Supporting Information

Metal-Organic Frameworks Coated Photonic Crystals for High-Performance Thin Layer Chromatography

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1. FTIR spectra of calcinated SiO_2, SiO_2-OH, SiO_2-NH_2, and SiO_2-COOH particles.

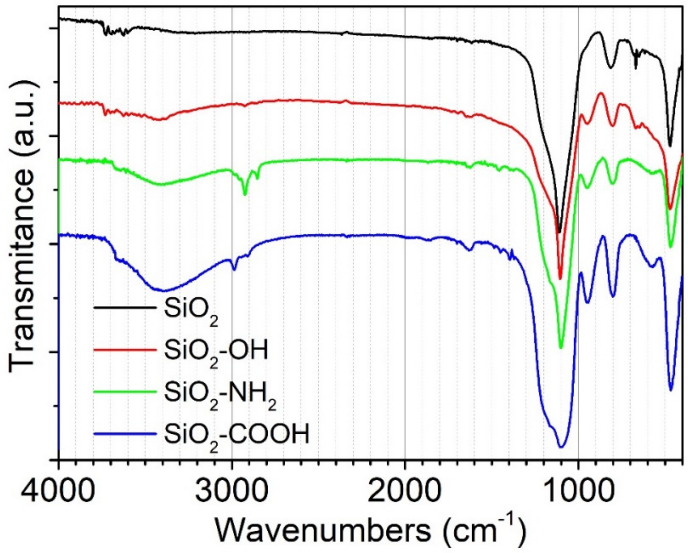

Figure S1. FTIR spectra of calcinated SiO_2, silanol recovered SiO_2, SiO_2-NH_2 and SiO_2-COOH particles. 1) For silanol recovered SiO_2 (red line), Si-OH stretching and bending vibration at 3400 cm^{-1} and 950 cm^{-1} demonstrated the recovery of silanol group. 2) For SiO_2-NH_2 particles (green line), N-H stretching vibration at 3400 cm^{-1}, C-H stretching at 2924 cm^{-1} and 2854 cm^{-1}, and C-N stretching at 1167 cm^{-1} proved the modification of NH_2 group. 3) For SiO_2-COOH particles (blue line), the C=O stretching vibration of amide at 1628 cm^{-1} and O-H bending of carboxylic acid at 1402 cm^{-1} proved the modification of COOH group.

2. Digital photos of SiO_2 PC, HKUST-1/PC, MIL-100/PC, and ZIF-8/PC films.

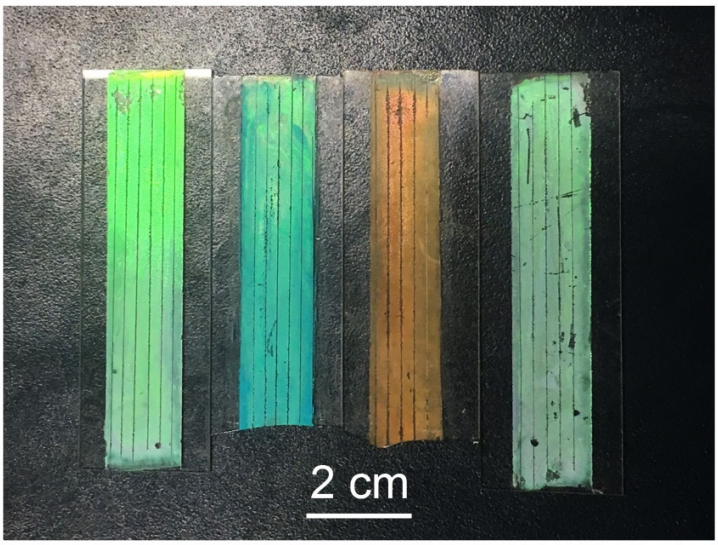

Figure S2. Digital photos (from left to right) of SiO_2 PC, HKUST-1/PC, MIL-100/PC, and ZIF-8/PC films. The natural colors of HKUST-1, MIL-100, and ZIF-8 are blue, yellowish-brown, and white.

