

Supporting Information

Effect of Ligand Aromaticity on Cyclohexane and Benzene Sorption in IRMOFs: A Computational Study

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Table of contents

1. Model of benzene and cyclohexane	2
2. Equilibration for calculation of K_H and coadsorption	3
3. Estimation of adsorption enthalpy using Van 't Hoff plot.....	4
4. Density plot of IRMOF-10 and IRMOF-16.....	5
5. Selectivity curves of IRMOFs.....	6

1. Model of benzene and cyclohexane

Table S1: Bond lengths, angles and positions of pseudo-atoms for benzene and cyclohexane molecules.

Benzene				
C-C length: 1.392 Å				
C-H length: 1.08 Å				
C-C-C angle: 120°				
H-C-C angle: 120°				
# Pseudo-atom	Type	<i>x</i>	<i>y</i>	<i>z</i>
0	C_benz	0	0	0
1	C_benz	1.392	0	0
2	C_benz	2.088	1.20551	0
3	C_benz	1.392	2.41101	-0.0012
4	C_benz	0	2.41101	-0.00167
5	C_benz	-0.696	1.20551	-6.8061E-4
6	H_benz	-0.54	-0.93531	4.4182E-4
7	H_benz	1.932	-0.93531	0.00129
8	H_benz	3.168	1.20551	6.2273E-4
9	H_benz	1.932	3.34632	-0.00125
10	H_benz	-0.54	3.34632	-0.0026
11	H_benz	-1.776	1.20551	-8.5731E-4

Cyclohexane			
CH ₂ -CH ₂ length: 1.527 Å			
CH ₂ -CH ₂ -CH ₂ angle: 111°			
# Pseudo-atom	<i>x</i>	<i>y</i>	<i>z</i>
0	-1.3715	-0.4792	-0.2349
1	-0.2707	-1.4273	0.2349
2	1.1008	-0.9481	-0.2349
3	1.3715	0.4792	0.2349
4	0.2707	1.4273	-0.2349
5	-1.1008	0.9481	0.2349

2. Equilibration for calculation of K_H and coadsorption

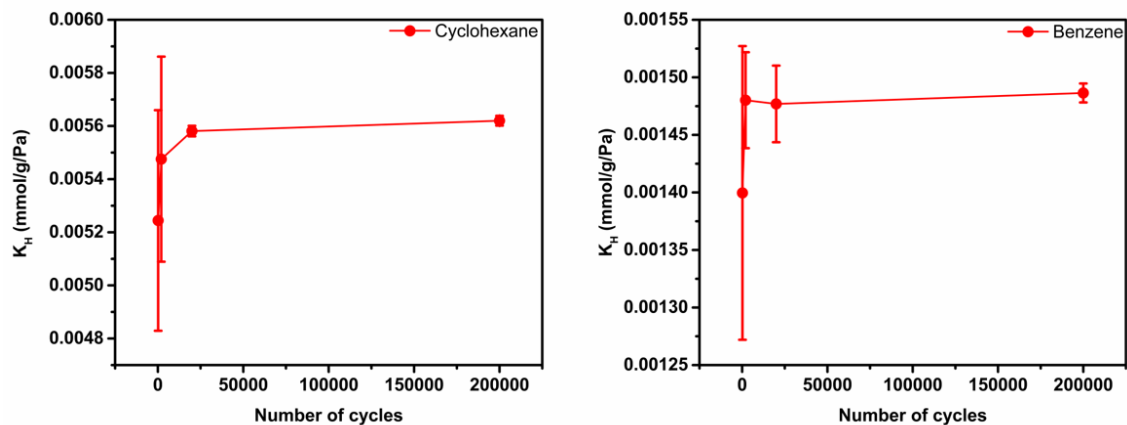


Figure S1: Values of Henry's constant and error bar after each range of GCMC cycles for IRMOF-1 in the presence of cyclohexane or benzene.

