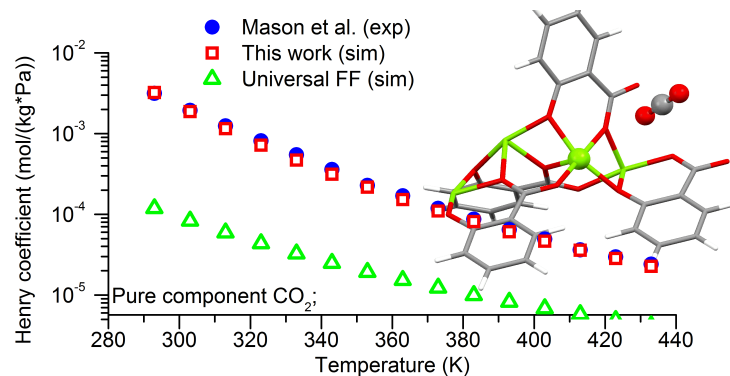
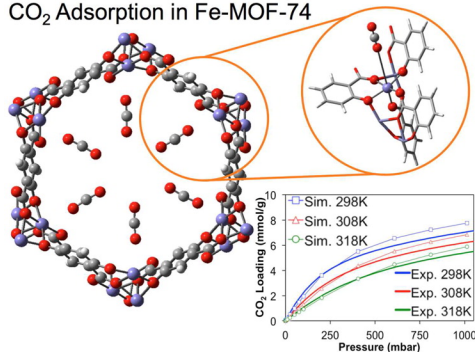


