CO_2 capture is required to mitigate climate change

Inorganic solids have potential to capture CO_2, but they are not yet economically viable. ☹

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Role of Pore Chemistry and Topology in the CO_2 Capture Capabilities of MOFs: From Molecular Simulation to Machine Learning

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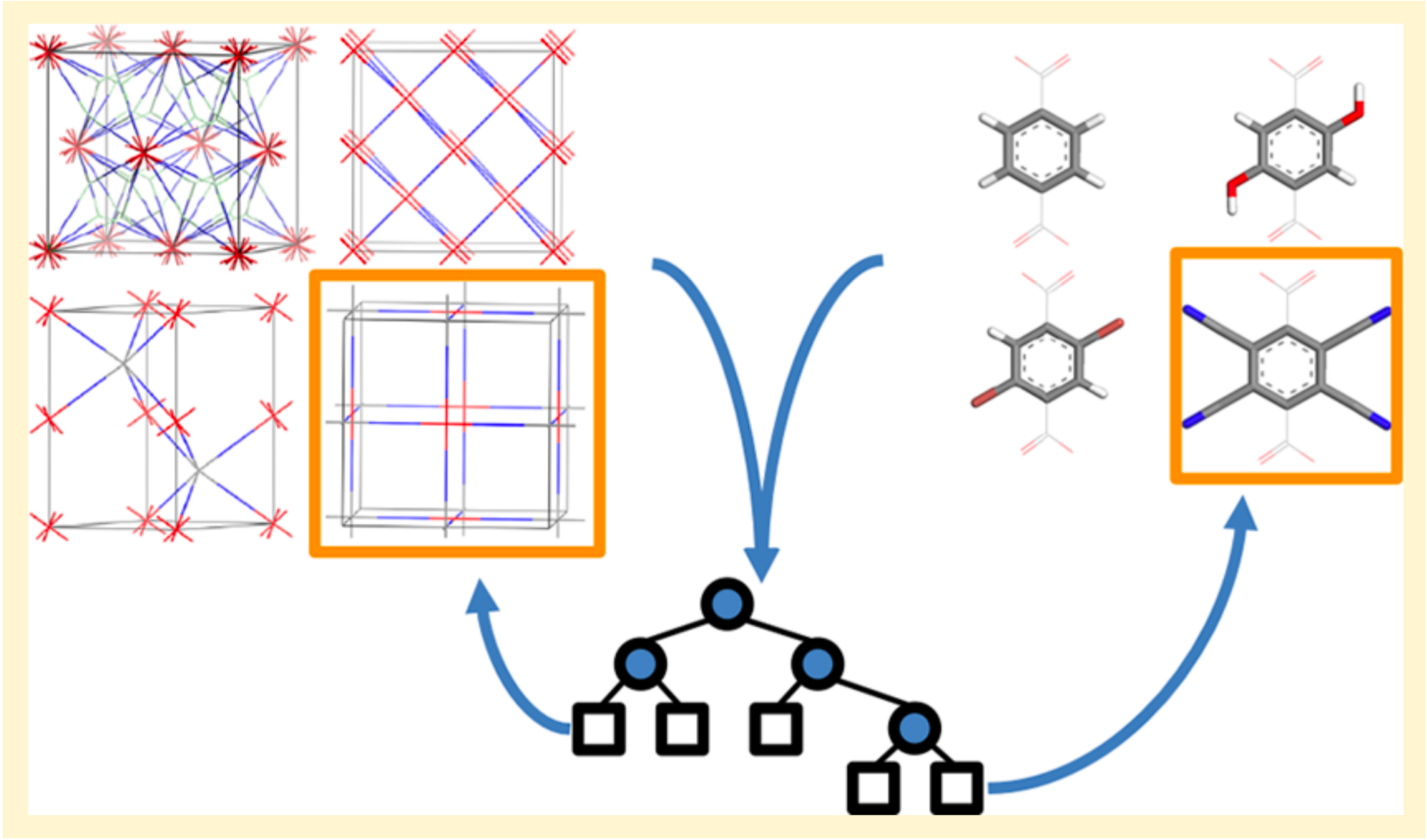
Role of Pore Chemistry and Topology in the CO_2 Capture Capabilities of MOFs: From Molecular Simulation to Machine Learning

