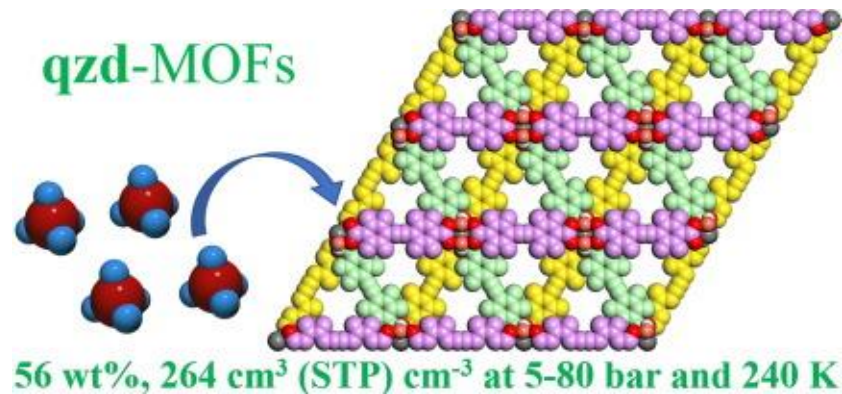


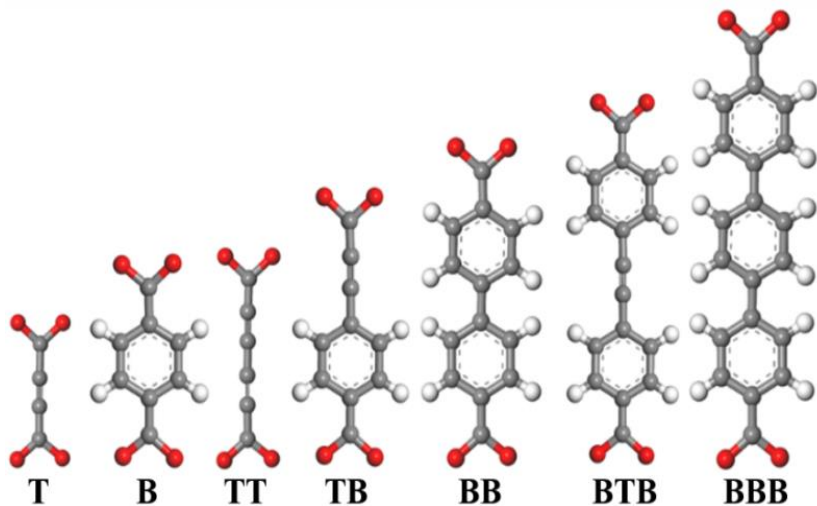
Methane Sorption in a Family of qzd-MOFs: A Multiscale Computational Study

Mikhail Suyetin, Maxim V. Peskov, Udo Schwingenschlögl



Suyetin, M., Peskov, M. V., Schwingenschlögl, U. Methane Sorption in a Family of **qzd**-MOFs: A Multiscale Computational Study. **Chemical Engineering Journal**. 2020, 123296.

