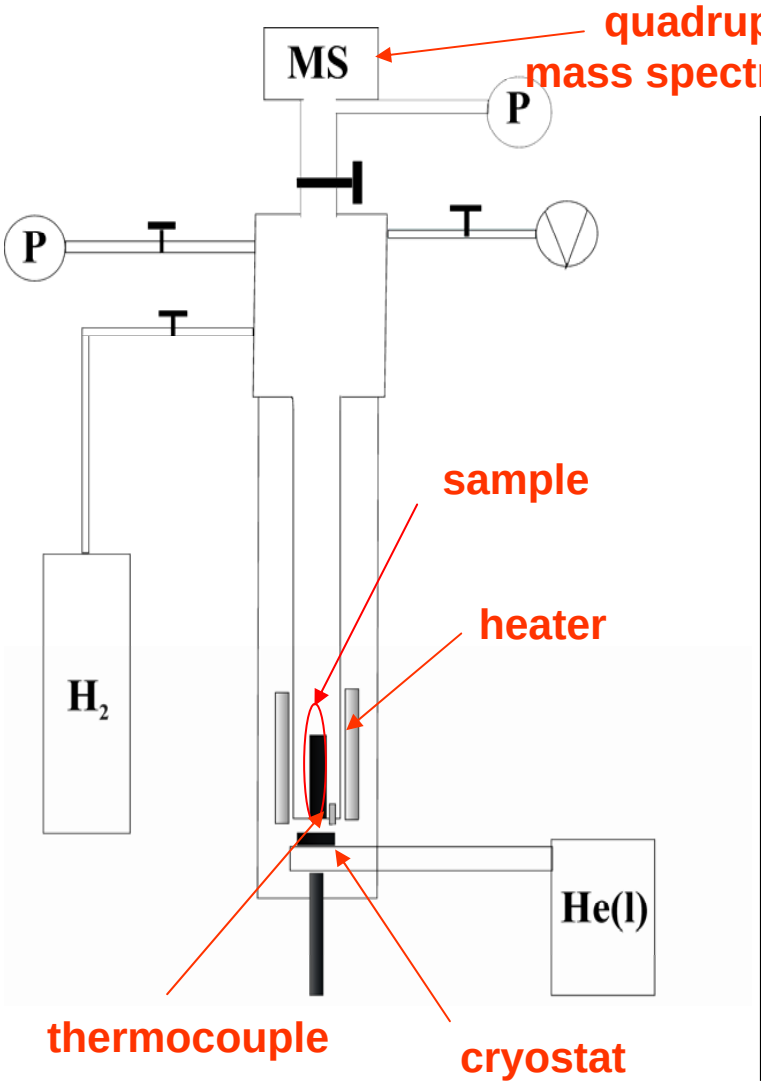
Cu-BTC

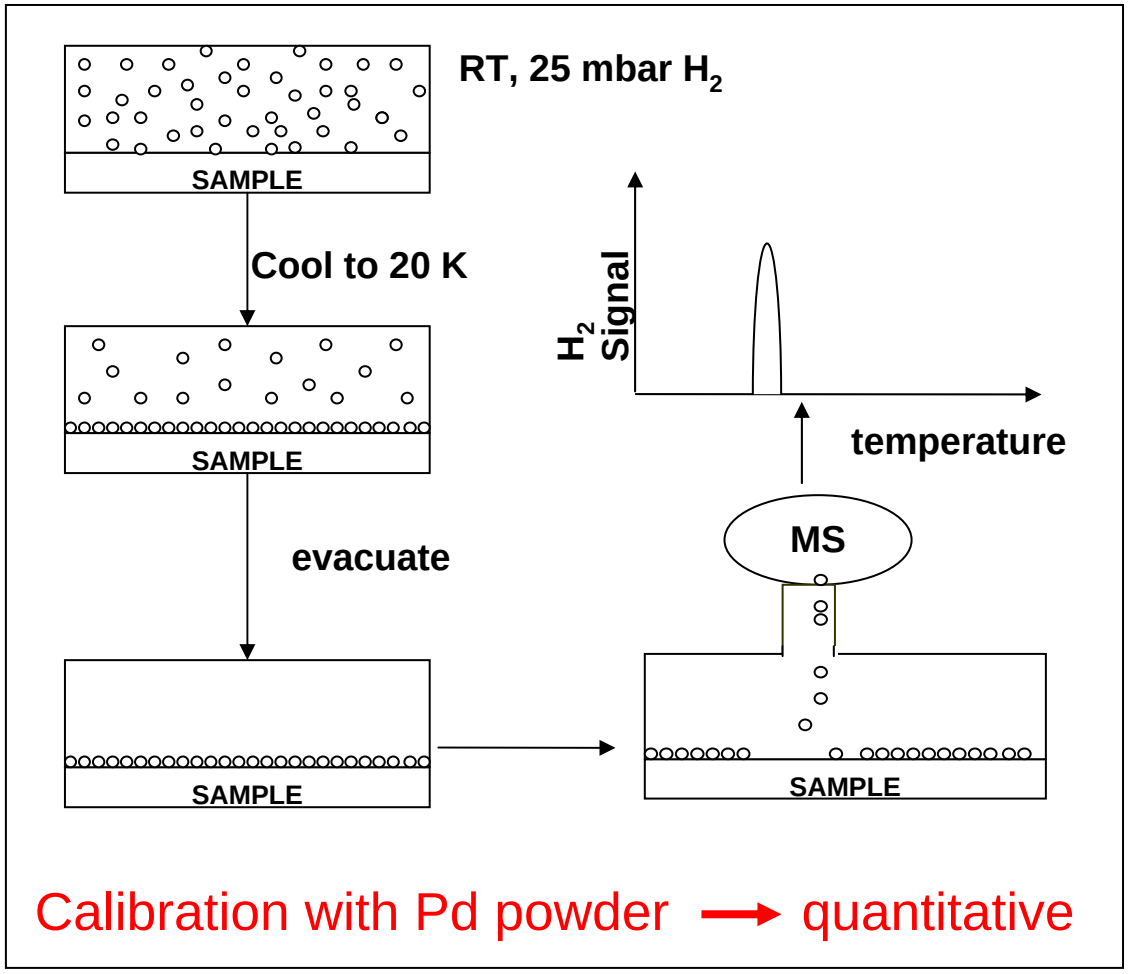


P. Krawiec et al., *Adv. Eng. Mater.* **8** (2006) 294

