Computational study of CO_2 capture in meal-organic frameworks

Qingyuan Yang, Chongli Zhong, Jianfeng Chen

Supporting Information

Crystal structures for the studied metal-organic frameworks (MOFs)

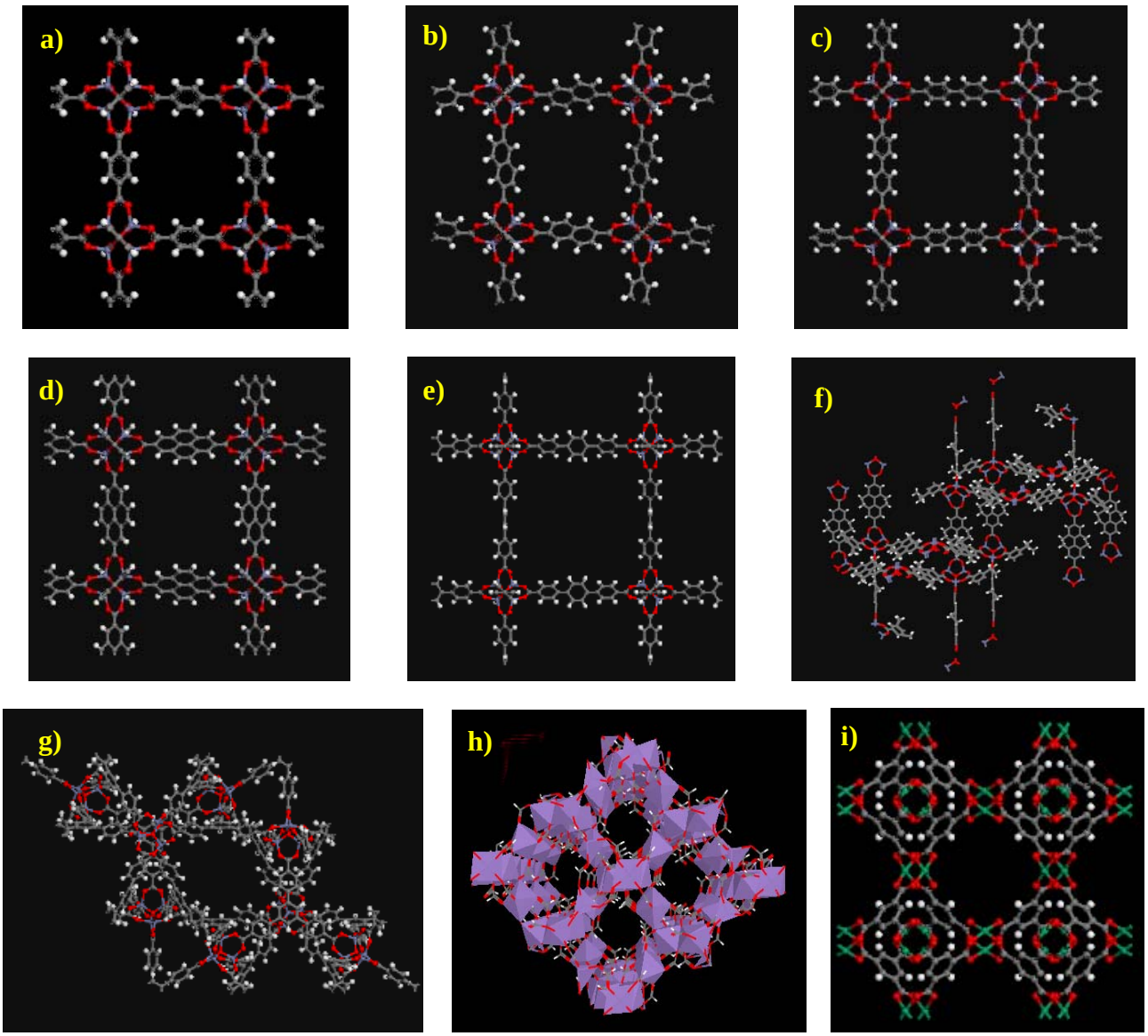
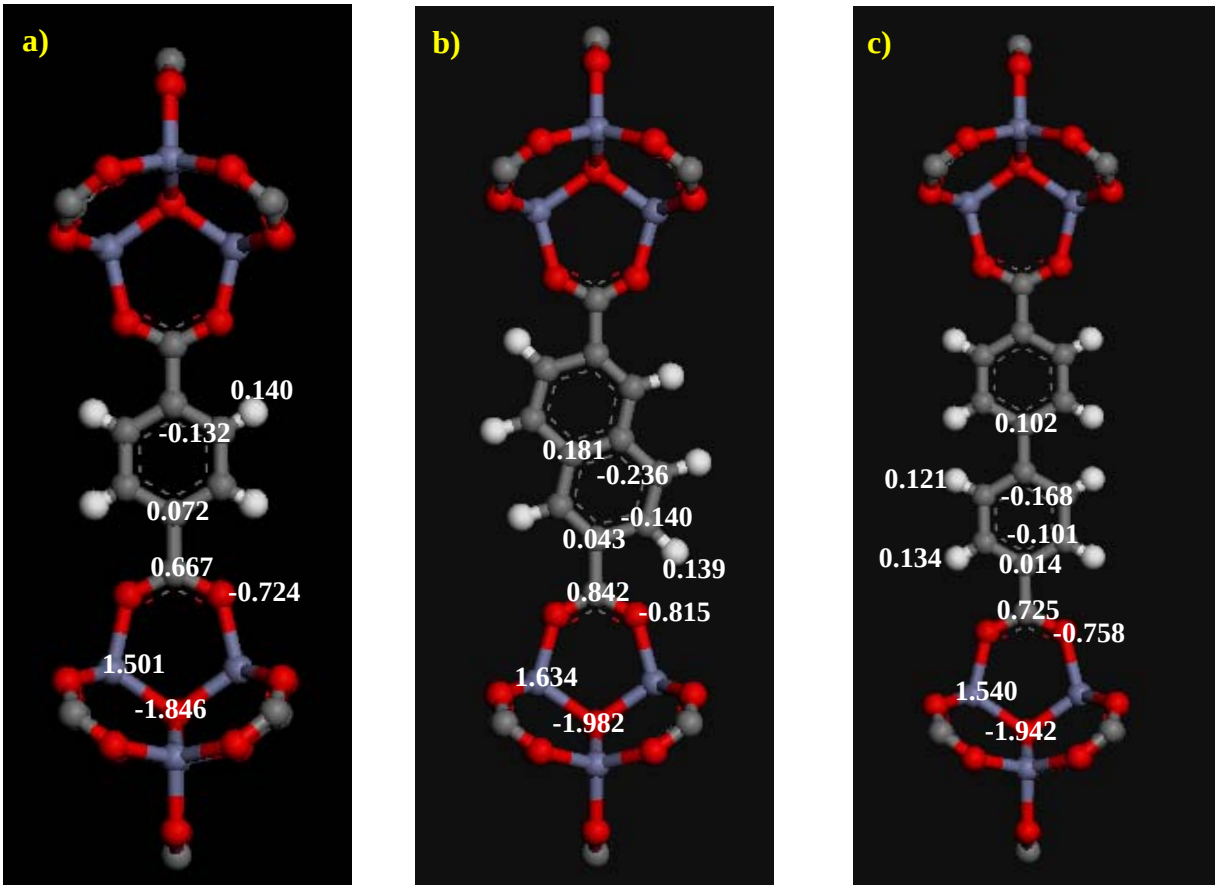
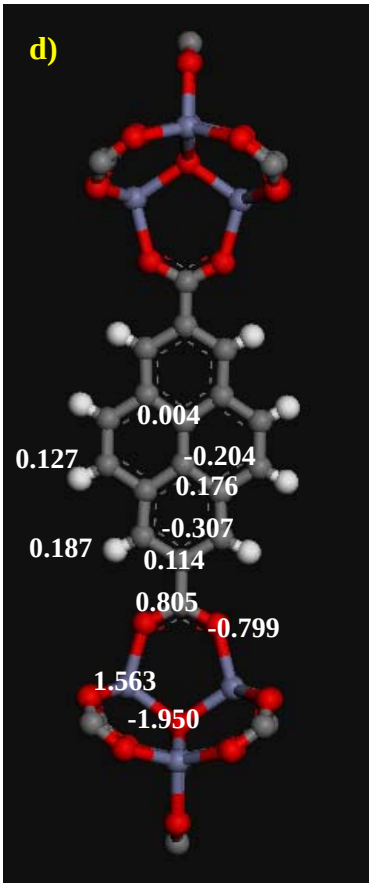