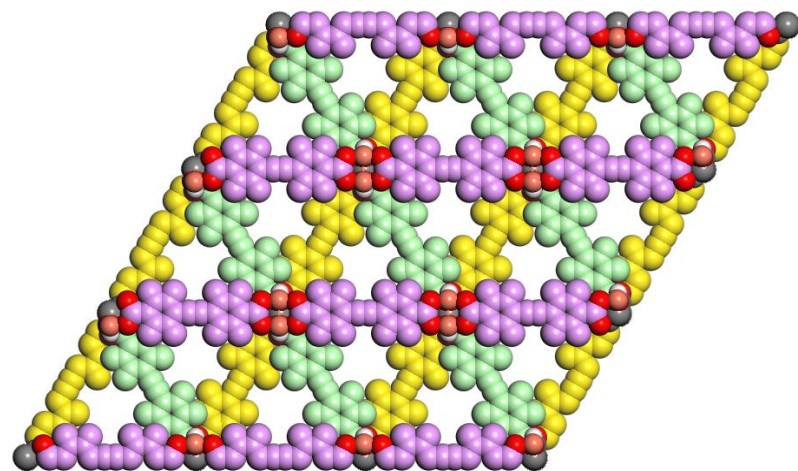
DOI: 10.1016/j.cej.2019.123296



Organic linkers used to obtain a series of **qzd**-

MOFs. White, grey, and red spheres denote H,

C, and O atoms, respectively

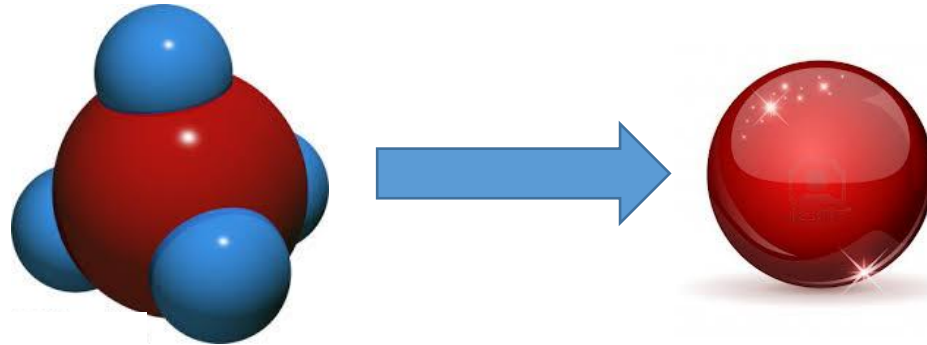


BB framework of **qzd** topology.

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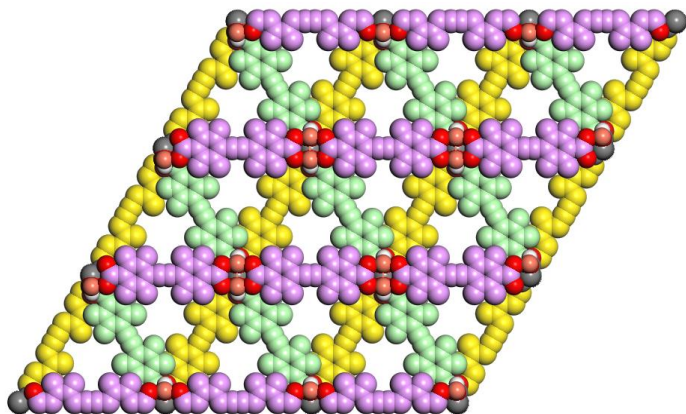
CH₄ model