- MOF = metal organic framework
- Machine learning: input = property, output = descriptors



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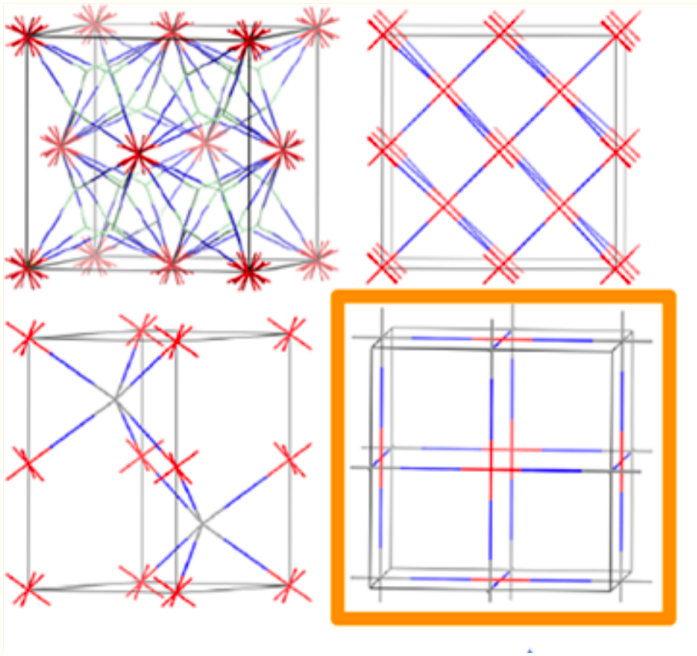
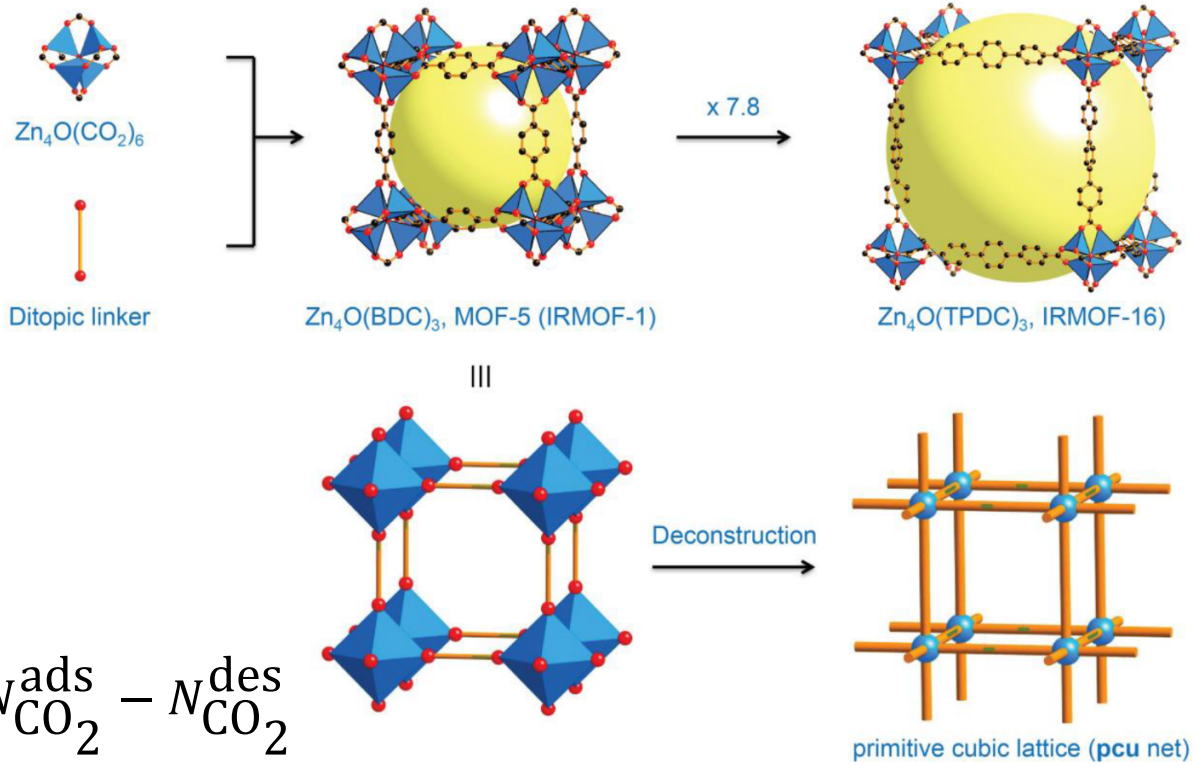
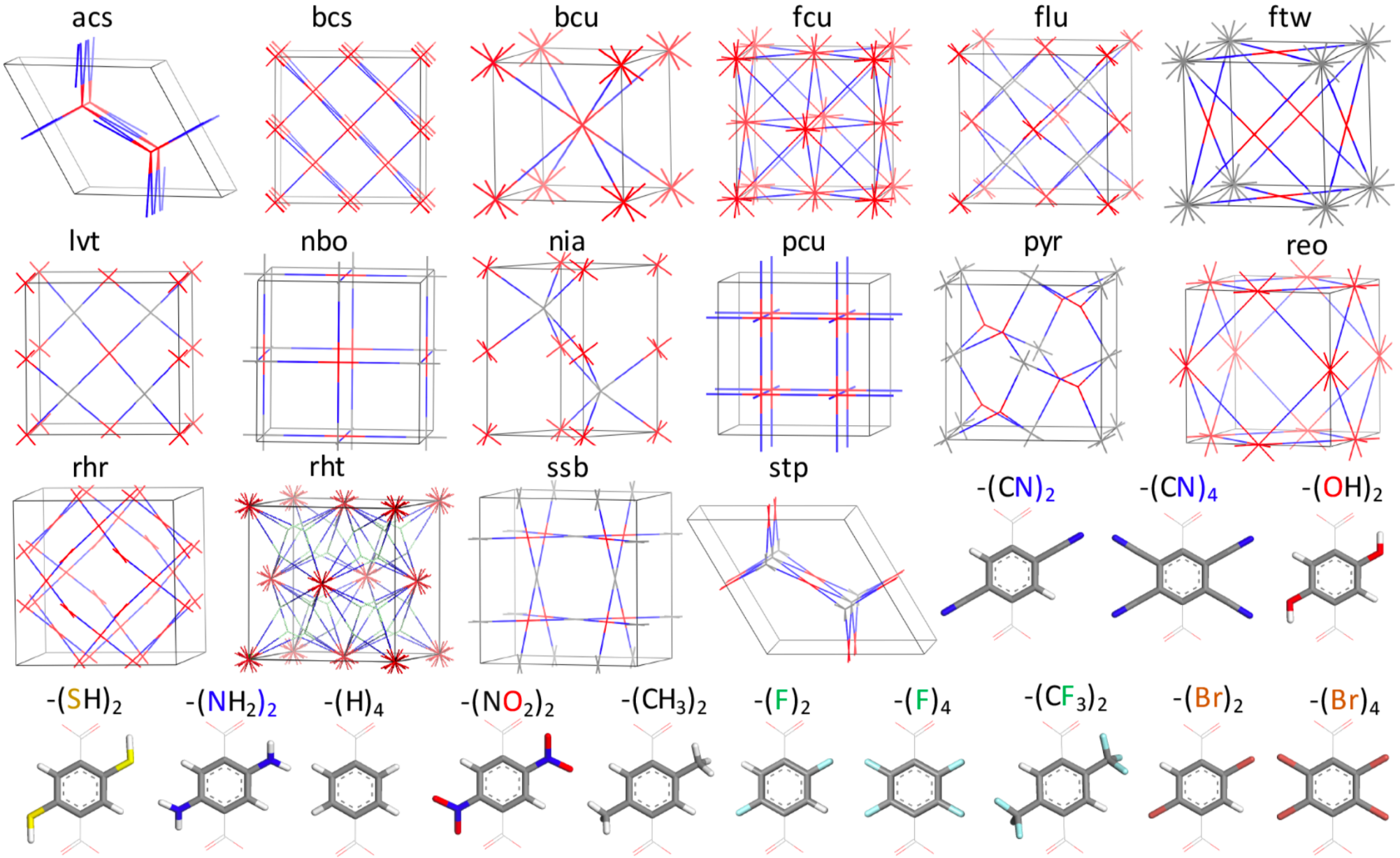




