Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Electronic Supplementary Information

Real-Time Colorimetric Water Content Monitoring of Organic Solvents by an Azo Dye Incorporated into $AlPO_4$-5 Nanochannel

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SI.1 N_2 isotherm of ground $AlPO_4$-5

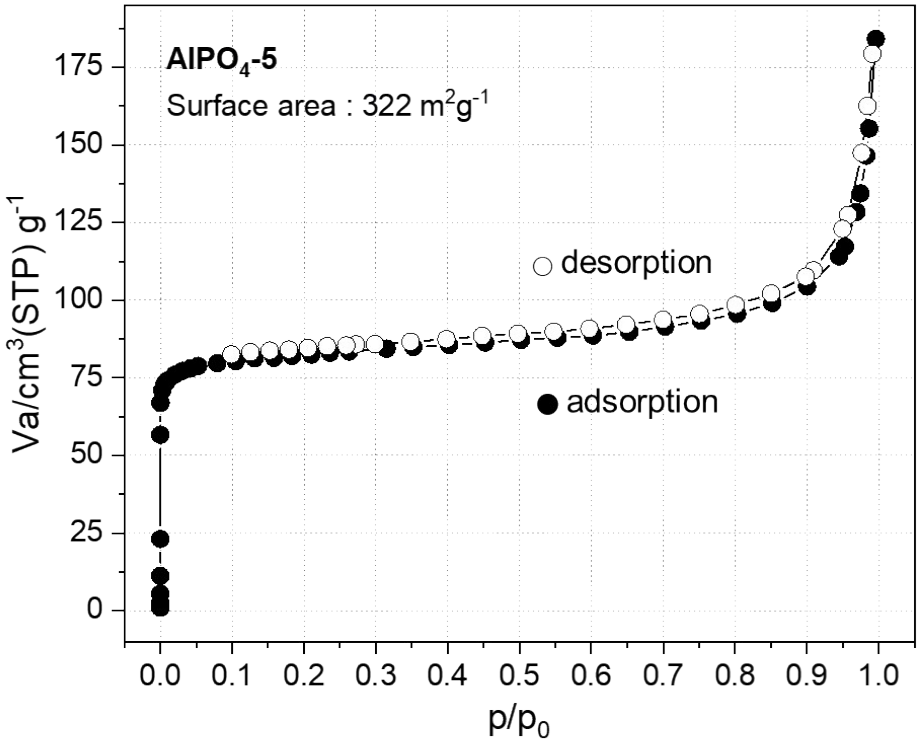


Fig. S1 N_2 isotherm of ground $AlPO_4$-5 from BET as indicated.

