

Supporting Information for

Temperature Responsive Channel Uniformity Impacts on Highly Guest-Selective Adsorption in a Porous Coordination Polymer

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Methods;

Dubinin- Radushkevich Equation

Dubinin-Radushkevich (DR) equation^[1] was widely used to express the adsorption isotherms in micropores. The DR equation is given by

$$W/W_0 = \exp \{ - (A / \beta E_0)^2 \}$$

where W and W_0 are the amount of adsorption at a relative pressure (P/P_0) and the saturated amount of adsorption, respectively, E_0 is a characteristic adsorption energy, and the parameter A is Polanyi's adsorption potential, defined as $A = RT \ln(P_0/P)$. The parameter β is the affinity coefficient, and is related to the adsorbate-adsorbent interaction.

Figure legends

Figure S1. Size, physical and physico-chemical properties of argon and oxygen.

Figure S2. In situ synchrotron XRPD patterns of dehydrated (black line) and hydrous (red line) CPLs at 300 K and the value of FWHM of the 020 peak for CPLs. XRPD patterns of CPL-1, -2 and -11 are **(A)**, **(B)** and **(C)**, respectively.

Figure S3. The variation of the values of FWHM for 020 peaks in the XRPD pattern of CPLs at 300 K. The values from hydrous and dehydrated CPL are shown by blue and red bar, respectively.

Fig. S1

Fig. S1

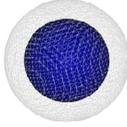
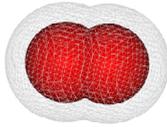
	Argon	Oxygen
		
Kinetic Diameter	3.40 Å	3.46 Å
Pauling Length	3.84 Å	3.9 Å
Pauling Width	3.84 Å	2.8 Å
Critical Temperature	150.687 K	154.581 K
Normal Boiling Point	87.302 K	90.1878 K