$$S = \frac{N_{CO_2}^{ads} / y_{CO_2}}{N_i^{ads} / y_i}$$

$$WC = N_{CO_2}^{ads} - N_{CO_2}^{des}$$

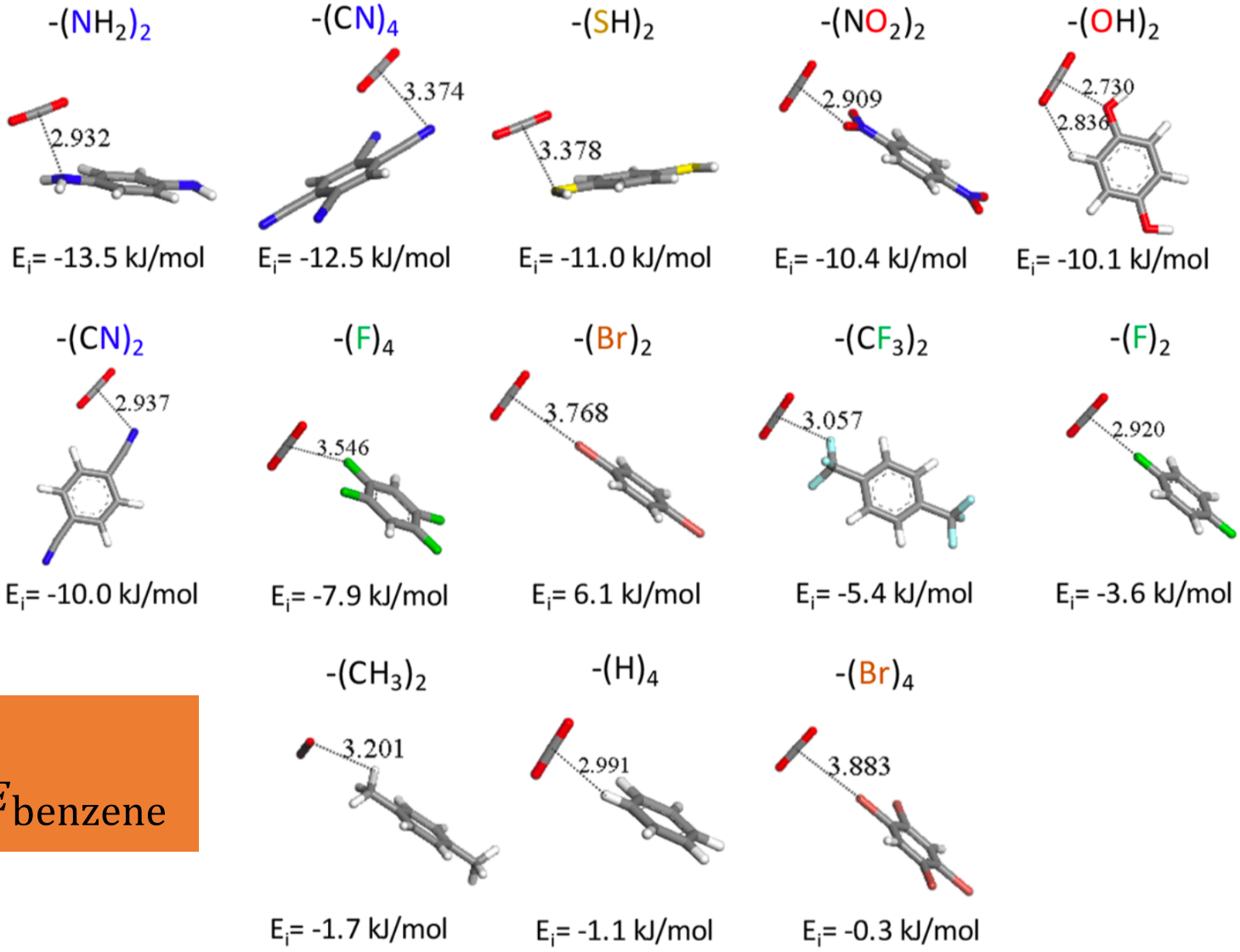
Test many MOFs, many linkers



DFT binding energies and geometries

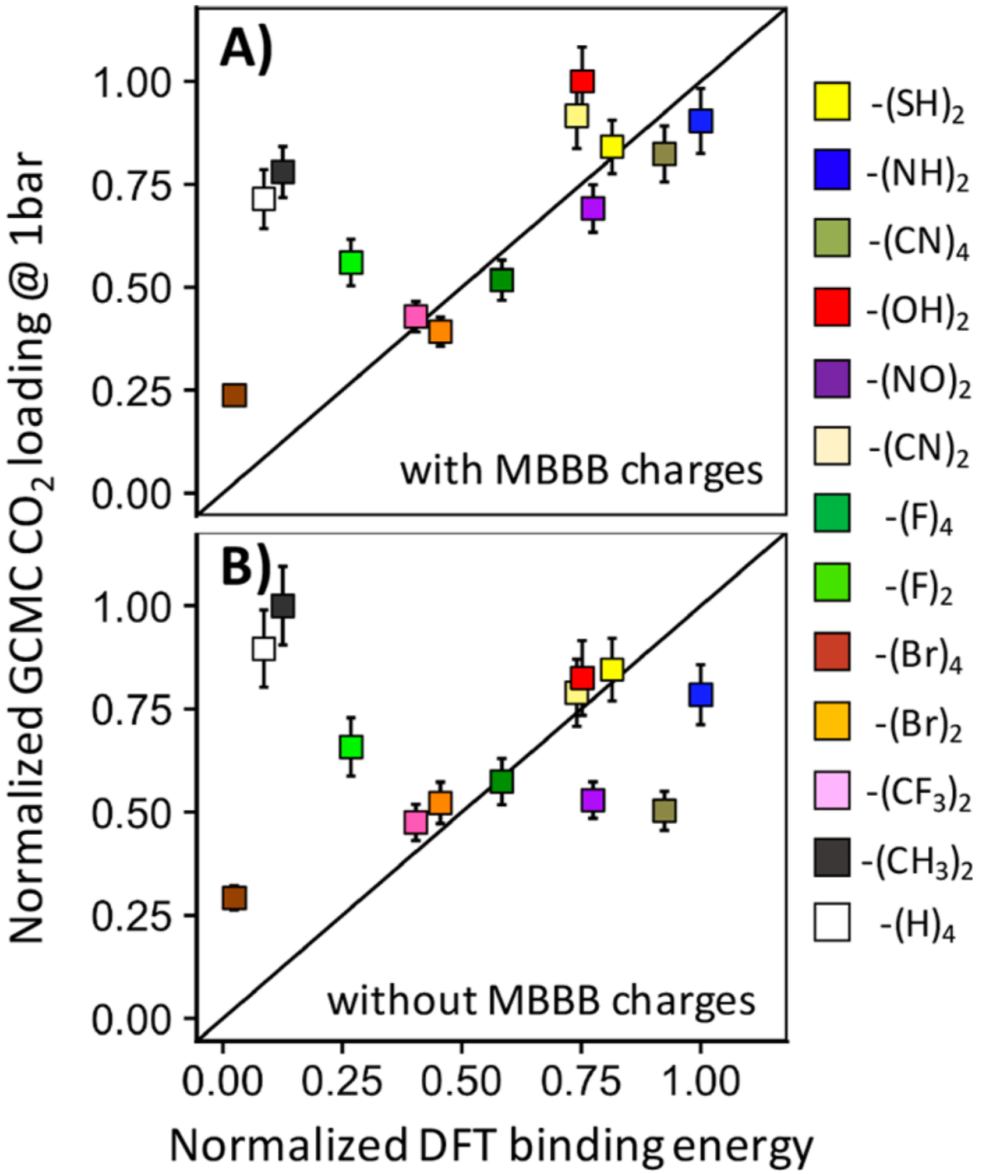
- DFT can estimate exchange-correlation energy
- A self consistent field method is still used to find the energies and wavefunctions.

$$E_{\text{binding}} = E_{\text{complex}} - E_{CO_2} - E_{\text{benzene}}$$



The calculation is pretty good

- CO_2 loading = mole of CO_2 per mole of MOF
- GCMC = Grand canonical Monte Carlo, a computational method to statistically investigate a reaction (such as CO_2 adsorption)