SI. 2 The water vapor adsorption isotherm of $AlPO_4$-5 and AZO@$AlPO_4$-5

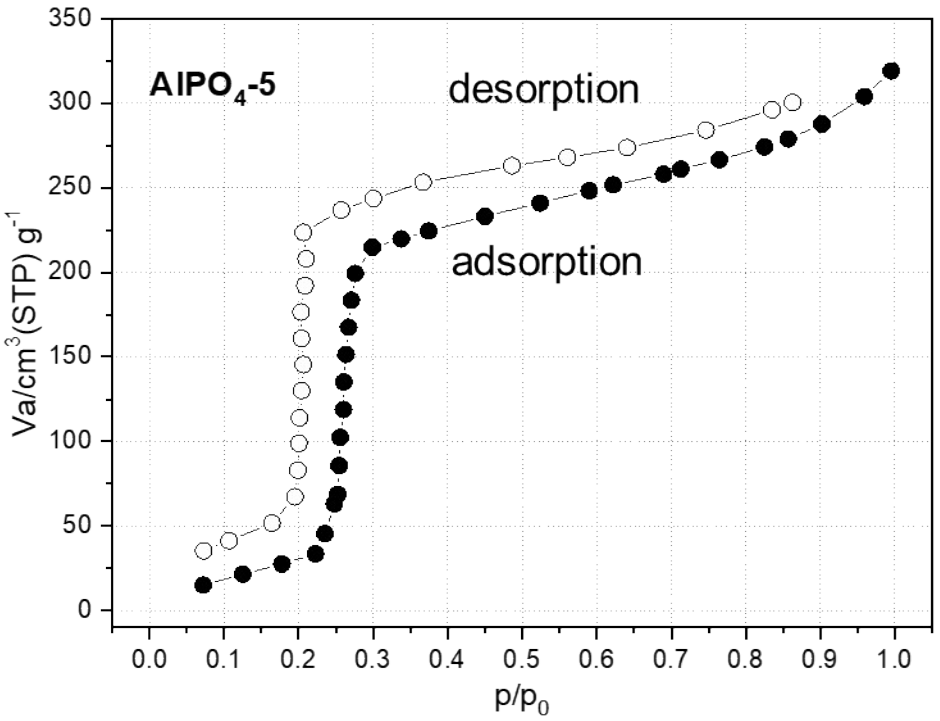


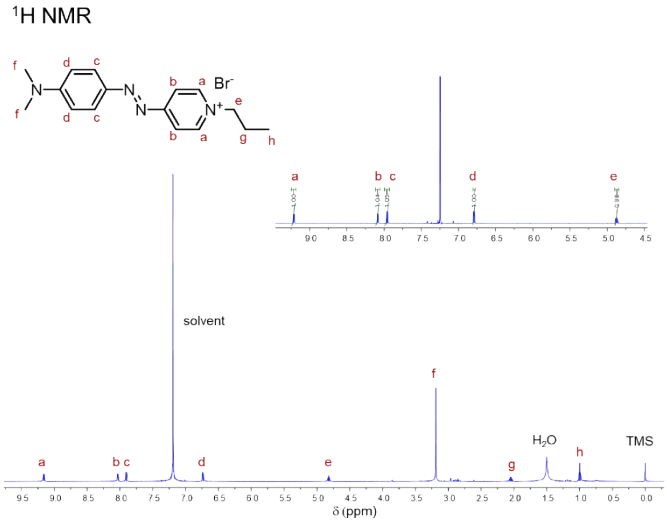
Fig. S2 The water vapor adsorption isotherm of $AlPO_4$-5.

SI. 3 Characterization of synthesized AZO dye.

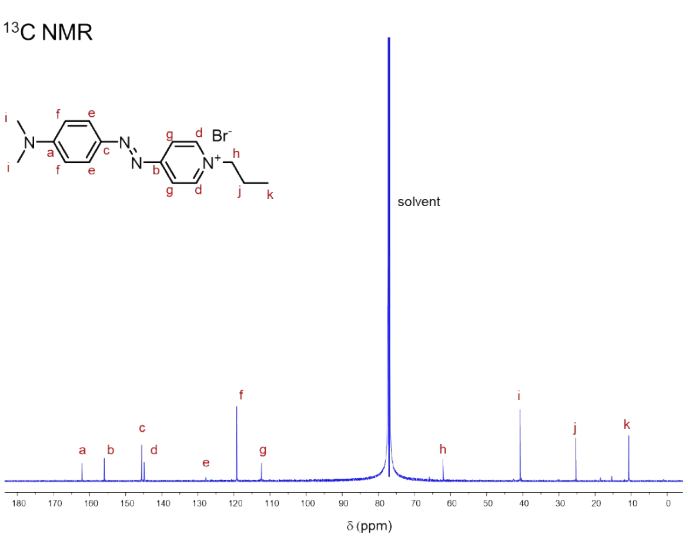
Table S1. Results of ^{1}H NMR, ^{13}C NMR and HR-MS

^{1}H NMR ($CDCl_3$) Chemical shift, δ/ppm, J/Hz	^{13}C NMR ($CDCl_3$) Chemical shift, δ/ppm	MS-ESI-TOF (m/z) $C_{16}H_{21}N_4$
δ_H (600 MHz) 9.16 (2 H, d, *J* 7.1), 8.03 (2 H, d, *J* 7.0), 7.90 (2 H, d, *J* 9.4), 6.74 (2 H, d, *J* 9.4), 4.82 (2 H, s), 3.19 (6 H, s), 2.04 (2 H, m), 1.00 (3 H, t, *J* 7.4).	δ_C (151 MHz) 162.07, 155.95, 145.58, 144.87, 127.76, 119.26, 112.37, 62.06, 40.58, 25.32, 10.68	Calculated: 269.1761 Found:269.1758

