Support Information

Single-layer Membranes for Organic Solvent Nanofiltration：A Molecular Dynamics Simulation Study and Comparative Experimental

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Table S1. Force field parameters of MoS_2[1-3]

Atom	charge	σ/Å	ε/(kJ mol^{-1})
Mo	0.76	4.43	0.485
S	0.38	3.34	2.085

bonds	r_0/Å	k_r/(kJ mol^{-1} Å^{-2})
Mo−S	2.41	430.3

angles	θ_0/deg	k_θ/(kJ mol^{-1} rad^{-2})
S−Mo−S	83.8	1187.7
Mo−S−Mo	83.8	2050.0

Table S2. Solvents and solute.

Solvent	Mw (g / mol)	Density (kg / L)	diameter $d_{kinetic}$ (Å)[4,5]	Viscosity μ (MPa · s)	Hansen Solubility parameter δ (MPa$^{1/2}$)[3]
Acetonitrile	41.05	0.757	3.4	0.32[5,6]	24.6
Methanol	32.04	0.778	3.8	0.49[4,7]	29.7
Hexane	86.18	0.653	4.3	0.29[6]	14.9
Ethanol	46.07	0.794	4.5	1.17[4,7]	26.6
Acetone	58.08	0.797	4.7	0.29[7]	20.1
Propanol	60.10	0.80	6.3	2.27[7,8]	23.4

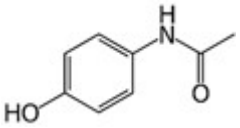
acetaminophen		
Formula	*M*w (g/mol)	Structure
C8H9NO2	151.16	

Figure. S1 Pore size distribution of MoS_2 nanosheets in experiment

In this study, the pore size distribution of MoS_2 nano sheets prepared by hydrothermal method was tested and analyzed by autosorb IQ N_2 adsorption desorption instrument (Beijing jinepu Technology Co. Ltd.). The measured aperture range is full hole. Prepare the sample in situ at about 80.9h under the condition of MoS_2, and put it into the nano tube for degassing.

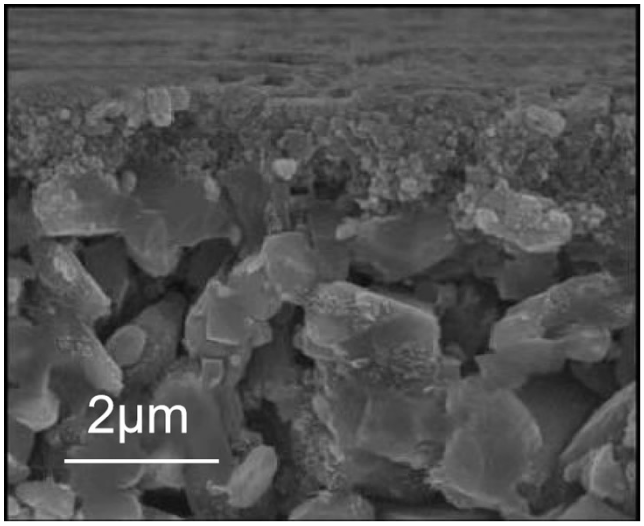


Fig. S2 SEM of the cross-sectional of MoS_2 membranes

(Preparation conditions: reaction temperature, 220℃; reaction time, 30h)

Scanning electron microscopy (SEM) was used to characterize the cross-sectional micro morphology of MoS2 tubular ceramic film. The results are shown in Figure S3. It can be seen from the figure that the thickness of MoS2 thin layer is about 200nm,

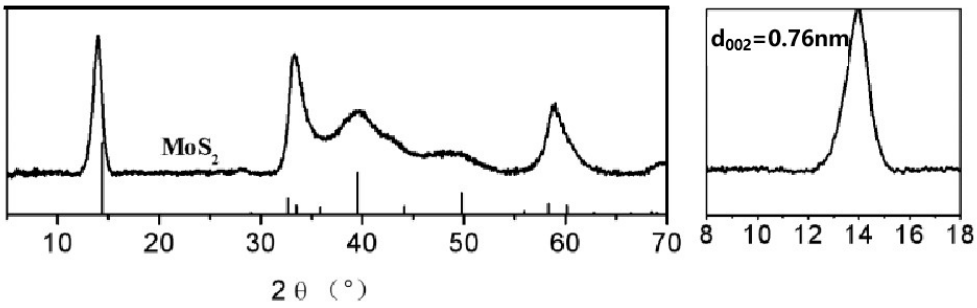


Fig. S3 XRD characterization of MoS_2 nanosheets (reaction time 30 h; reaction temperature 220 ℃)

It can be seen from figure S3 that during hydrothermal reaction, the hydrothermal products are θ MoS_2 characteristic peaks appeared at about 14 °, 32 °, 39 ° and 58 °, indicating that MoS2 nanosheets were prepared in hydrothermal solvent. According to the Bragg equation, the spacing of MoS_2 nano flakes is 0.76 nm. The thickness of each molybdenum disulfide molecular layer is about 0.626 nm. Therefore, the layer spacing of MoS_2 is 1.4nm

Table S3. force field parameters of solvents

			charge	sigma	epsilon
Methanol	C	opls_157	+0.145	0.350	0.276
	H	Opls_140	+0.040	0.250	0.126
		Opls_155	+0.418	0.000	0.000
	O	Opls_154	-0.683	0.312	0.711
Ethanol	C	Opls_157	+0.145	0.35	0.276
		Opls_135	-0.180	0.350	0.276
	H	Opls_155	+0.418	0.00	0.000
		Opls_140	+0.040	0.25	0.126
	O	Opls_154	-0.683	0.312	0.711
Propanol	C	Opls_157	+0.145	0.350	0.276
		Opls_136	-0.120	0.3500	0.276
		Opls_135	-0.180	0.3500	0.276
	H	Opls_155	+0.418	0.000	0.000
		Opls_140	+0.040	0.250	0.126
	O	Opls_154	-0.683	0.3120	0.711
acetonitrile	C	Opls_754	+0.460	0.3300	0.276
		Opls_755	-0.080	0.3300	0.276
	H	Opls_140	+0.040	0.250	0.126
	N	Opls_753	-0.560	0.3200	0.711
N-hexane	C	Opls_135	-0.180	0.3500	0.276

	H	Opls_136	-0.120	0.3500	0.276
		Opls_140	+0.040	0.250	0.126
acetone	C	Opls_455	-0.500	0.350	0.276
		Opls_623	+0.732	0.355	0.293
	H	Opls_376	+0.139	0.2500	0.209
	O	Opls_771	-0.566	0.296	0.879

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