Supporting information

Peptide nanotube for carbon dioxide chemisorption with

regeneration property and water compatibility

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Experimental section

Materials. Ac-KLVFFAL-NH₂ (KL-7) and Ac-RLVFFAL-NH₂ (RL-7) were purchased from GL Biochem Ltd (Shanghai). The peptide purity was assessed by HPLC (>98%) and characterized by electrospray ionization mass spectrometry. The other chemicals and solvents were purchased from Sigma and used as provided.

Peptide assembly. Purified lyophilized peptides (3.5 mM) were dissolved in 4:6 CH_3CN/H_2O with 0.1% TFA solution and slowly titrated by drop-wise addition of 200 mM NaOH to pH 7.0. Dissolution was generally assisted by 2 min of continuous vortex, followed by 15 min sonication until solution became clear. Peptides were allowed to assemble for approximately 24 h at 37 °C until mature.

Fourier transform infrared spectroscopy (FTIR). The lyophilized powder peptide samples were mixed with dehydrated KBr crystals at ratio of 1:10 (w/w), and the KBr/peptide pellets were analyzed on a Nicolet iS50 FT-IR spectroscopy (Thermo Scientific, USA). For solution sample, a drop of sample was directly mixed with dehydrated KBr, and the mixture was analyzed after drying.

Transmission electron microscopy (TEM). Peptide assemblies were allowed to be adsorbed on carbon-coated copper grids (from Zhongjingkeyi Technology Co. Ltd, China) for 1 min before excess peptide solution was wicked away with filter paper. Freshly prepared 2 wt% uranyl acetate solutions were then added, and staining was allowed to proceed for 1.5 min, followed by removal of excess solution. Finally, the grids were left to dry covered by a Petri dish at room temperature. TEM micrographs were collected on a HT7700 transmission electron microscope (Hitachi. Ltd, Japan) with 100 kV acceleration voltages.

X-ray powder diffraction (XRD). About 50 mg KL-7 nanotube powder was used, and the XRD patterns were measured with D8 ADVANCE X-ray powder diffractometer (Bruker, German).

X-ray photoelectron spectroscopy (XPS). The element contents were measured by ESCALab 220-Xi (VG, UK) with 500 µm spot size and 0.050 eV energy step size.

Gas adsorption measurements. Carbon dioxide isotherms were collected on a FlowSorb III automatic volumetric gas adsorption analyzer (Micromeritics Instrument

Corp, USA). 100 mg of the sample was loaded into a preweighted sample tube, and the sample was outgassed to 10^{-6} Torr, after which the evacuated tube was weighted to determine the mass of the degassed sample. The sample was then transferred to the analysis port of the adsorption analyzer. Ultrahigh purity-grade nitrogenand carbon dioxide gases (99.995% purity) were used throughout the adsorption experiments.

Solid-State NMR. High-resolution solid-state NMR spectra were recorded at ambient temperature on a Bruker DSX-600 spectrometer (Bruker, Germany) using a standard Bruker magic-angle-spinning (MAS) probe with 4-mm (outside diameter) zirconia rotors. The ¹³C chemical shifts are given relative to tetramethylsilane as 0 ppm, calibrated using the methylene carbon signal of adamantane assigned to 37.77 ppm as a secondary reference.

Before exposure to ¹³C carbon dioxide, the sample was outgassed. ¹³C carbon dioxide (Sigma-Aldrich, 99 atom % ¹³C; <3 atom % ¹⁸O) was then injected into the sample at 1 bar. The sample was then transferred to zirconia NMR rotors right before the NMR measurement.



Fig. S1. XRD patterns of KL-7 nanotube before and after CO_2 uptake.



Fig. S2. TEM image of lyophilized powder of KL-7 nanotube.



Fig. S3. Photographic image of the KL-7 nanotube after the CO₂ uptake.



Fig. S4. TEM image of RL-7 nanotube solution.



Fig. S5. BET surface area plot of solid buffer component (A) and KL-7 nanotube (B).



Fig. S6. FTIR spectra of KL-7 nanotube before (black) and after (red) carbon dioxide adsorption.



Fig. S7. Temperature dependent CO₂ uptake of KL-7 nanotubes at 750 mmHg.



Fig. S8. The CP/MAS ¹³C NMR spectrum of KL-7 nanotube after regeneration, the peak of carbamate at 162.9 ppm disappeared.



Fig. S9. TEM image of regenerated KL-7 nanotubes.

Samples	C (%)	O (%)	Na (%)	N (%)	F (%)	P (%)
KL-7 nanotubes	47.97	24.14	10.46	8.34	6.12	2.97
KL-7 nanotubes	46.72	26.31	10.24	8.02	5.90	2.81
after CO ₂ uptake						

Table S1. Elemental content of KL-7 nanotubes before and after CO₂ uptake by XPS measurement.

KL-7 nanotubes after carbon dioxide uptake, the content of C was decreased and the content of O was increased, and the content of other elements barely changed (Na and P were from PB buffer, F was from the TFA in peptide assembly solution). Note that the elemental content of XPS analysis is the relevant content, therefore, although the absolute content of C after carbon dioxide uptake was increased, the relevant content of C was decreased actually. Thus, the XPS analysis is consistent with the carbon dioxide uptake.

	CO ₂ adsorption	Effect of H ₂ O			
Absorbents	capacities	on CO ₂ uptake	Regenerability	Notes	Ref.
	(mmol $CO_2 g^{-1}$)				
Zeolites	0.18~4.61 (310	Decreased	Good	-	1, 2
	K, 0.1 bar)	CO ₂ uptake			
30% MEA	~3 (303 K, 0.15	Almost no	Significant	-	3,4
	bar)	influence	decomposition		
Calcium oxide	1.5~11.6 (723	Almost no	Capacity loss as a	-	5,6
	K, 0.4 bar)	influence	function of cycling		
Hydrotalcite-	< 1.0(673 K, 1	Increased	Capacity loss as a	-	7, 8, 9
like	bar)	CO2 uptake	function of cycling		
compounds					
Amine-grafted	0.05~2.56 (298	Almost no	Good	-	10, 11,
silica sorbents	K, 0.1 bar)	influence			12
Amine-	1.1~4.2 (298 K,	Almost no		Complicated	13, 14,
functionalized	1 bar)	influence	Good	synthesis	15, 16
MOFs					
Nitrogen-Rich	1~5.37 (273 K,	Almost no	Good	Complicated	17, 18,
POPs	1 bar)	influence		synthesis	19, 20
KL-7	0.74 (298 K, 1	Almost no	Good	-	This
nanotubes	bar)	influence			work

Table S2. Comparison of absorbents for carbon dioxide uptake.

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