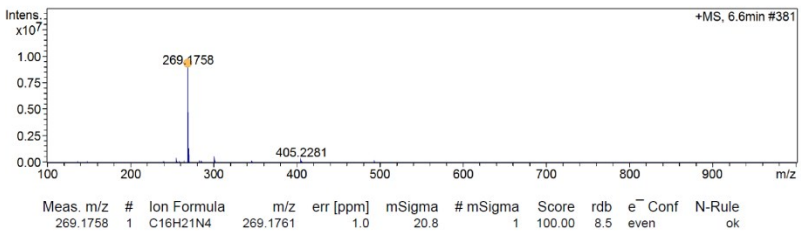
(a)



(b)



(c)



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
269.1758	1	C16H21N4	269.1761	1.0	20.8	1	100.00	8.5	even	ok

Fig. S3 The spectra of (a) ^{1}H NMR (b) ^{13}C NMR and (c) HR-MS as indicated.

SI. 4 Inclusion of the AZO dye into $AlPO_4$-5 nanochannel in methanol

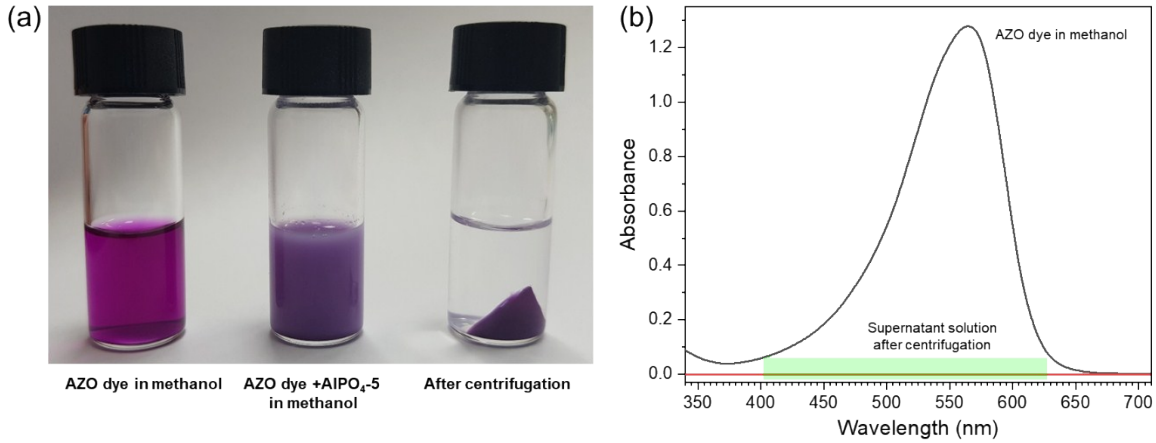


Fig. S4 (a) Digital photographic images (before, after incorporation of the AZO dye and after centrifugation) and (b) UV-vis spectra of the supernatant solution that depicts the process of the complete incorporation of the AZO dye into $AlPO_4$-5.

SI. 5 The calculation of concentration for AZO dye encapsulated in $AlPO_4$-5

Chemical composition of $AlPO_4$-5's unit cell:

Molecular weight of $AlPO_4$-5's unit cell:

(1) The # mole of unit cell in $AlPO_4$-5 (1.00g)

→ 1.00 / (molecular weight of unit cell)

→ **6.83×10^{-4} mole**

(2) We have confirmed that AZO dye in methanol solution (10 mL, 0.23 mM) completely incorporated into $AlPO_4$-5 (1.00 g) using UV-vis spectroscopy analysis. The total # mole of AZO dye incorporated into $AlPO_4$-5 (1.00g)

→ **2.30×10^{-6} mole**

(3) The number of AZO dye in a $AlPO_4$-5's unit cell

→ [value from (2)] / [value from (1)]

