new materials for capture…
new methods to characterize…
new ways to compute…
new ways to communicate…
new materials for capture...

Pore size suitable for $H_2$ only

Larger pores

Cyclic Peptide Nanotube

$0.7 - 0.8 \text{ nm}$
new methods to characterize...
new ways to compute...
new ways to communicate...
MOF-5

ZnO$_4$ tetrahedra

"MOF-5"
"MOF-5"

ZnO$_4$ tetrahedra

organic linker

- O\_2

- C=O
MTV-MOFs: MOFs with multivariate organic linkers
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- Certain MTV-MOFs have better H₂ and CO₂ adsorption properties than MOFs with a single type of linker.

Deng. et al. Science 2010
MTV-MOFs: MOFs with multivariate organic linkers

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*Deng. et al.*  
*Science* 2010
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Deng. et al. Science 2010
Apportionment matters
Apportionment matters

MTV-MOF-5-EHI

- Alternating
- Large cluster
- Experiment

CO₂ uptake [cm³/g]

Pressure [Torr]

33%
25%
42%

Alternating

Kong et. al. Science, in press
Apportionment matters

\[
\text{CO}_2\text{ uptake [cm}^3\text{/g]}
\]

\begin{align*}
\text{Pressure [Torr]} & \quad 0 & \quad 200 & \quad 400 & \quad 600 & \quad 800 \\
\text{MTV-MOF-5-EHI} & \\
\bullet \text{Alternating} & \quad \circ \text{Large cluster} & \quad \otimes \text{Experiment}
\end{align*}

Kong et. al. Science, in press
CO$_2$ has strong affinity for open metal sites, Mg$^{2+}$
Mg₂(2,5-dioxido-1,4-benzenedicarboxylate)  

“Mg-MOF-74”

CO₂ has strong affinity for open metal sites, Mg²⁺
The spectrum of CO in Mg-MOF-74 demonstrates the effect of temperature on the NMR signal. After demagnetization, the signal-toc+noise ratio is enhanced, and the optical polarization is maintained. The spectrum for CO is observed at 82.5°C, which is slightly less than the theoretical value of 232.8°. The ratio for the 0.3 CO spectral lineshape of the 0.3 CO molecule is 6.4×10^−2. The simulation was performed with a mode of rotation, and the atoms when adsorbed have been suggested by previous adsorption isotherms reported previously (see Figure S3). Interestingly, two populations of adsorbed CO are observed, with the relative amount of gaseous CO increasing as the degree of loading increases. The NMR-derived angles agree with the degree of loading. The NMR-derived angles agree with the degree of loading. The NMR-derived angles agree with the degree of loading. The NMR-derived angles agree with the degree of loading.
MD trajectories of a single CO$_2$ at 200 K with the time period of 5 ns in Mg-MOF-74 structure.
**13CO₂ NMR in Mg-MOF-74**

MD trajectories of a single CO₂ at 200 K with the time period of 5 ns in Mg-MOF-74 structure.
High-Throughput Discovery of Robust Metal-Organic Frameworks for CO₂ Capture

Jeffrey A. Reimer,¹ Tae-Hyun Bae,¹,² Adam H. Berger,³ Joseph Chen,⁴ Justin J. Dutton,⁵ Kuldeep Jariwala,² Jihan Kim,² Sean Kong,² Li-Chiang Lin, Richard L. Martin,⁶ Jarad A. Mason,¹ Thomas M. McDonald,¹ Ken J. Micklash,⁵ Roger Sathre,⁷ Kenji Sumida,¹ Joseph A. Swisher,²,⁶ Abhoyjit S. Bhown,³ Maciej Haranczyk,⁶ Steven Kaye,⁵ Jeffrey R. Long,¹,² Eric Masanet,⁷ Berend Smit¹,²,⁴

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Tuesday, July 9, 2013 - Grand Station I & II

5:00 p.m. Poster Session/Reception – Grand Station III
a dizzying array of possibilities...
a dizzying array of possibilities...

Cu₃[(Cu₄Cl)₃(BTTr)₈]₂·xH₂NCH₂CH₂NR₂
a dizzying array of possibilities...

2,5-dioxidoterephthalate (DOBDC$^{2-}$) + $\text{M} (\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ → solvent exchange activation

$\text{Cu}_3[(\text{Cu}_4\text{Cl})_3(\text{BTTri})_8]_2 \cdot \text{xH}_2\text{NCH}_2\text{CH}_2\text{NR}_2$

$\text{M}_2(\text{DOBDC})$ (M-MOF-74) (M = Mg, Co, Ni, Zn)