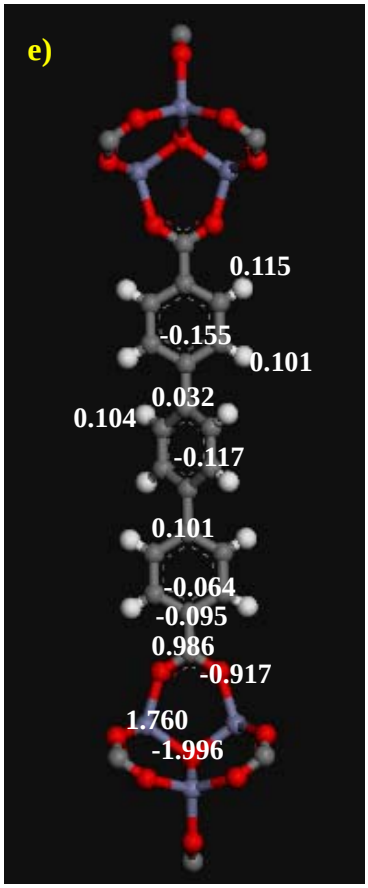
Figure *S1*. Unit cell crystal structures of the studied MOFs: a) IRMOF-1. b) IRMOF-8. c) IRMOF-10. d) IRMOF-14. e) IRMOF-11. f) IRMOF-16. g) MOF-177. h) Mn-MOF. i) Cu-BTC (Zn, blue; Mn, purple; Cu, green; O, red; C, gray, and H, white).