→ **3.37×10^{-3}**

(4) The volume of $AlPO_4$-5's unit cell

→ 1420.6 $Å^3$

→ 1.4206×10^{-27} m^3

→ **1.4206×10^{-24} L**

(5) The concentration of AZO dye encapsulated in $AlPO_4$-5

→ [value from (3) / (# of Avogadro)] / [value from (4)]

→ 3.94×10^{-3} mole·L^{-1}

→ **3.94 mM**

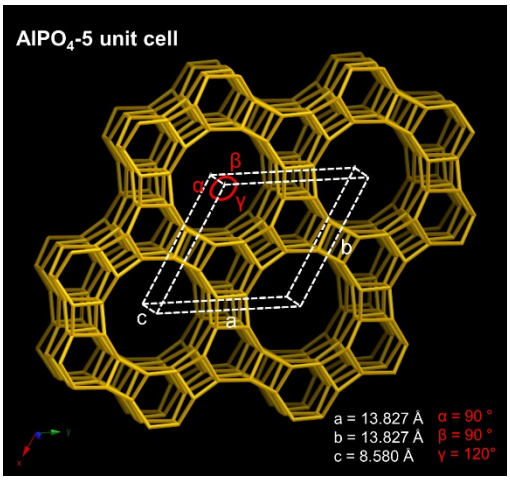


Fig. S5 The description for $AlPO_4$-5 unit cell

SI. 6 The relationship between relativity polarity and sensitivity of for AZO@$AlPO_4$-5 in primary alcohol.

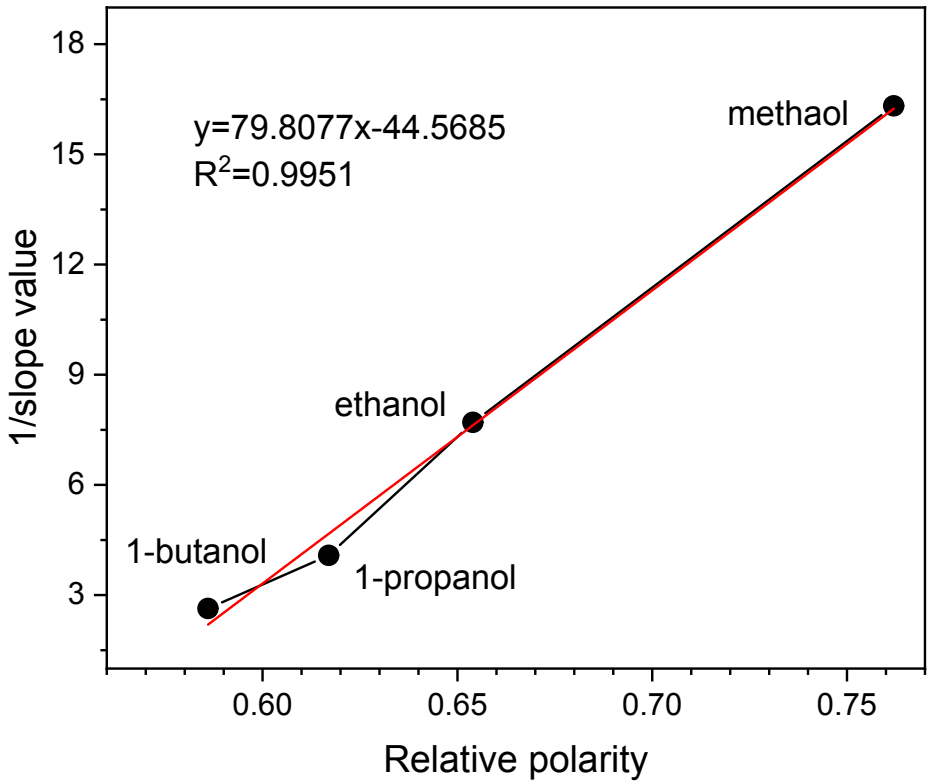


Fig. S6 The plot for relationship between relativity polarity and sensitivity of AZO@$AlPO_4$-5 in linear primary alcohol.