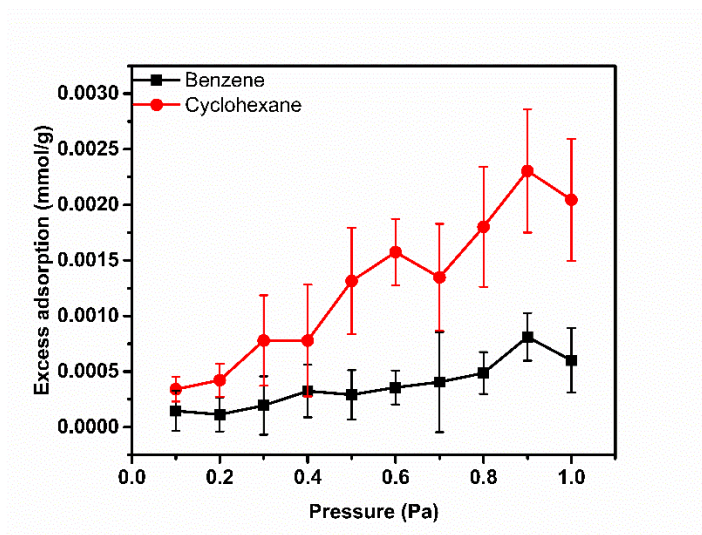


Figure S2: Coadsorption isotherms for IRMOF-1 using 10000 equilibrium cycles and 10000 production cycles.

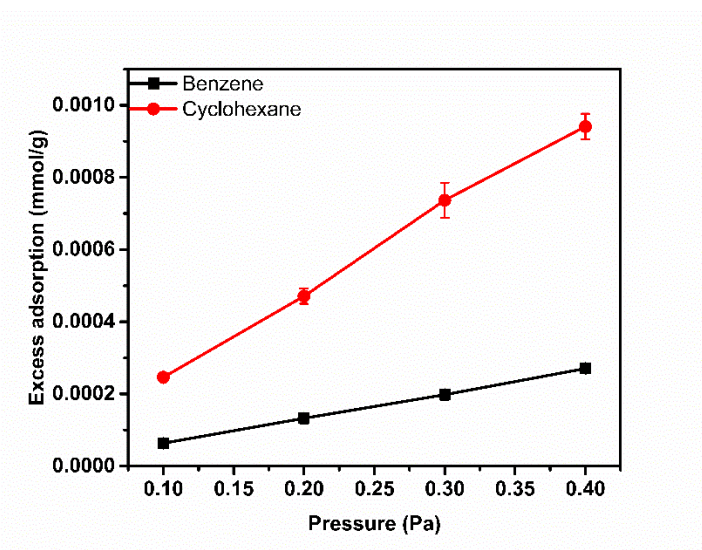


Figure S3: Coadsorption isotherms for IRMOF-1 using 10000 equilibrium cycles and 100000 production cycles.

3. Estimation of adsorption enthalpy using Van 't Hoff plot

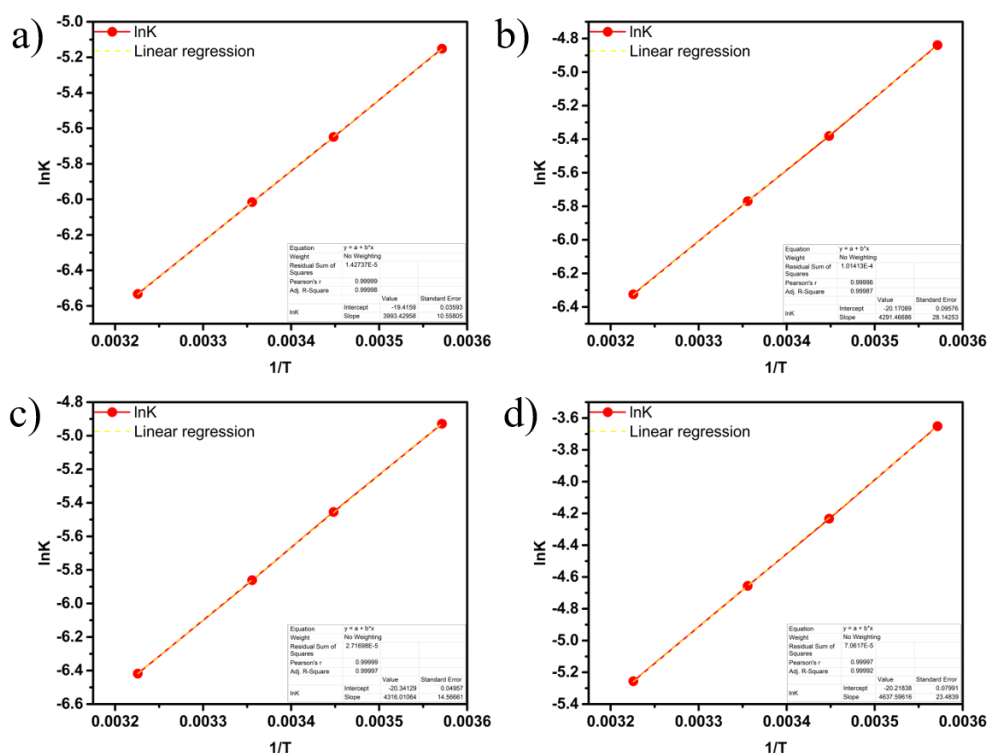


Figure S4: Estimation of enthalpy of adsorption for cyclohexane in the case of a) IRMOF-1, b) IRMOF-10; c) IRMOF-16 and d) IRMOF-14.