Atom type	σ_j (Å)	ϵ_j/k_B (K)	q (e)
United	3.73	148	0



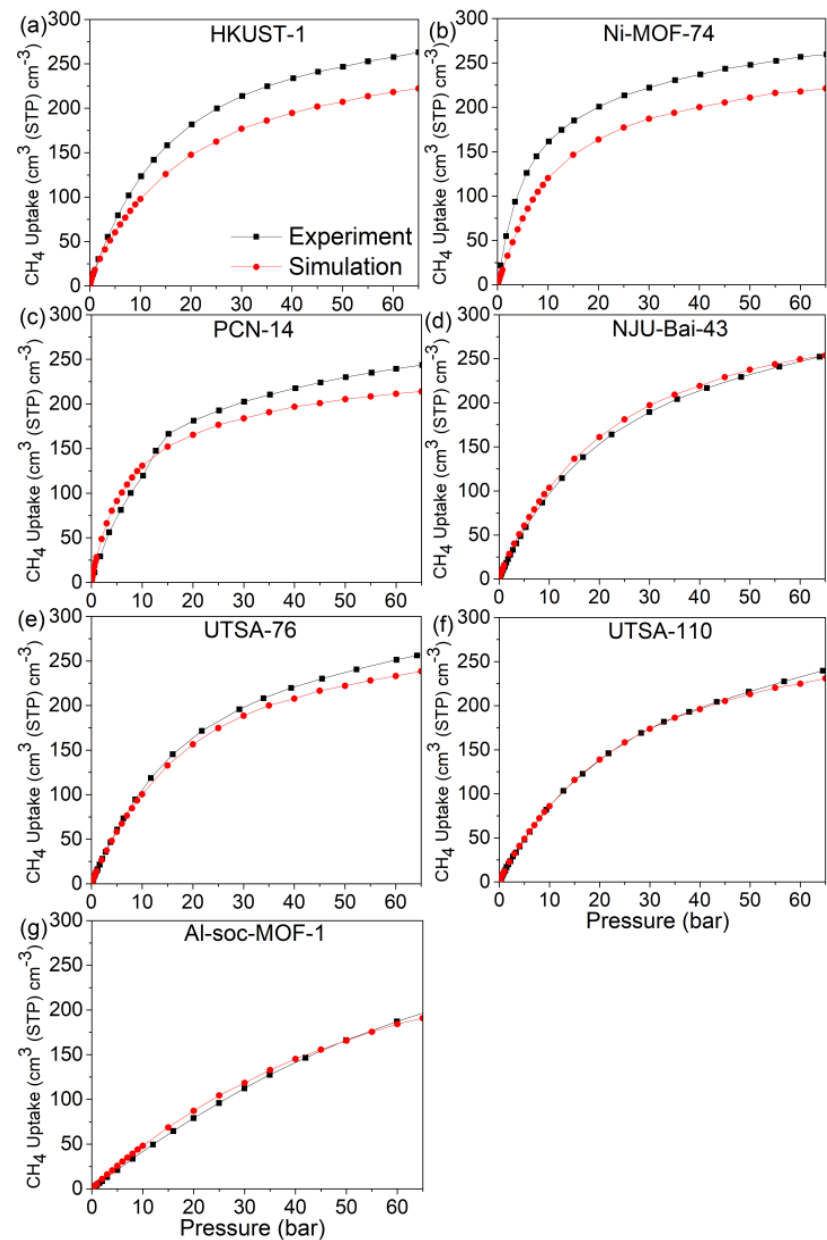
MOF model: Dreiding Force Field, Universal Force Field

Atom type	σ_i (Å)	ϵ_i/k_B (K)
C	3.473	47.856
O	3.033	48.158
H	2.846	7.649
Cu	3.114	2.516