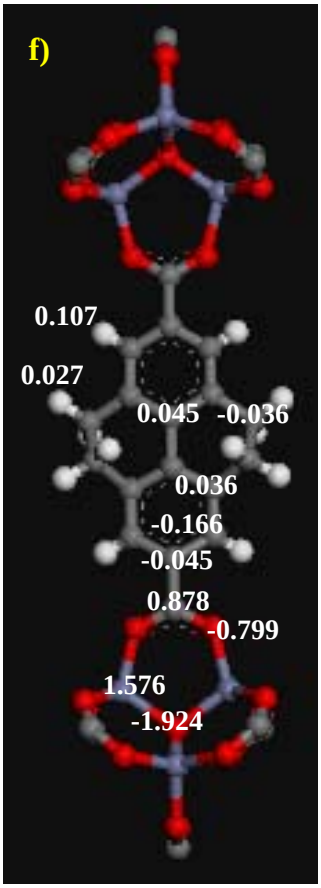
Atomic partial charges for the studied MOFs

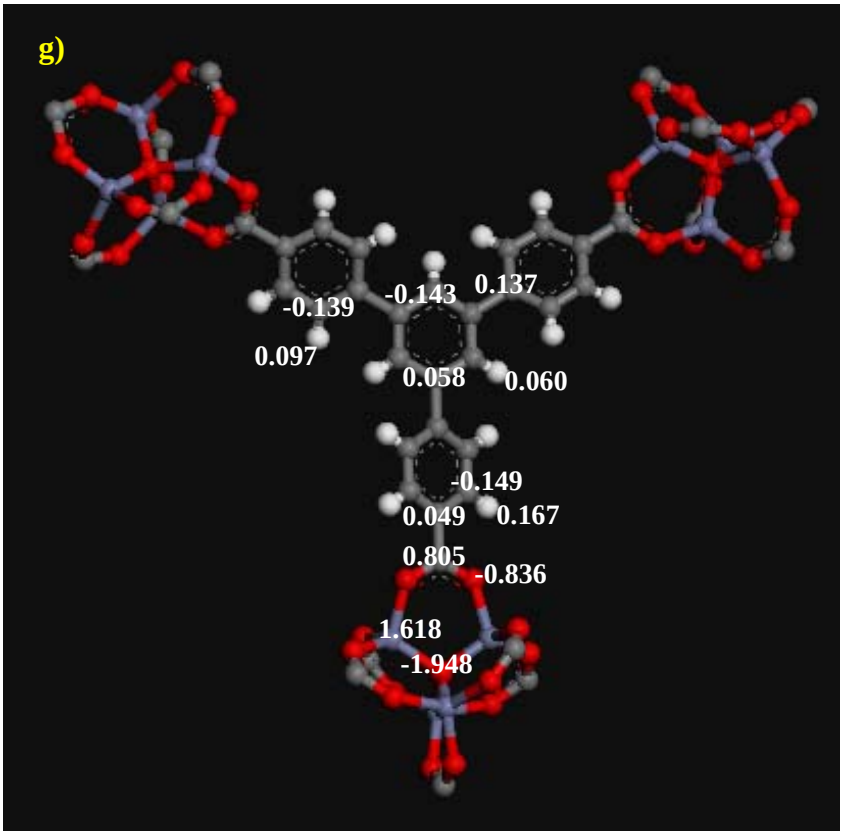
In this work, based on the ChelpG method, density functional theory (DFT) calculations combined with unrestricted B3LYP functional were carried out to calculate the atomic partial charges of the studied metal-organic frameworks (MOFs), using the structural models shown in Figure S2. To compensate better the termination effects, the terminations for the model cluster of Mn-MOF were saturated with lithium atoms as Sagara et al. (*J. Chem. Phys.*, 2004; 121: 12543-12547.), while methyl groups were employed for the model clusters of other MOFs. For these calculations, basis set LANL2DZ was used for atoms Zn, Cu and Mn, while 6-31+G* for the rest atoms. The calculations were carried out using GAUSSIAN 03 suite of programs (GAUSSIAN 03, 2003, Gaussian, Inc.), and all the calculated results are also shown in Figure S2 together with their corresponding structural models.