How to get any microscopic information?

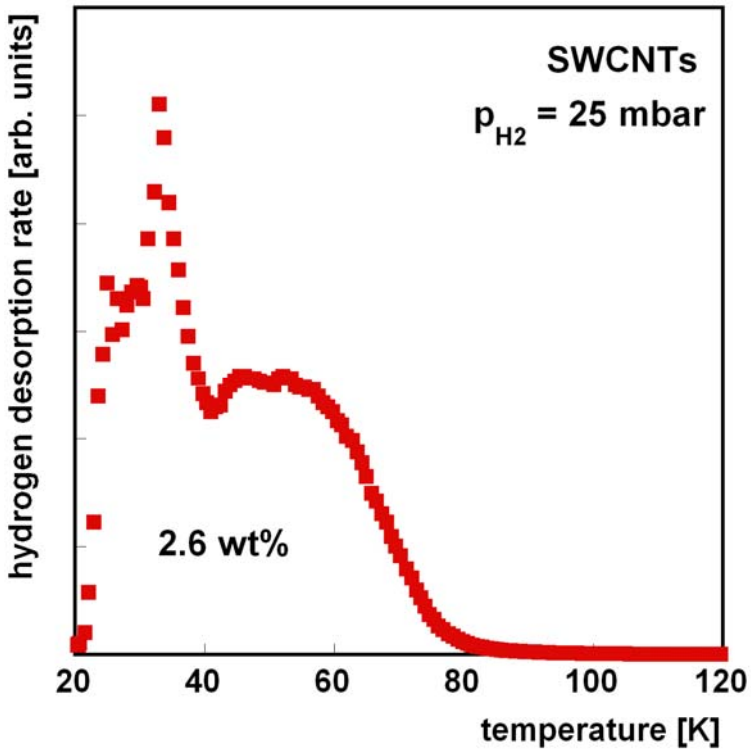
Low-temp. thermal desorption spectroscopy