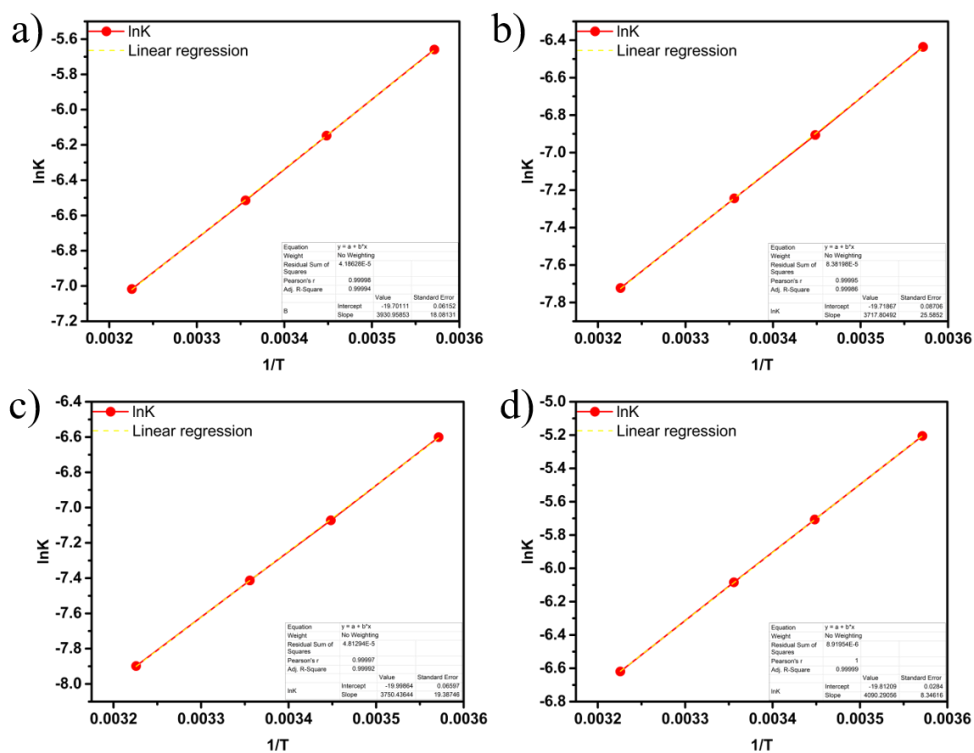


Figure S5: Estimation of enthalpy of adsorption for benzene in the case of a) IRMOF-1, b) IRMOF-10; c) IRMOF-16 and d) IRMOF-14.

4. Density plot of IRMOF-10 and IRMOF-16

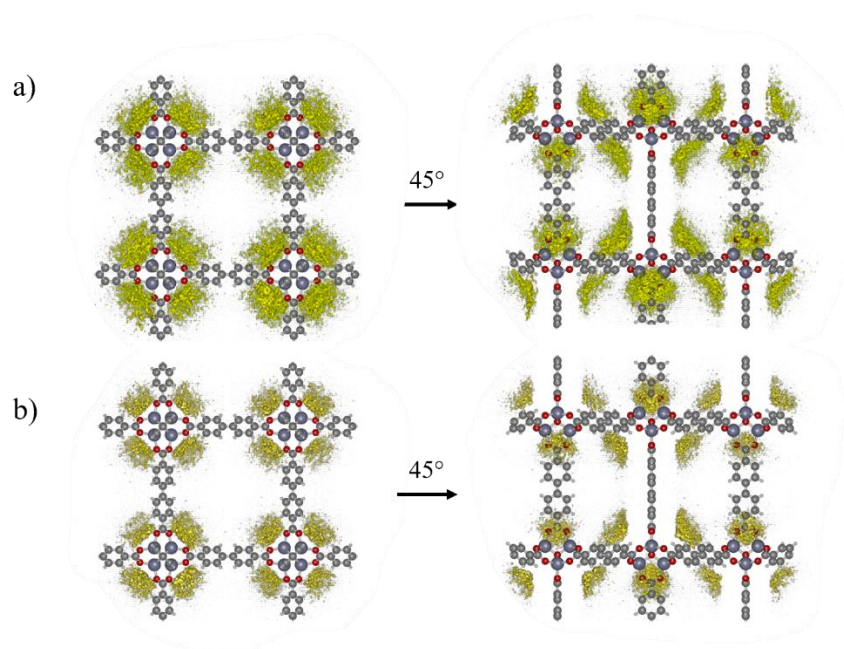


Figure S6: Density plots for a) benzene and b) cyclohexane in IRMOF-10 structure. Zinc: dark grey, carbon: light grey, oxygen: red and hydrogen: white.