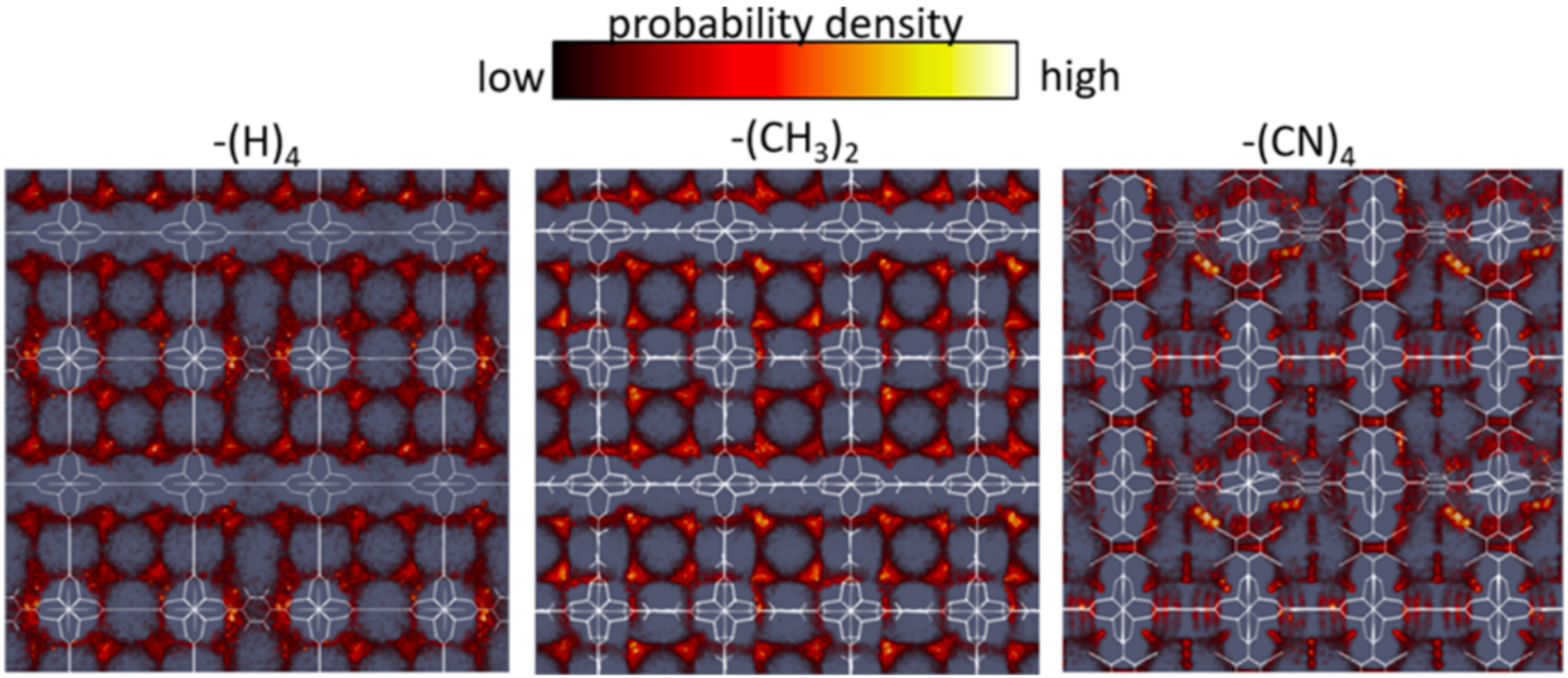
The DFT functional for systems with dispersion forces!

- Literature: M06-L with Def2SVP
  - I suggested: B3LYP and 6-31+G(d,p) because I got errors when I tried to run

```
#P M06L/def2SVP opt iop(1/7=30) integral=ultrafine
```

- However, the benzene and CO_2 molecules did not "bind" with B3LYP and 6-31+G(d,p)!
  - Eureka! M06-L is better than B3LYP for dispersion.
  - With testing, I found the error was Def2VSP (not M06-L).
- Please run M06L and 6-311+G(d,p) or 6-31+G(d,p).
  - I think the larger basis set will be more accurate, but it takes twice the amount of time (I tested on benzene geo opt).
  - New input files and analysis script is on iLearn.

Locations of CO_2 binding in MOF



Finding the best MOFs and linkers