3. Transmission spectra of SiO_2 PC, HKUST-1/PC, MIL-100/PC, and ZIF-8/PC films.

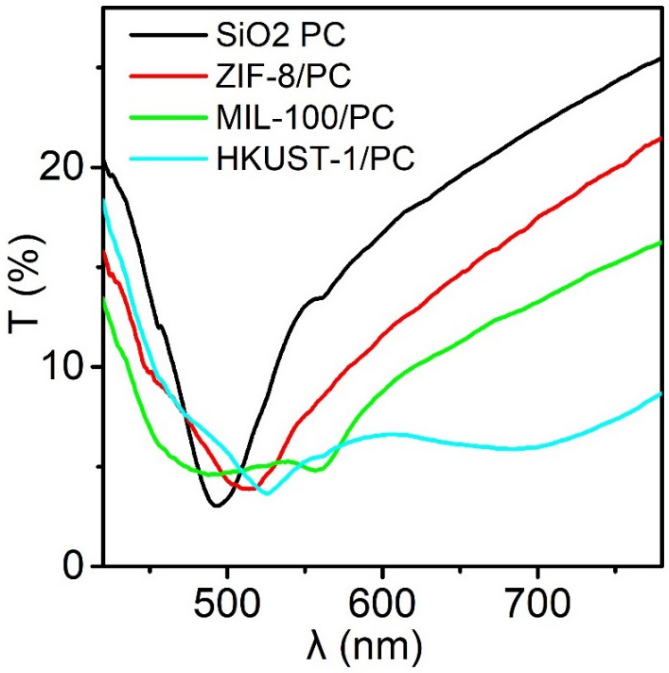

Figure S3. Transmission spectra of SiO_2 PC, HKUST-1/PC, MIL-100/PC, and ZIF-8/PC films.

4. Separation of cresol isomers by commercial gas chromatography.

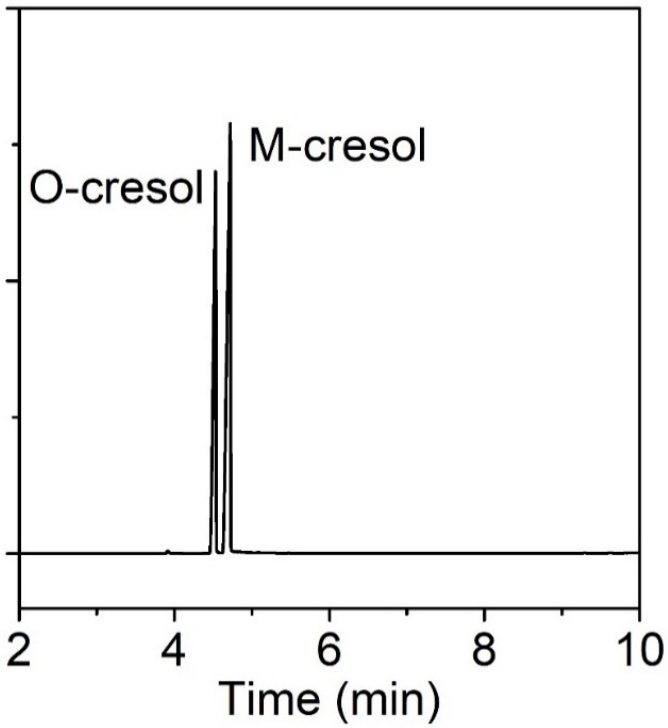

Figure S4. Separation of cresol isomers by commercial gas chromatography (GC) using methanol as the mobile phase and HP-5MS silica gel column as the stationary phase.