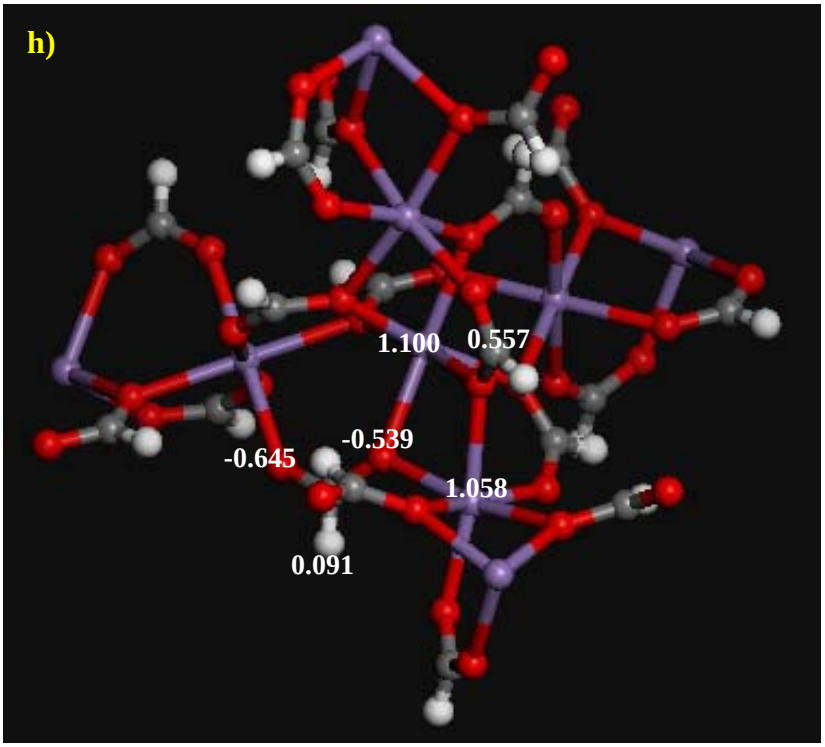



d)
0.004
0.127
-0.204
0.176
-0.307
0.187
0.114
0.805
-0.799
1.563
-1.950


e)
0.115
-0.155
0.101
0.032
0.104
-0.117
0.101
-0.064
-0.095
0.986
-0.917
1.760
-1.996


f)
0.107
0.027
0.045
-0.036
0.036
-0.166
-0.045
0.878
-0.799
1.576
-1.924


g)
-0.139
-0.143
0.137
0.097
0.058
0.060
-0.149
0.049
0.167
0.805
-0.836
1.618
-1.948



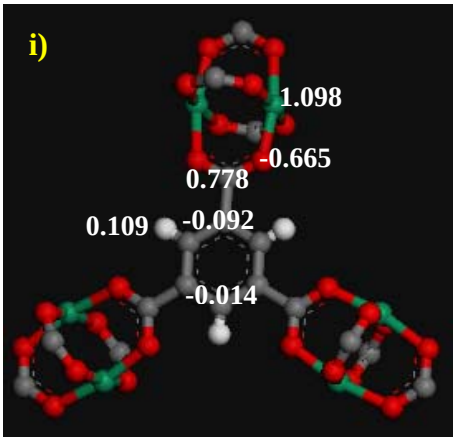


Figure S2. Model clusters of the studied MOFs used for the calculations of atomic partial charges. a) IRMOF-1. b) IRMOF-8. c) IRMOF-10. d) IRMOF-14. e) IRMOF-11. f) IRMOF-16. g) MOF-177. h) Mn-MOF. i) Cu-BTC (Zn, blue; Mn, purple; Cu, green; O, red; C, gray, and H, white).