Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Electronic Supplementary Information (ESI)

Volume shrinkage of metal organic framework host induced by the dispersive attraction of guest gas molecules

Jaeyong Joo,[a] Hyungjun Kim*[b] and Sang Soo Han*[a]

[a] *Center for Computational Science, Korea Institute of Science and Technology (KIST), Seoul 136-791, Republic of Korea. E-mail: sangsoo@kist.re.kr*

[b] *Graduate School of EEWS, Korea Advanced Institute of Science and Technology, Daejeon 305-701, Republic of Korea. E-mail: linus16@kaist.ac.kr*

A comparison of the DFT-*ulg* method (PBE-ulg) with a post Hartree-Fock calculation such as Møller-Plesset perturbation (MP2)

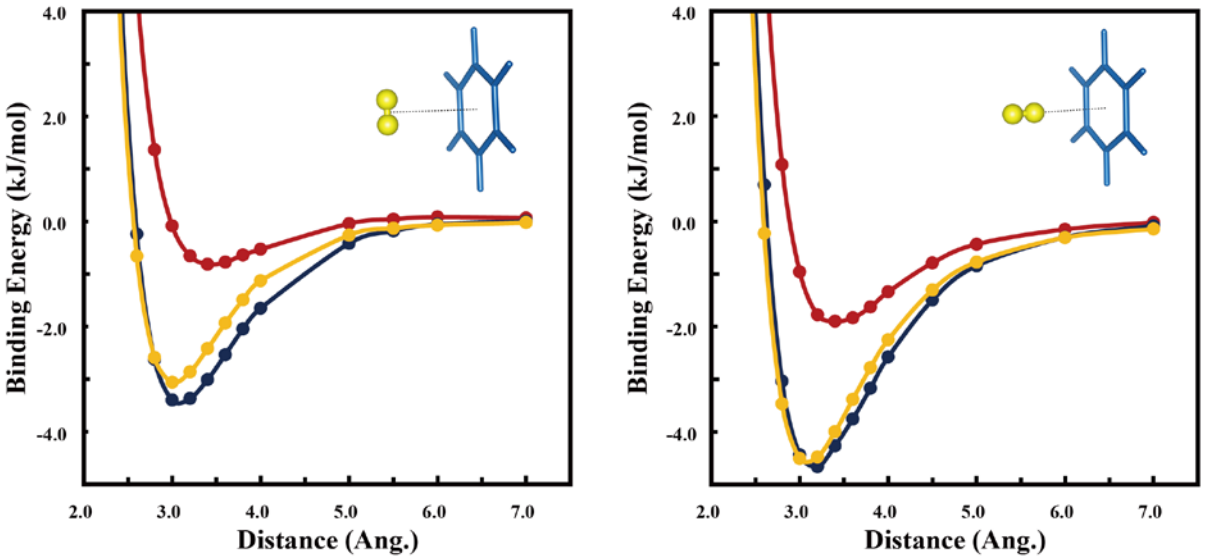

Fig. S1. Calculated H_2-C_6H_6 binding energies for the parallel (left) and vertical (right) configurations by PBE (red), PBE-ulg (blue), and MP2 (yellow) with a basis set of cc-pVQZ. The MP2 calculations were performed with the Q-CHEM software.

Variations of bonds and angles in MOF-5 after H_2 adsorption

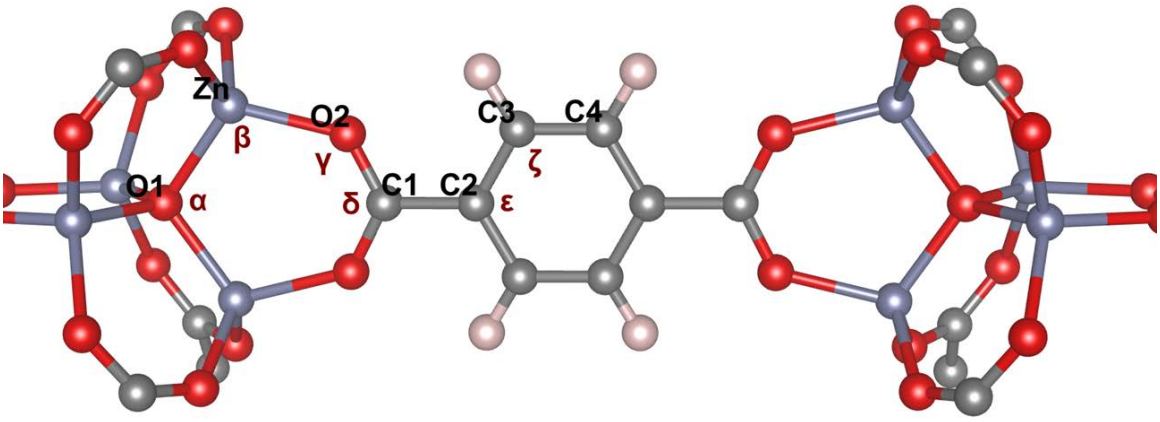

Fig. S2. Bonds and angles in MOF-5

Table S1. Variations of bonds in MOF-5 after H_2 adsorption, where the codes are in Fig. S2.

H_2 adsorption	O1-Zn	Zn-O2	O2-C1	C1-C2	C2-C3	C3-C4
No adsorption (Å)	1.967	1.967	1.277	1.495	1.403	1.391
Site 1 (%)	0.0	-0.1	0.0	-0.1	0.0	0.0
Site 1+2 (%)	0.0	-0.1	0.0	-0.1	0.0	0.0
Site 1+2+3 (%)	-0.4	-0.3	0.0	-0.3	0.0	-0.1
Site 1+2+3+4 (%)	-0.4	-0.5	0.0	-0.4	-0.1	-0.1

Table S2. Variations of angles in MOF-5 after H_2 adsorption, where the codes are in Fig. S2.

H_2 adsorption	α	β	γ	δ	ε	ζ
No adsorption (°)	109.48	111.52	130.61	126.25	119.95	120.02
Site 1 (%)	0.0	0.0	0.0	0.0	0.1	0.0
Site 1+2 (%)	0.0	0.0	0.0	0.0	0.1	0.0
Site 1+2+3 (%)	0.0	0.1	0.0	-0.1	0.2	-0.1
Site 1+2+3+4 (%)	0.0	0.1	-0.2	0.1	0.3	-0.1

Table S3. Variations of Bader charges in MOF-5 after H_2 adsorption, where the codes are in Fig. S2.

H_2 adsorption	O1	Zn	O2	C1	C2	C3
No adsorption (e)	-0.1500	1.2909	-1.1523	1.5379	-0.0265	0.0488
Site 1 (e)	-1.1491	1.2884	-1.1520	1.5387	-0.0245	0.1103