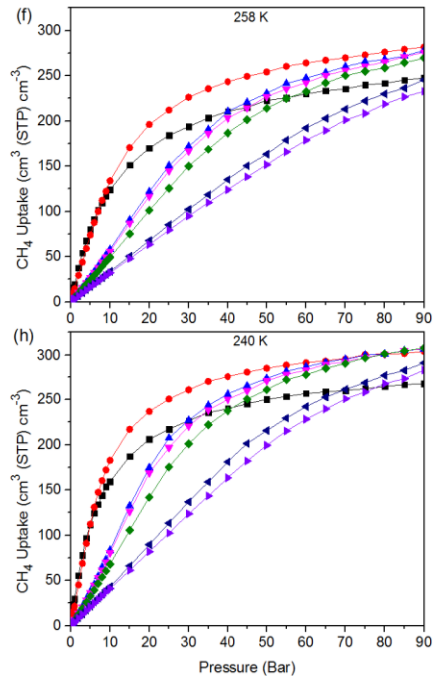
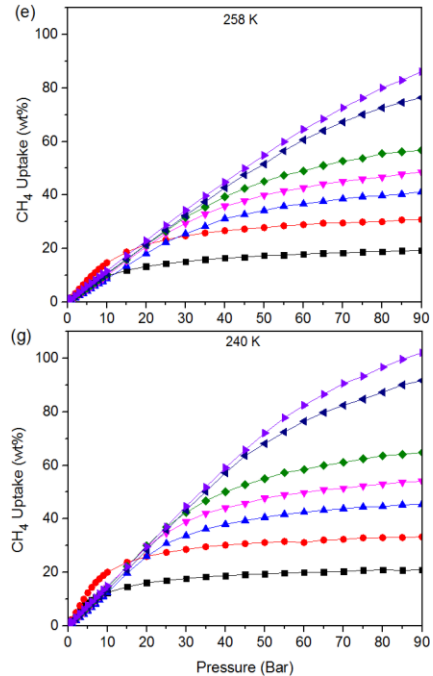
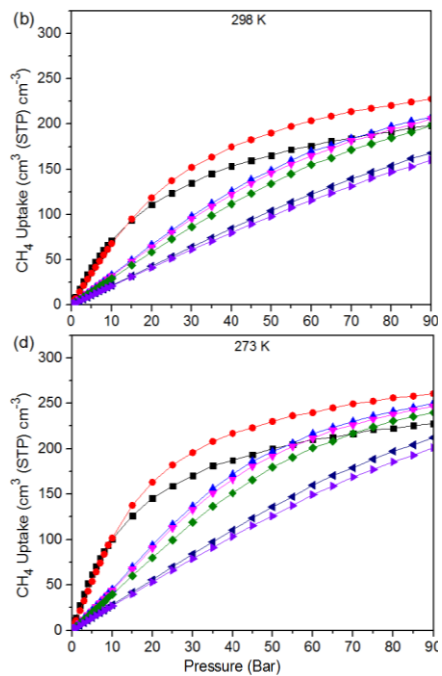
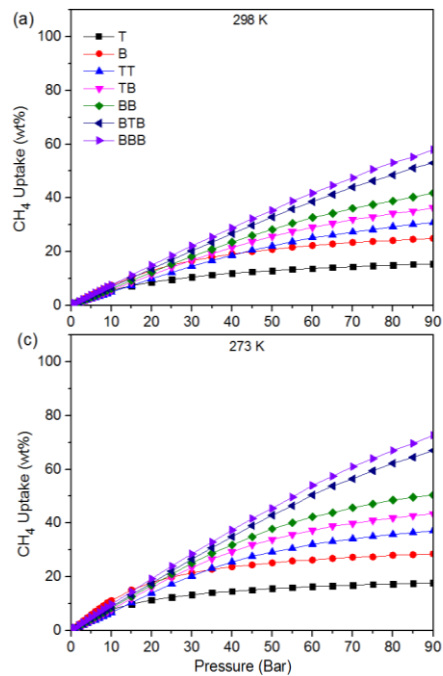


BB framework of **qzd** topology.