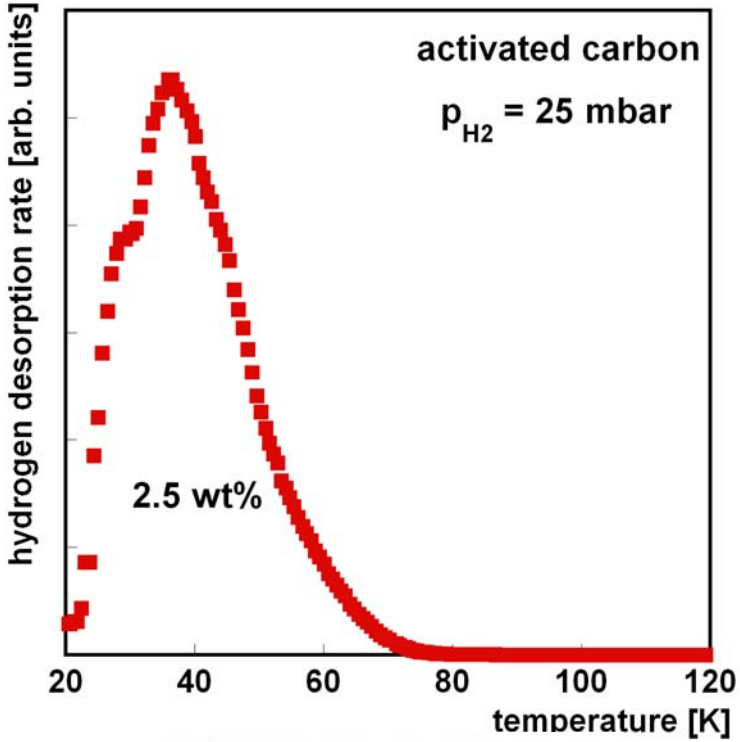


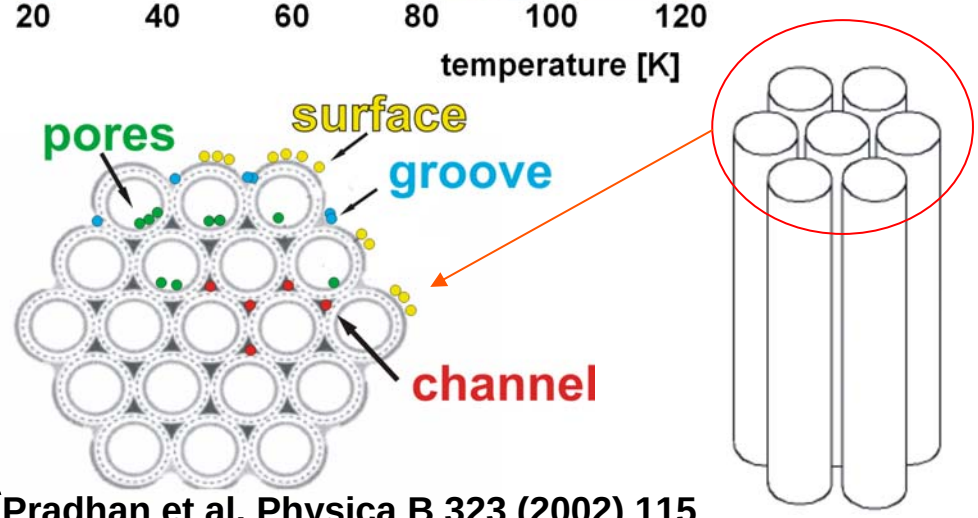


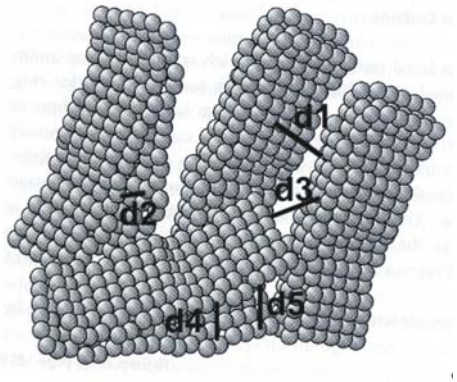
B. Panella et al. *Micropor. Mesopor. Mater.* **103** (2007) 230