Fig. S2

Fig. S2

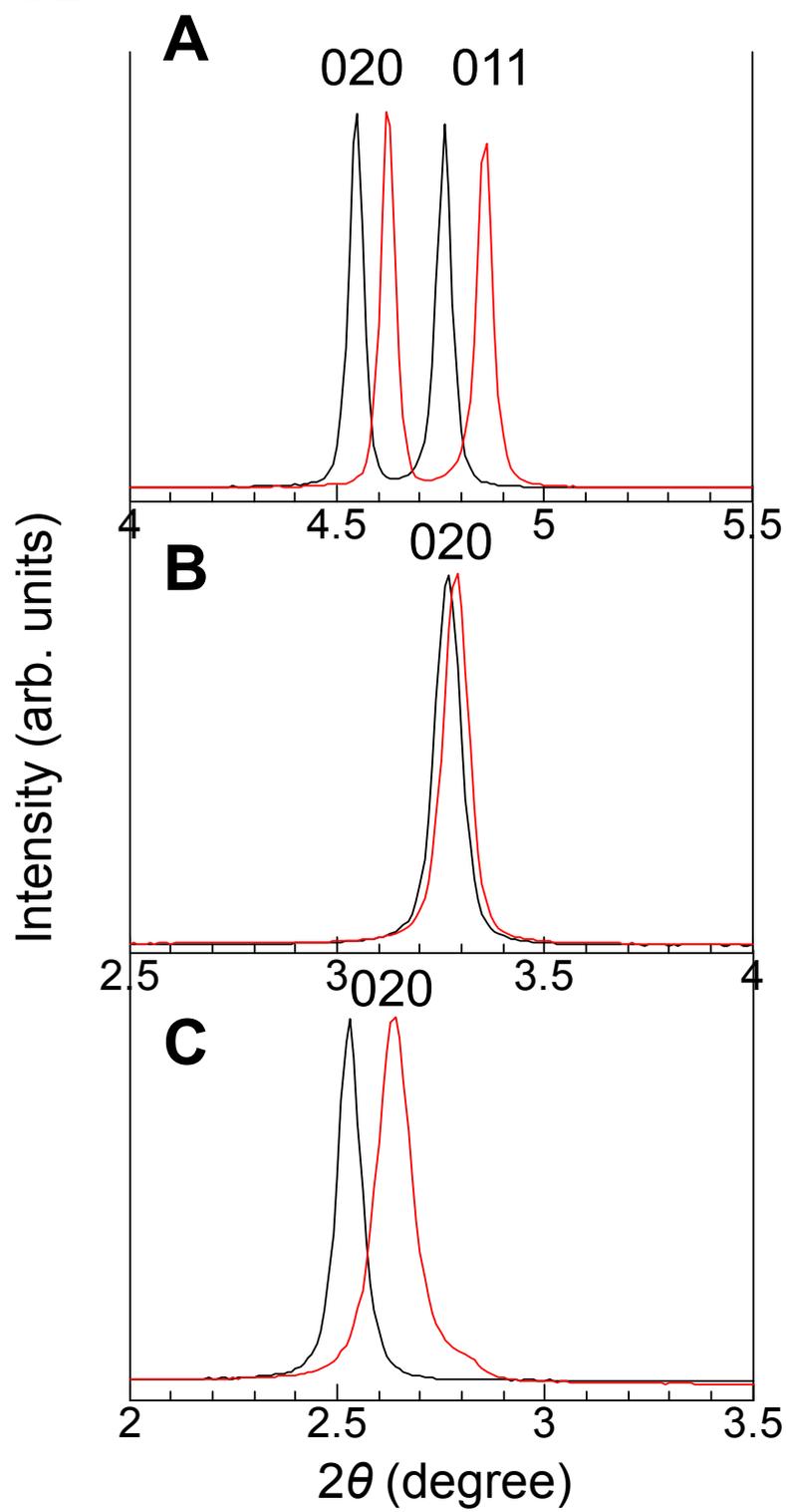


Fig. S3

Fig. S3

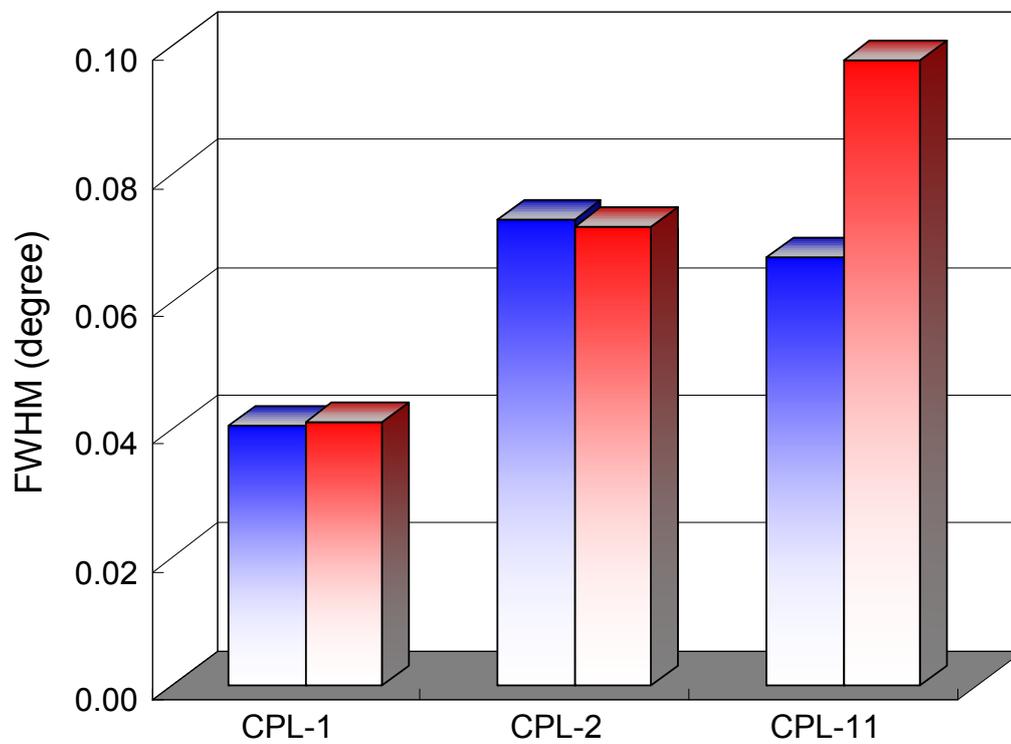


Table S1 Crystallographic data and Rietveld refinement summary for CPL-11 without guest molecule at 300 K.

CPL-11	
Formula	C ₁₂ H ₆ CuN ₅ O ₄
Formula Weight	347.75
Crystal System	monoclinic
Space Group	<i>P</i> 2 ₁ / <i>c</i> (#14)
<i>a</i> (Å)	4.6507 (15)
<i>b</i> (Å)	34.683 (4)
<i>c</i> (Å)	10.8118 (11)
β (degree)	95.80 (2)
<i>V</i> (Å ³)	1735.0 (6)
<i>Z</i>	4
Diffractometer	Debye-Scherrer
Radiation (Å)	0.80101
2 θ range	2.0 ° < 2 θ < 30.00 °
Temperature (K)	300
R_1 ^[a]	0.0362
R_{wp} ^[b]	0.0436

^[a] $R_{wp} = [\sum w|y_o - y_c|^2 / \sum w y_o^2]^{1/2}$, ^[b] $R_1 = \sum |I_o - I_c| / \sum I_o$.