# Force Field Parameterization



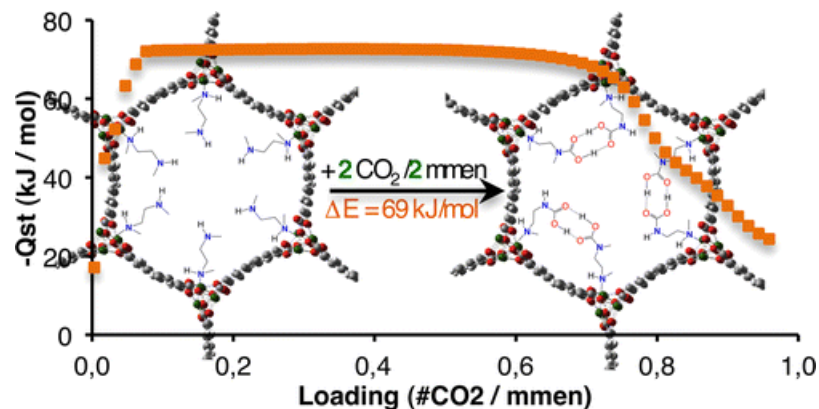
*Nature Chem.* **2012**, 4, 810

CO<sub>2</sub> Adsorption in Fe-MOF-74

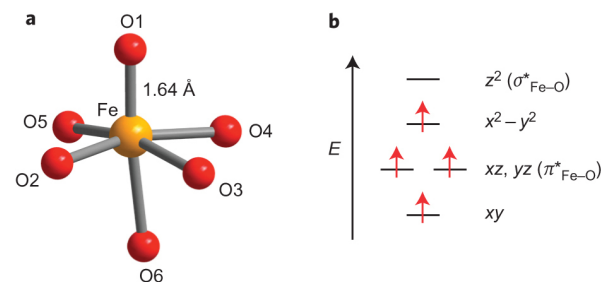


*J. Phys. Chem. C.* **2014**, 118, 12230

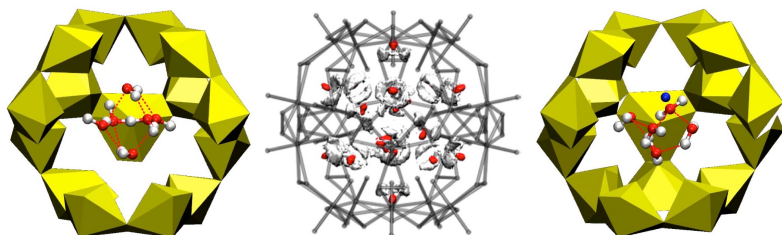
# Gas Reactivity within MOFs



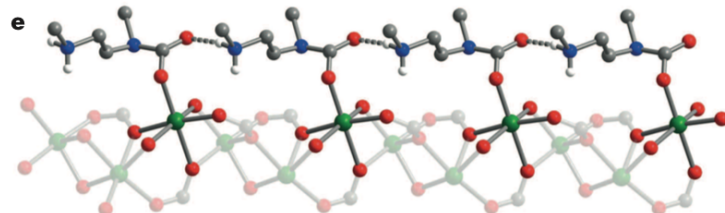
*J. Am. Chem. Soc.* **2013**, 135, 7402



*Nature Chem.* **2014**, 6, 590

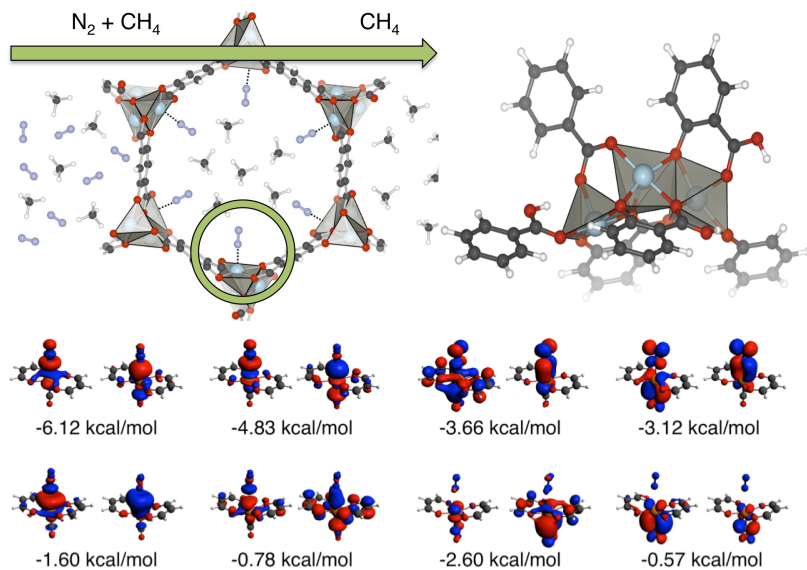


*J. Phys. Chem. C.* **2014**, 118, 24730

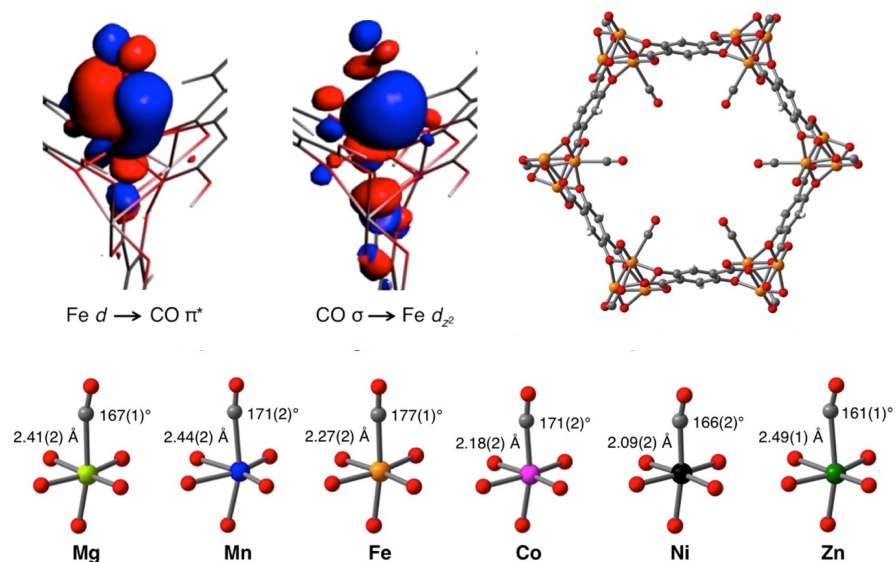


*Nature*, **2015**. Published Online

# Nature of Adsorbate-MOF Bonding

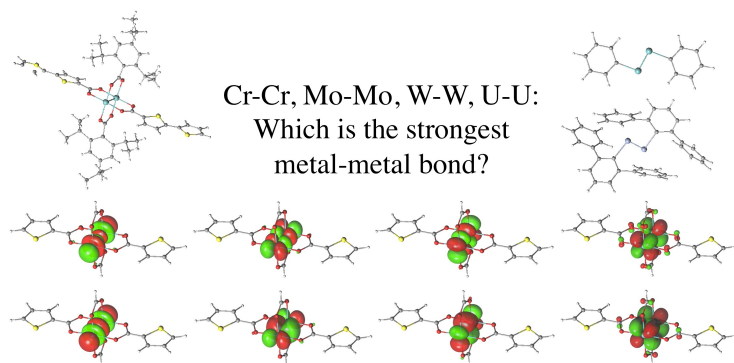


*J. Am. Chem. Soc.* **2014**, *136*, 698

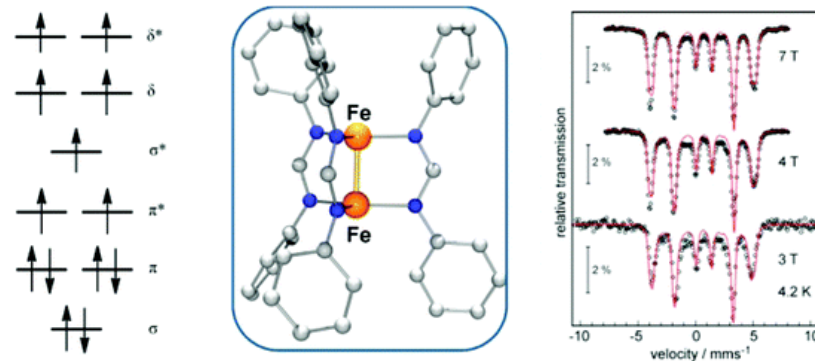


*J. Am. Chem. Soc.* **2014**, *136*, 10752

## Multireference Treatment of Metal-Metal Bonds



*Chem. Eur. J.* **2012**, *18*, 1737



*Inorg. Chem.* **2012**, *51*, 728