TDS of H_2 on carbon materials





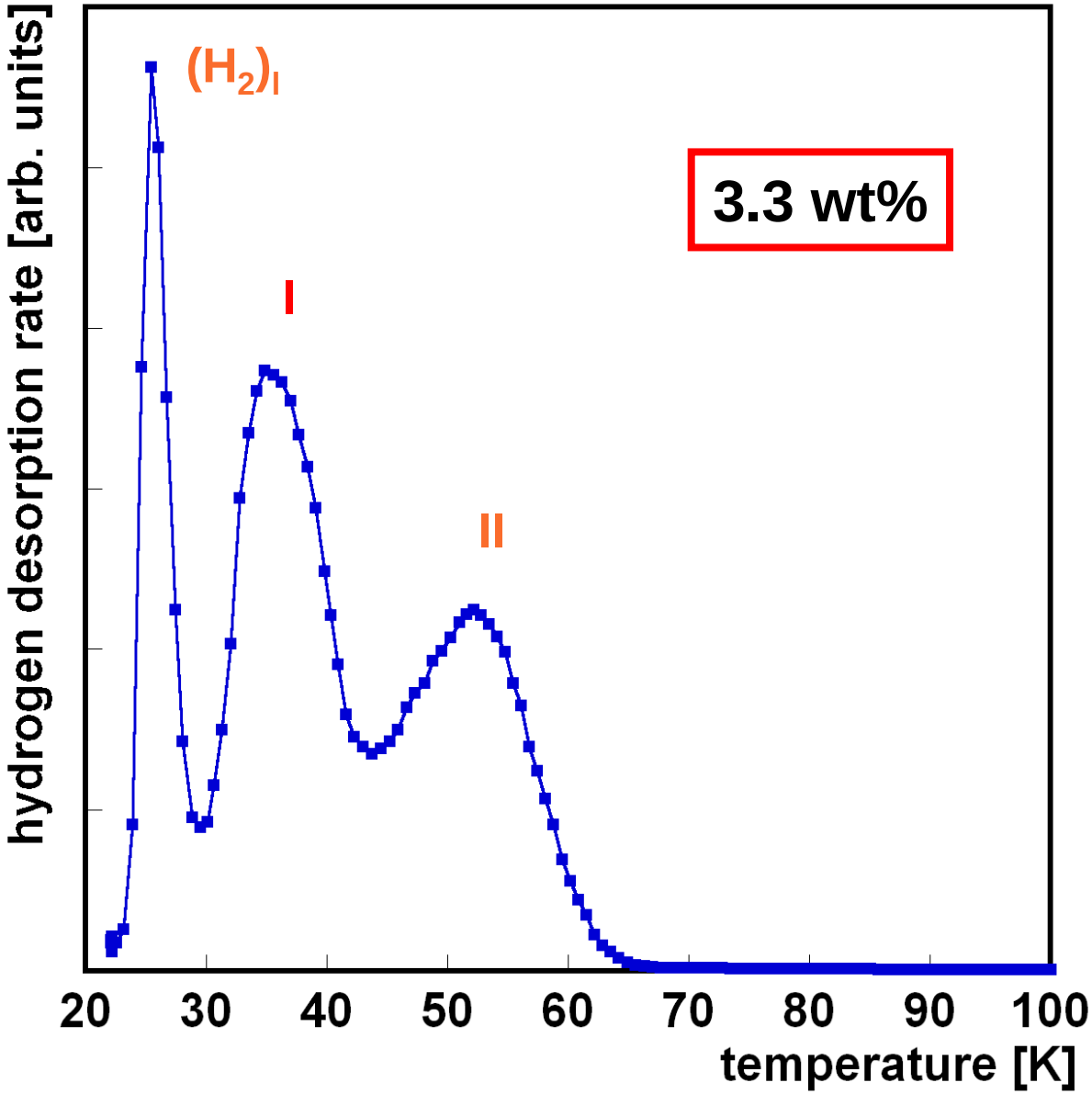




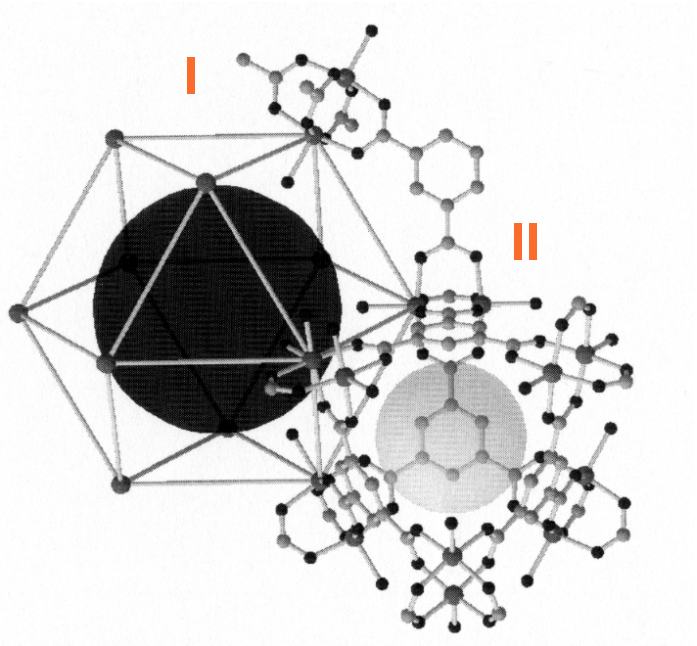
*Pradhan et al. Physica B 323 (2002) 115