5. SRRS of clean MOF/PC film and o-cresol loaded MOF/PC film

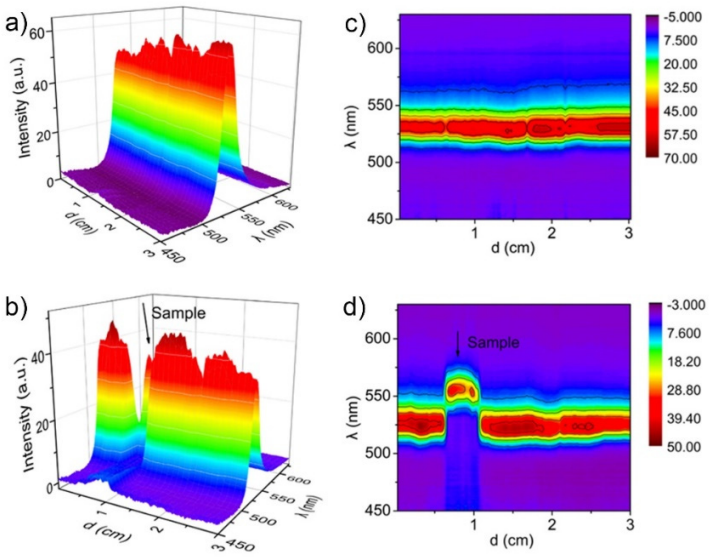

Figure S5. Spatially resolved reflection spectra (SRRS) are collected along the direction of development on a clean MOF/PC film and an o-cresol loaded MOF/PC film, which are further converted to (a, b) 3D surface maps and (c, d) contour maps.

6. Separation of o-cresol and m-cresol on MIL-100/PC plates in 3 repeated tests.

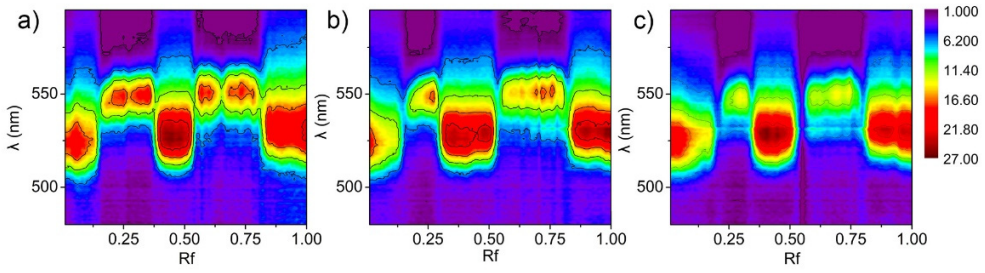

Figure S6. Spatial resolved 3D reflection spectra for the separation of o-cresol and m-cresol on a-c) three MIL-100/PC plates.

7. Stability and durability of MOF/PC plates.

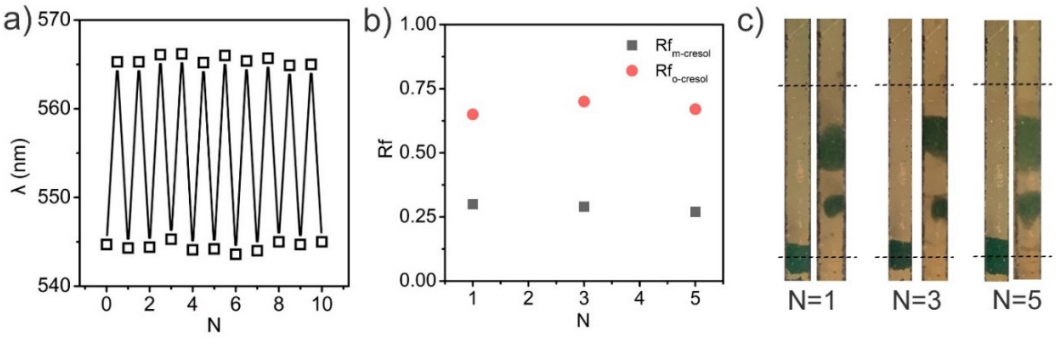

Figure S7. a) Periodic change of reflection wavelength of MIL-100/PC as m-cresol was repeatedly loaded and eluted. b) The retention factors of cresol isomers in c) the 1st, 3rd, and 5th separation on the same MIL-100/PC plate.