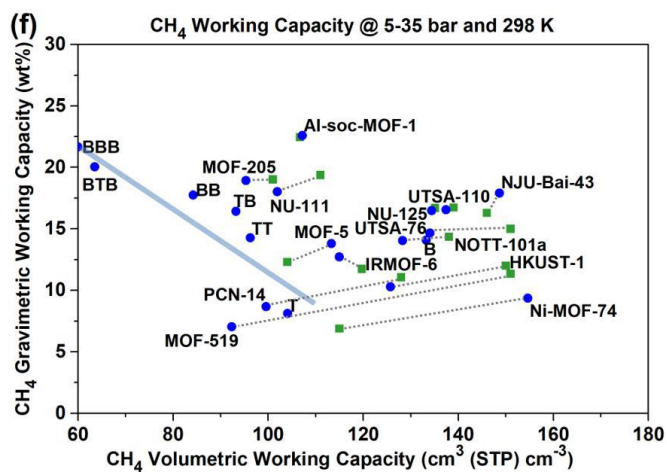
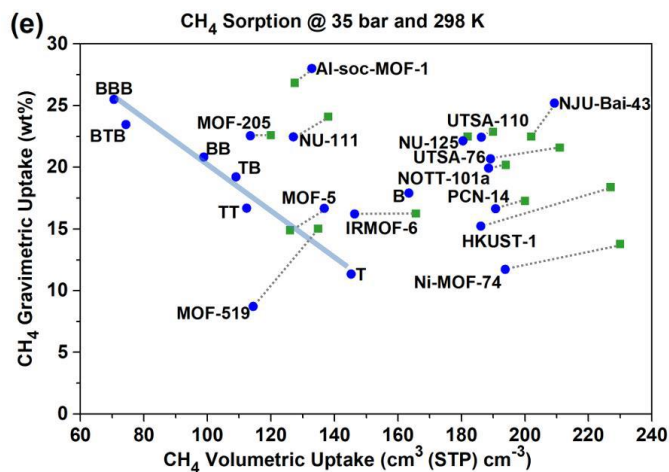
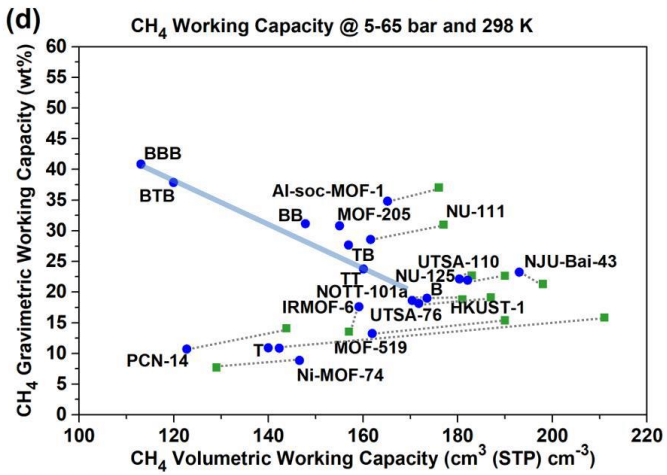
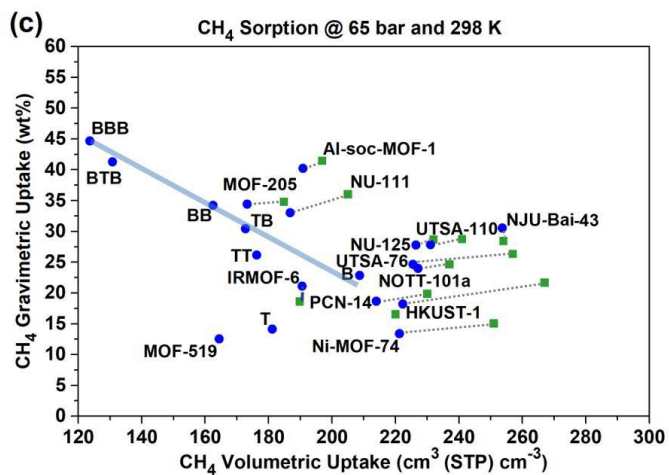
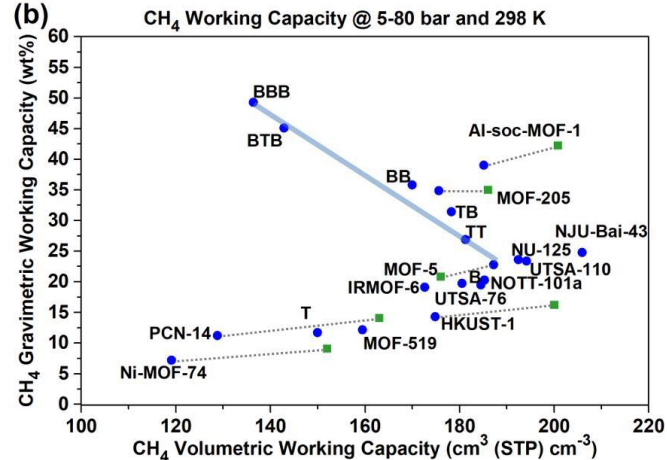
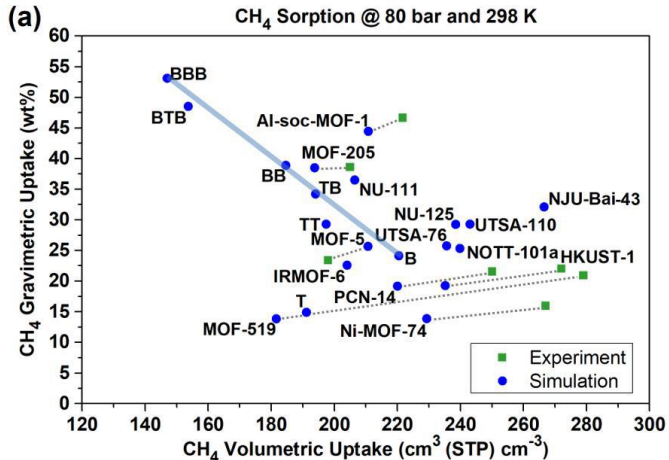
Comparison of experimental and simulated methane sorption isotherms for state-of-the-art MOFs.