* Handbook of porous solids, Wiley-VCH

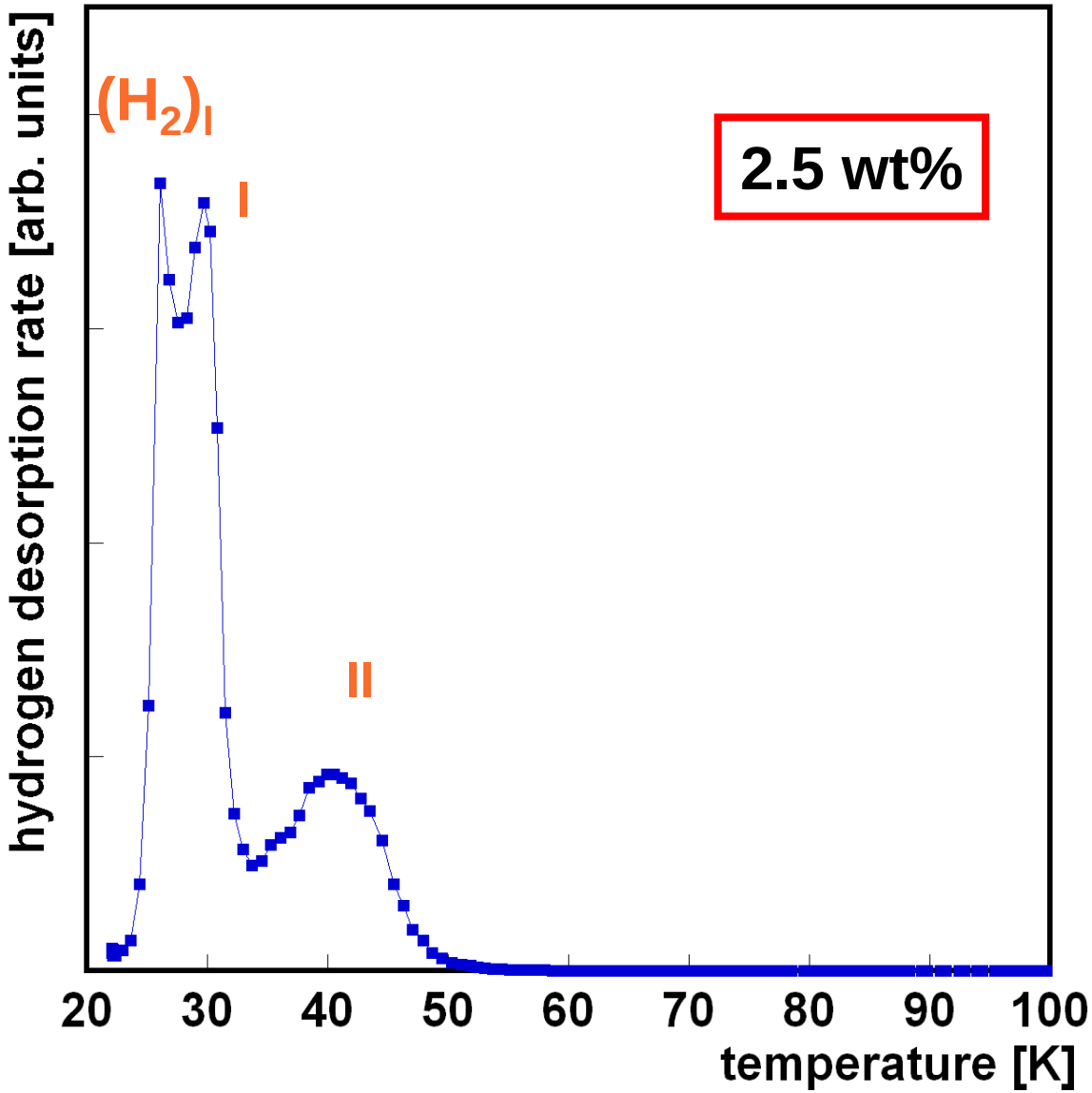
Cu-BTC

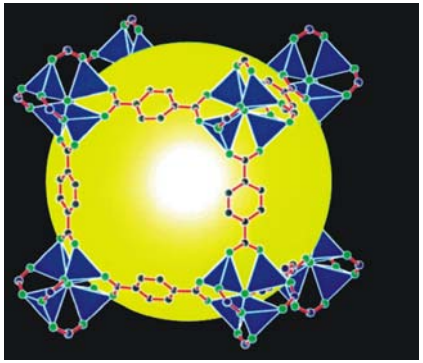


*** Krawiec et al. Adv. Eng. Mater. 8 (2006) 293**

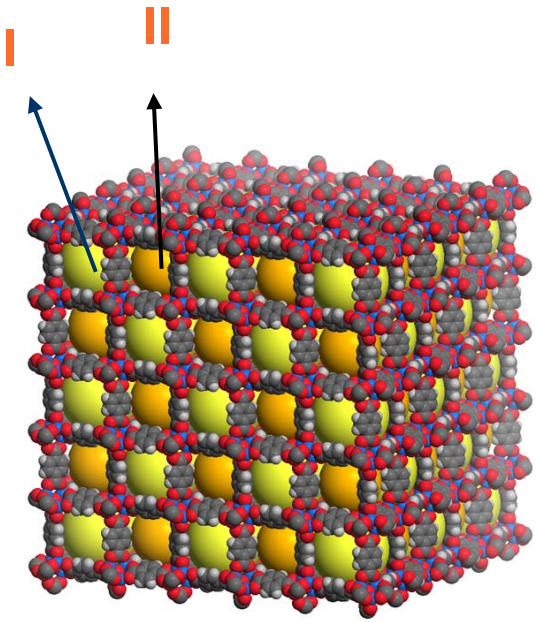


MOF-5



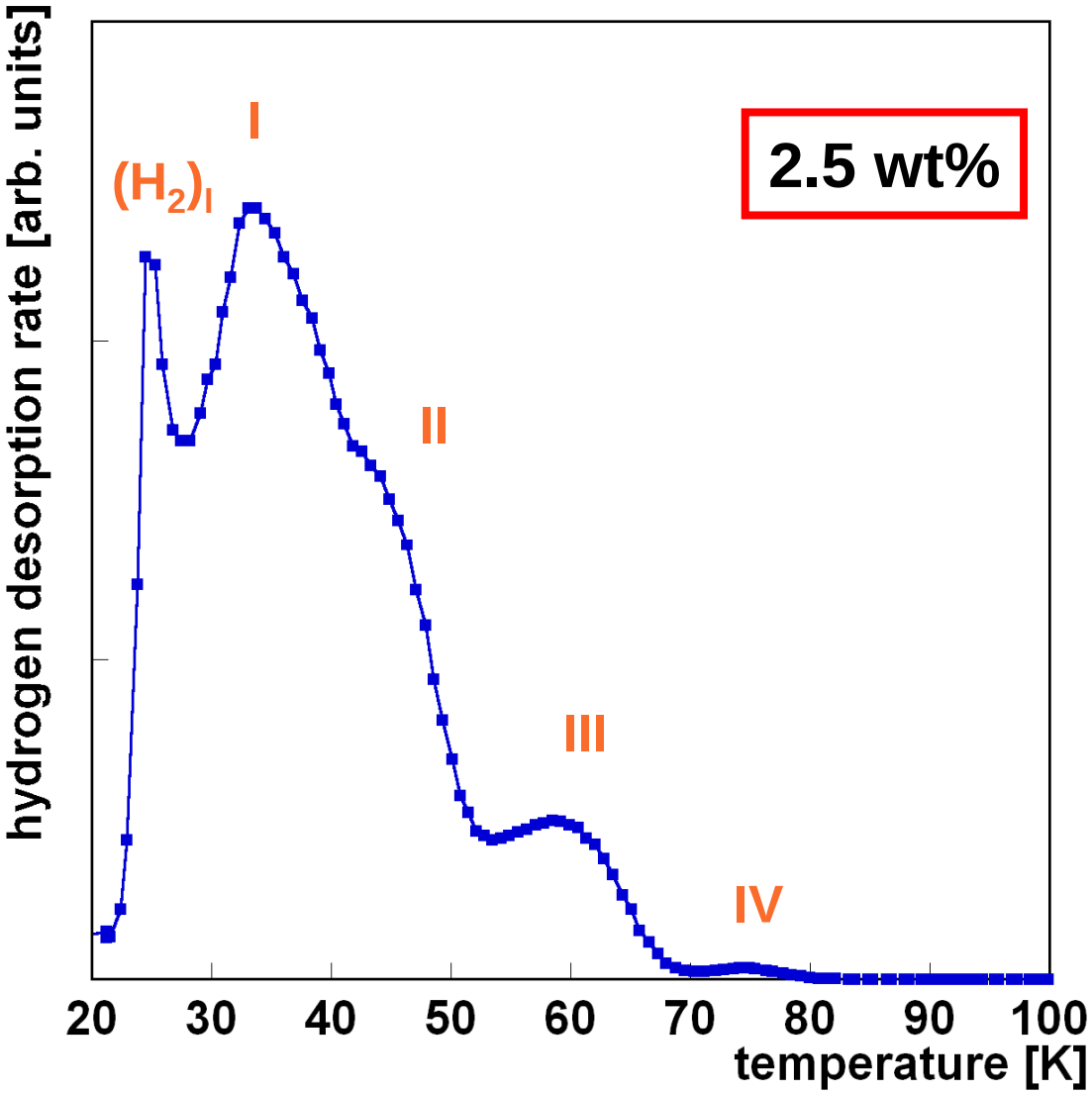