SI. 7 The effect of dye loading on water detection sensitivity

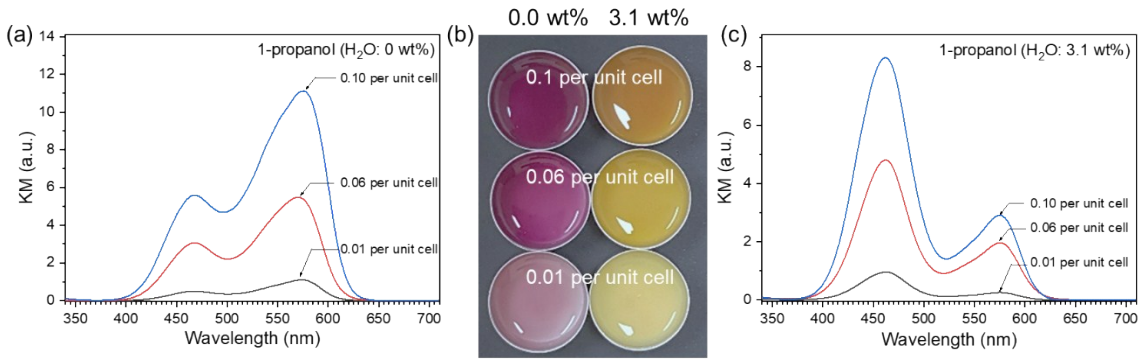


Fig. S7 UV-vis absorption (Kubelka-Munk, K/M) spectra of different AZO dye loaded $AlPO_4$-5 (0.01,0.06 and 0.1 per unit cell) in (a) ethanol sample (0.0 wt% H_2O), (c) ethanol sample (3.1 wt % H_2O) and (b) digital photographic images as indicated.

SI. 8 Evolution performance of recovered AZO@$AlPO_4$-5

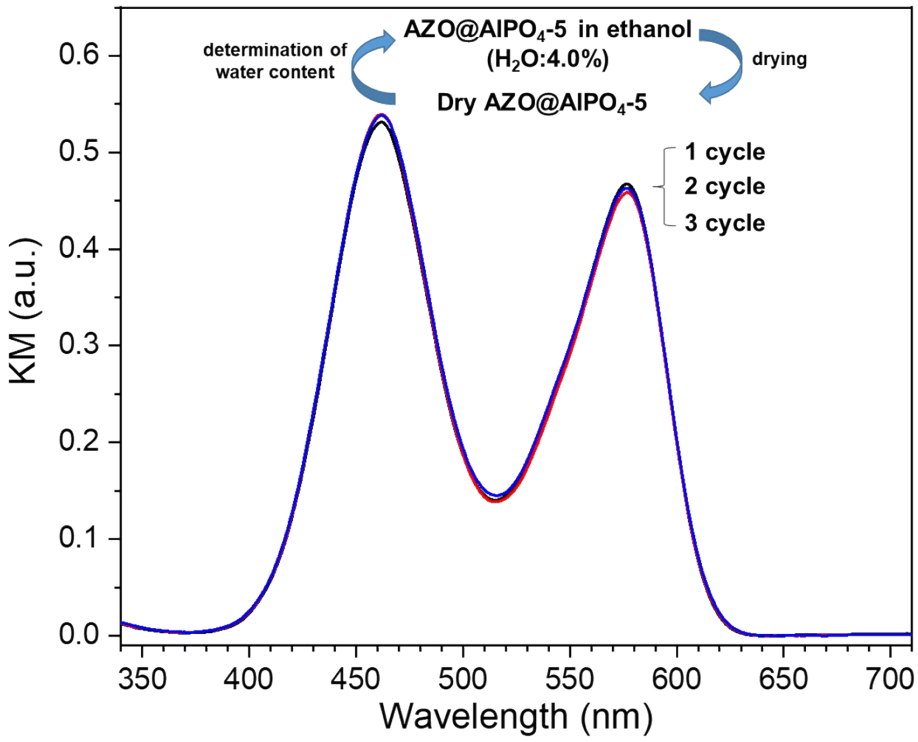


Fig. S8. UV-vis absorption spectra of fresh and recovered AZO@$AlPO_4$-5 dispersed ethanol sample (4.0 wt % H_2O).