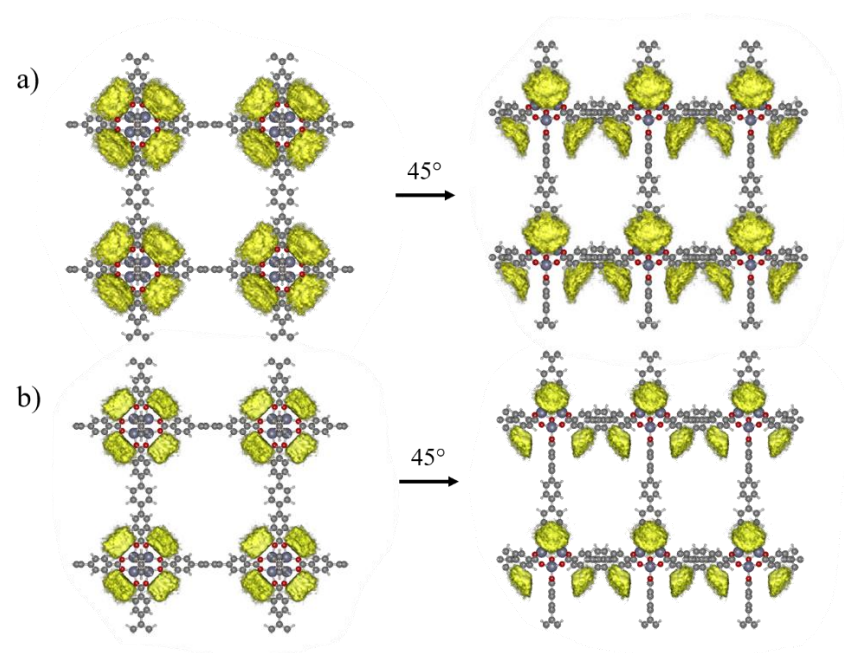


Figure S7: Density plots for a) benzene and b) cyclohexane in IRMOF-16 structure. Zinc: dark grey, carbon: light grey, oxygen: red and hydrogen: white.

5. Selectivity curves of IRMOFs

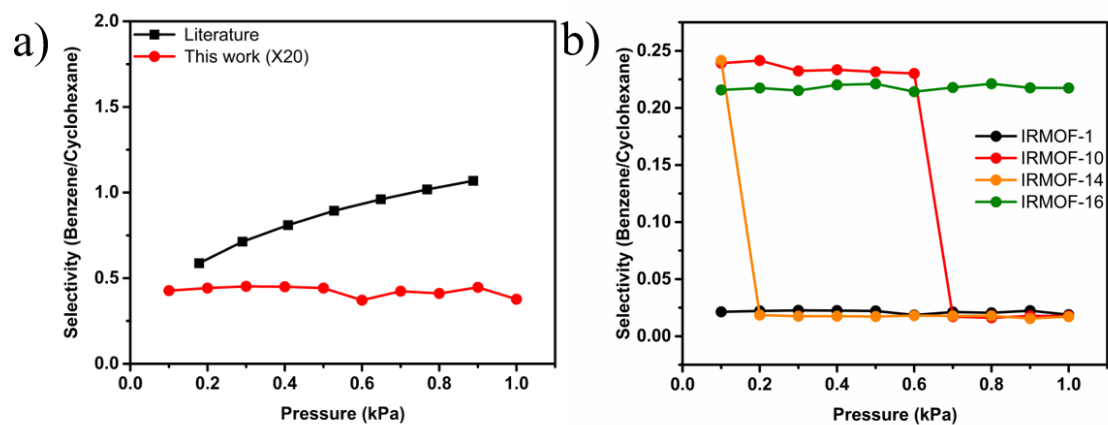


Figure S8: a) Selectivity curves of IRMOF-1 at 298K obtained by GCMC compared to an experimental curve reported in literature³². b) Comparison of theoretical selectivity curves at 298K of all IRMOF materials simulated in this work.