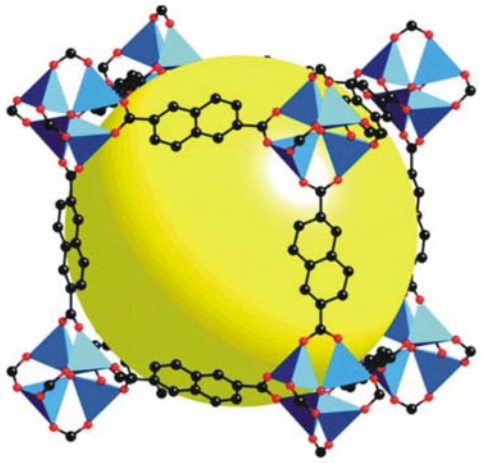
Li et al. Science 402 (1999) 276



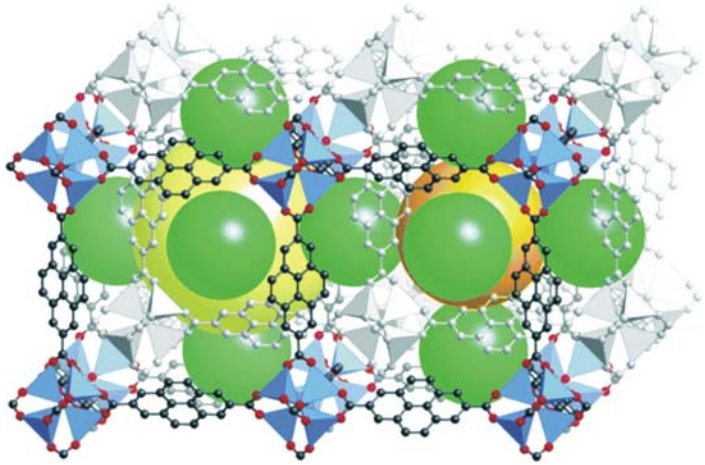
*Picture kindly provided by J. Rowsell

IRMOF-8



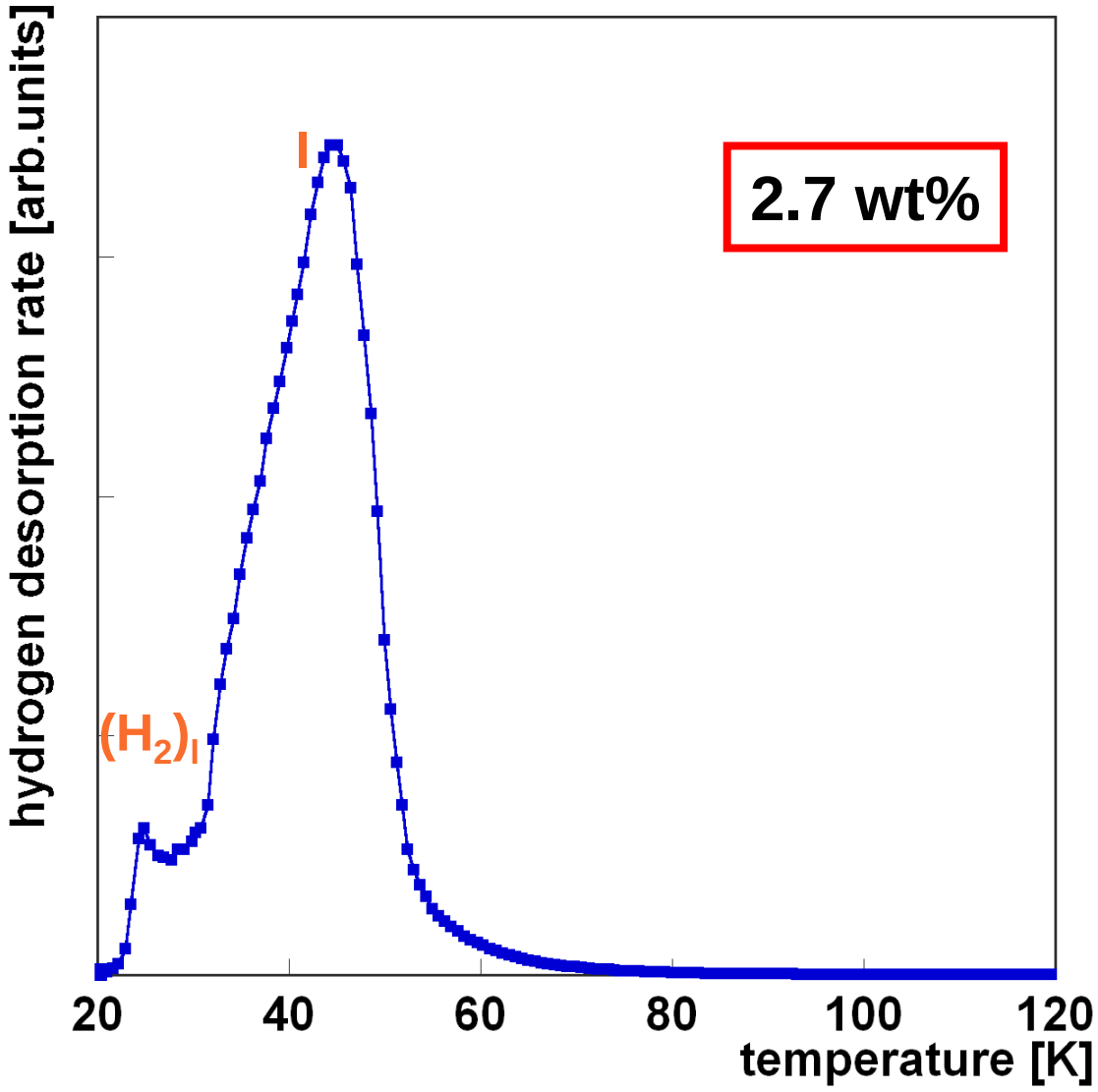


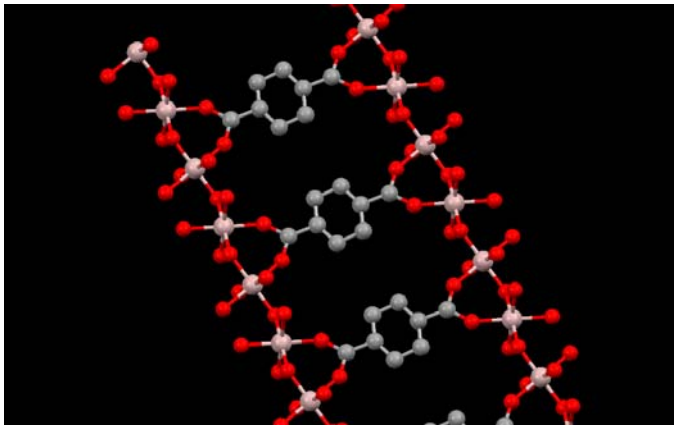