8. Development of cresols on MIL-100/PC plate with different cycles of MOF depositions.

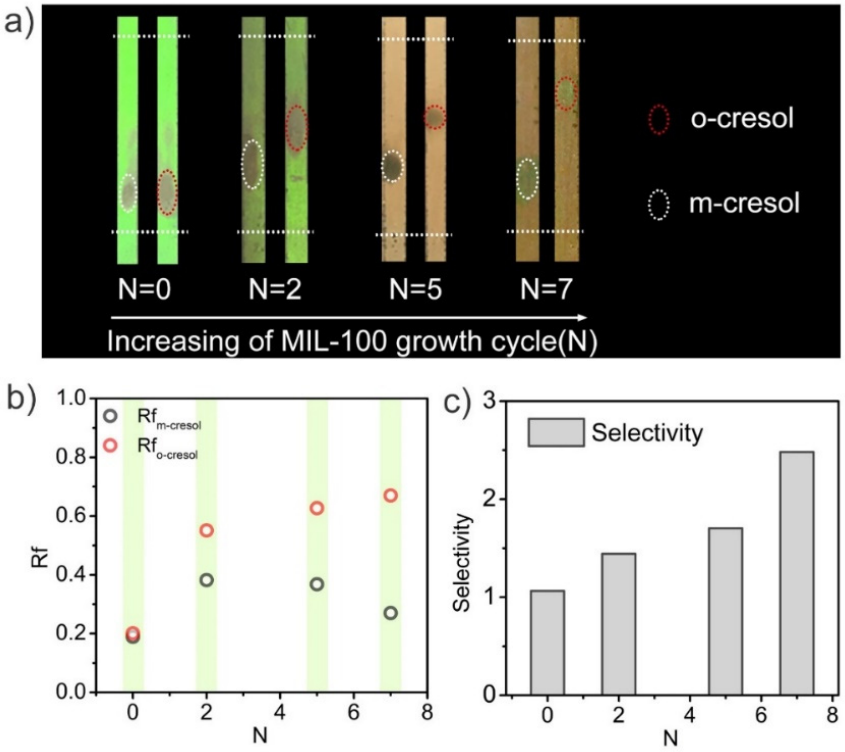

Figure S8. a) Development of o-cresol and m-cresol on MIL-100/PC plate prepared by 0, 2, 5, and 7 cycles of depositions in LBL growth. Comparison of b) R_f and c) selectivity of cresol isomers in the above developments.

9. Separation of chlorophenols, benzenediol isomers on MIL-100/PC TLC plate.

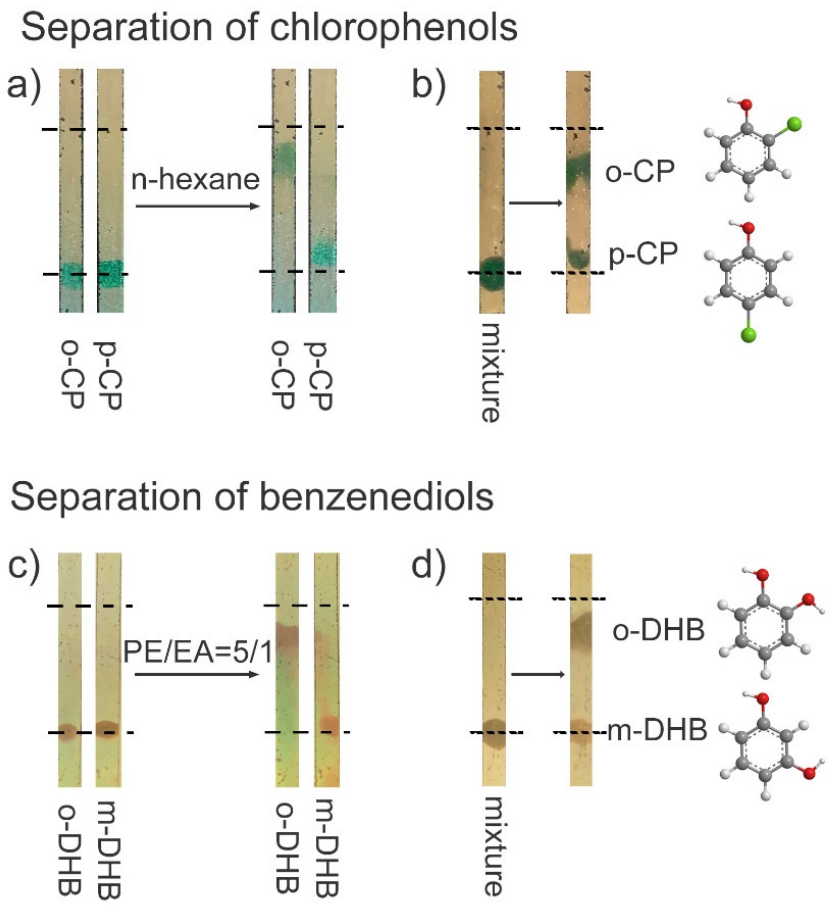

Figure S9. Development of a) 2-chlorophenol (o-CP) and 4-chlorophenol (p-CP) on MIL-100/PC by hexane and b) separation of their mixtures under same conditions. Development of c) 1,2-dihydroxybenzene (o-DHB) and 1,3-dihydroxybenzene (m-DHB) on MIL-100/PC by the mixing solvent of petroleum ether and ethyl acetate (5:1) and d) separation of their mixtures.

