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MDPI

Supplementary materials

Table 1. Structure properties of the MCM-41 model.

Properties	MCM-41
Cell parameters(Å)	(89.021, 89.021, 37.057)
Lattice angle(°)	(90, 90, 120)
Cell volume(Å^3)	254325
Number of O atoms only connecting Si	5612
Number of O atoms connecting H	1042
Number of Si atoms	3070
No. of H atoms	1042
Wall thickness(Å)	11.51
T sites(/1000Å^3)	7.5
Skeleton density(g/cm^3)	2.2134
Porosity density(g/cm^3)	1.2648
Pore radius(Å)	33
Connolly surface(Å^2)	22459.73
Surface Area(m^2/g)	698.269
-OH groups(/nm^2)	4.64

Table 2. Lennard-Jones potential parameters and atomic charges.

Molecule	Site	σ(Å)	ε/kB(K)	*q*(e)
MCM-41	Si	3.804	155.858	1.24152
	O	3.033	48.115	-0.73843
	H	2.846	0.0503	0.41006
naphthalene phenanthrene pyrene	C	3.473	47.813	See figure 2
	H	2.846	0.05	

Table 3. Properties of naphthalene, phenanthrene and pyrene.

Properties	Naphthalene	Phenanthrene	Pyrene
Molecular formula	C_8H_{10}	$C_{14}H_{10}$	$C_{16}H_{10}$
Molar mass(g/mol)	128.174	178.233	202.255
Standard boiling point	217.989	340.3	394.8
Critical temperature(K)	475.25	596.1	662.85
Critical pressure(MPa)	0.0698	0.0723	0.093
Acentric factor(kJ/(kg·K))	0.302	0.499	0.5088
Dipole moment(D)	0	0	0

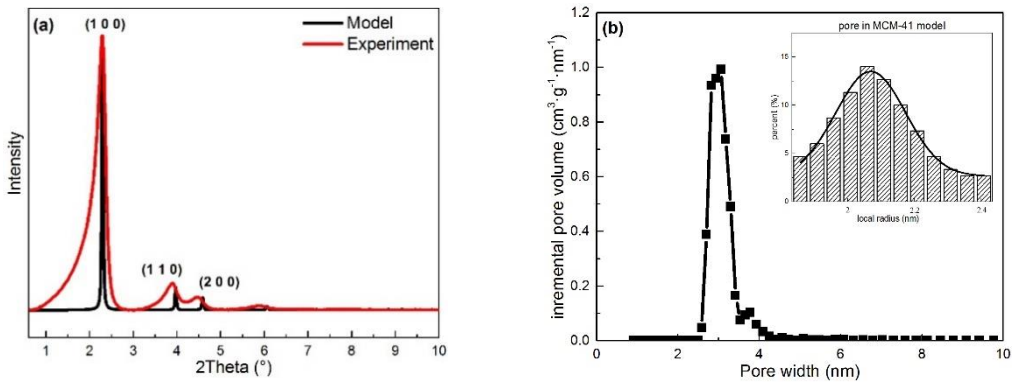

Figure 1. Characterization results of the MCM-41 model compared with experiments: (a) X-ray diffraction, (b) pore size distribution.