Rosi et al. Science, 300 (2003) 1127

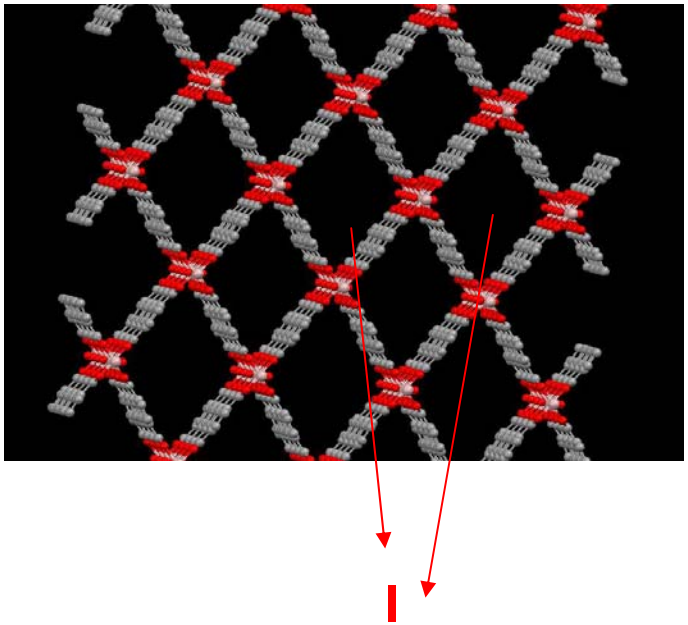


Rowsell et al. J. Am. Chem. Soc. 128 (2006) 1304

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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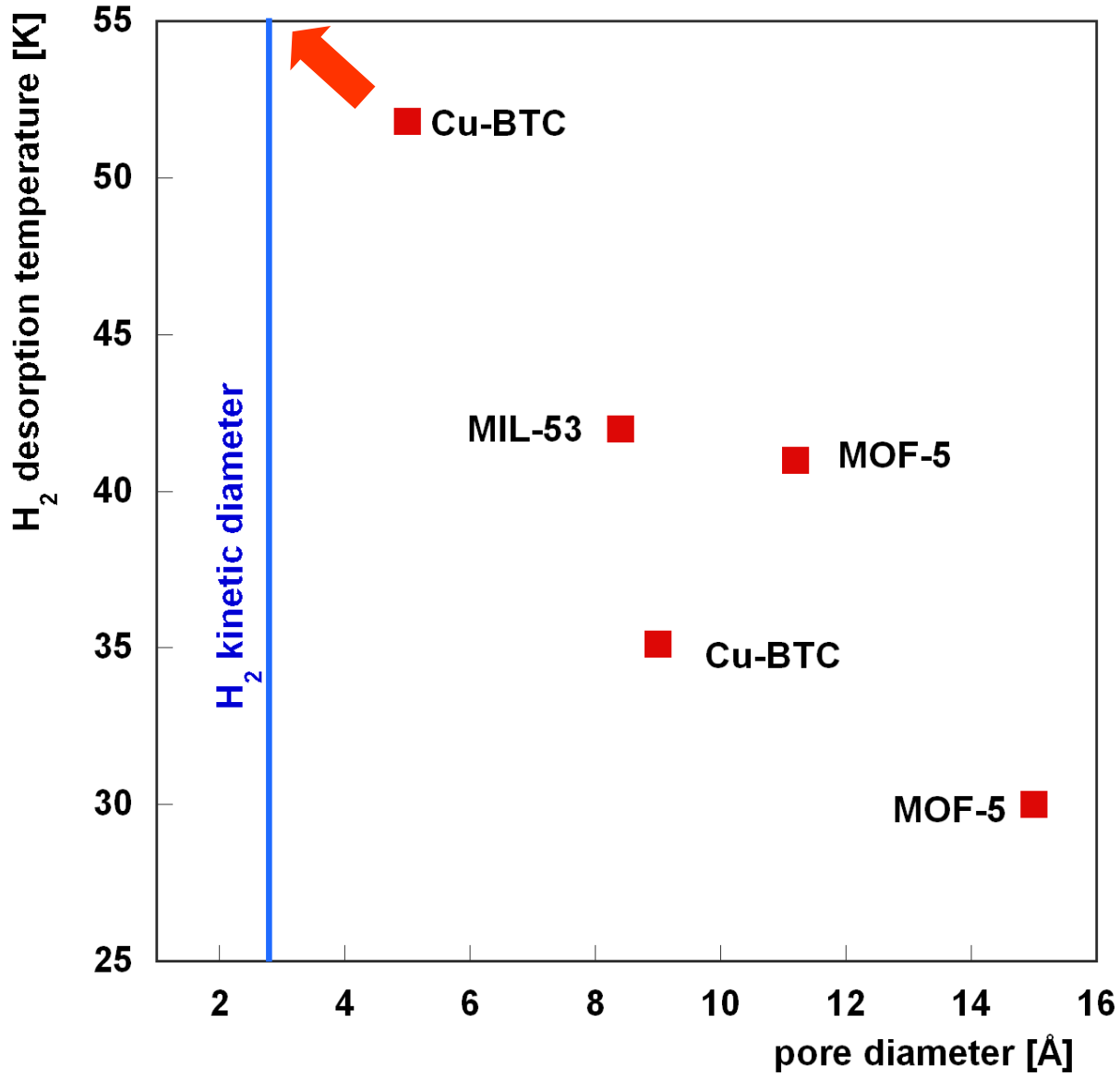
Effect of pore size



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 short refueling time 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? 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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