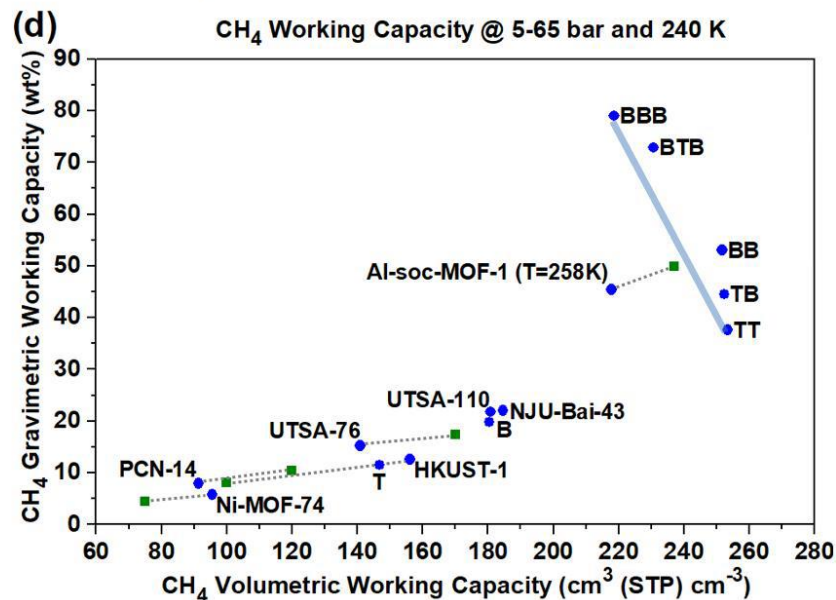
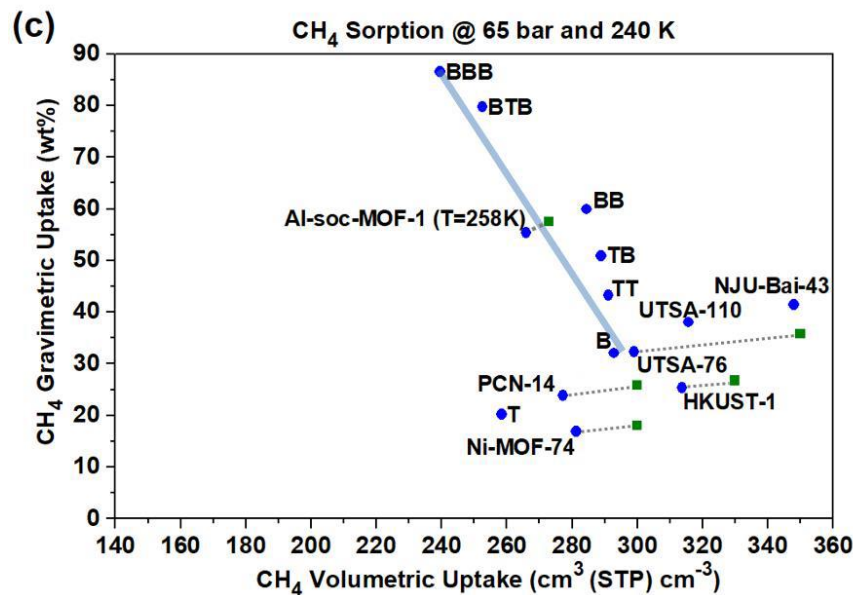
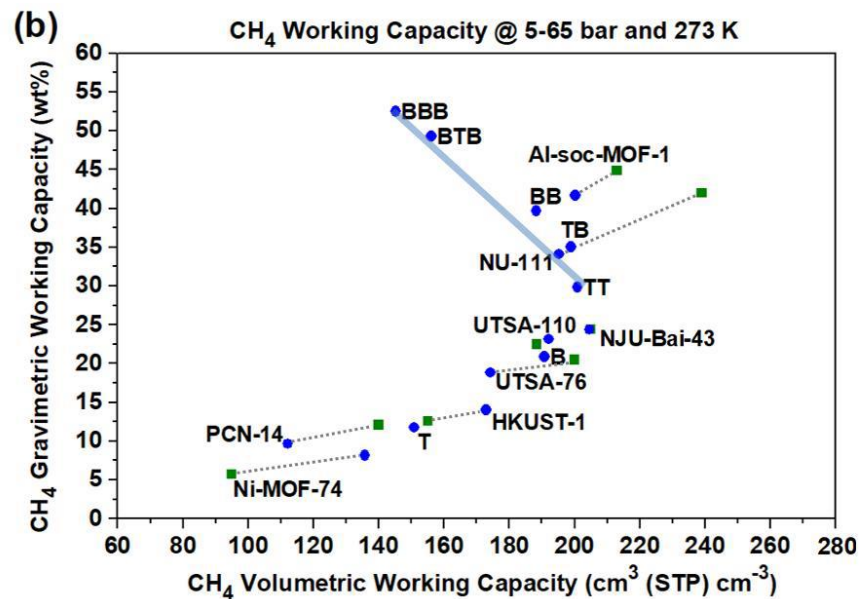
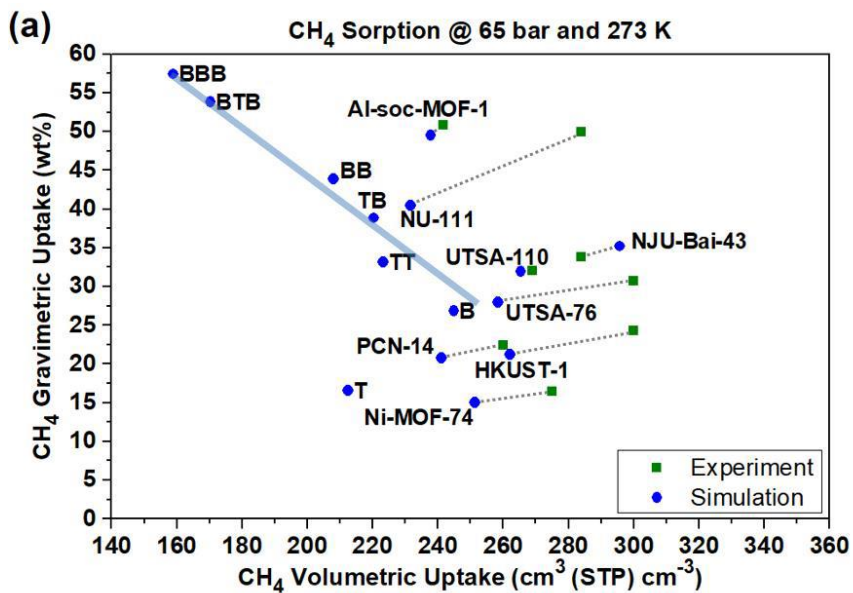


Methane sorption isotherms of the computationally designed MOFs with qzd topology.



Total methane uptake and working capacity at 35 bar, 65 bar, or 80 bar and 298 K.





Total methane uptake and working capacity of the computationally designed **qzd**-MOFs and outstanding MOFs from the literature at 65 bar and 273 K or 240 K.