10. Comparison of chromatographic parameters of MOF/PC TLC, TLC and GC

Table S1. Retention factor (Rf_m, Rf_o), theoretical plate number (N_m, N_o), selectivity factors (α) and resolution (R) for m-cresol and o-cresol, which are separated by HKUST-1, ZIF-8 and MIL-100 coated PC films, commercial silica gel TLC plate and commercial silica GC column (HP-5MS).

Method	Materials	Rf_m	Rf_o	w_m	w_o	N_m	N_o	α	R
PC TLC	HKUST-1	0.367	0.535	0.241	0.263	37.1	66.2	1.46	0.67
PC TLC	ZIF-8	0.402	0.533	0.251	0.199	41.0	114.8	1.33	0.58
PC TLC	MIL-100	0.267	0.67	0.148	0.263	52.1	103.8	2.51	1.96
TLC	SiO_2	0.67	0.746	0.217	0.238	152.1	157.2	1.11	0.33
GC	SiO_2	4.529†	4.733†	0.132	0.133	18835	20262	1.05	1.54

† Retention time (min) was taken for the calculation of selectivity and resolution for the case of GC.

11. Calculation of plate number (N), selectivity factor (α), and resolution (R)

In thin layer chromatography (TLC), the retention factor (R_f) is defined as the ratio of distance travelled by an individual chemical to the distance travelled by the developing reagent. In gas chromatography (GC), the retention time (t_R) is defined as the time required for an individual chemical to migrate through the column. Both of them are used to quantify the migration of chemicals on the stationary phase.

Theoretical plate number (N) is an index which describes the number of plates as defined by the plate theory, where the stationary phase is considered to be made up of a number of segments or

plates. For TLC, the theoretical plate number can be calculated by Equation (1), where L_s is the distance travelled by the sample on the TLC plate, and w_s is the width of the sample spot. For GC, the theoretical plate number can be calculated by Equation (2), where t_R is the retention time of the sample and w_s is its peak width in GC spectrum.

$$N = 16 \times \left(\frac{L_s}{w_s}\right)^2 \quad (1)$$

$$N = 16 \times \left(\frac{t_R}{w_s}\right)^2 \quad (2)$$

Selectivity factor (α) is usually defined as the ratio of the retention factors for two samples in the chromatogram. For TLC, the selectivity factor can be calculated by Equation (3), where R_{fm} and R_{fo} are the retention factors for m-cresol and o-cresol. For GC, the selectivity factor can be calculated by Equation (4), where t_{Rm} and t_{Ro} are the retention times for m-cresol and o-cresol.

$$\alpha = \frac{R_{fo}}{R_{fm}} \quad (3)$$

$$\alpha = \frac{t_{Ro}}{t_{Rm}} \quad (4)$$

Resolution (R) in chromatography is usually defined as the capability to separate two components, and it is a comprehensive factor to evaluate the performance of chromatography. In TLC, it is calculated by Equation (5), where L_m and L_o are the distances travelled by m-cresol and o-cresol on the TLC plate, and w_m and w_o are the sample spots widths of m-cresol and o-cresol respectively. For GC, the resolution is calculated by Equation (6), where t_{Rm} and t_{Ro} are the retention times for m-cresol and o-cresol, and w_m and w_o are the peak widths.

$$R = \frac{2(L_o - L_m)}{w_m + w_o} \quad (5)$$

$$R = \frac{2(t_{Ro} - t_{Rm})}{w_m + w_o} \quad (6)$$

For both TLC and GC, the resolution can be calculated by Equation (7) according to its relationship with peak/spot width, selectivity, and plate numbers. It can be concluded that the resolution increases along with the increasing of selectivity and plate numbers, when the peak/spot widths of m-cresol and o-cresol are close to each other.

$$R = \frac{2w_m}{w_m + w_o} \times (\alpha - 1) \times \frac{\sqrt{N_m}}{4} \quad (7)$$