

Supplementary Information

Scalable and Sustainable Cellulose Xerogels for High-Capacity Enrichment of Per- and polyfluoroalkyl Substances

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Section 1. General methods

Materials

Perfluoro-2,5-dimethyl-3,6-dioxanonoic acid (HFPO-TrA, 98%), Perfluorooctanoic acid (PFOA, 96%), Perfluoro(2-methyl-3-oxahexanoic) acid (HFPO-DA, 97%), Perfluorohexanoic acid (PFHxA, 98%), Perfluorobutyric acid (PFBA, 98%) and Pentafluoropropionic acid (PFPrA, 97%) were purchased from Aladdin. Polyethyleneimine (M.N. 70,000, 50% in water) was obtained from Macklin. 3-Glycidyloxypropyltrimethoxysilane (KH560, 98%) was purchased from Shanghai Yuanye Biotechnology Co., Ltd. Nanofibrillated cellulose (NFC, 2.5 wt%) was furnished by Zhongshan Nanofiber New Materials Co., Ltd. Methanol (MeOH) and ethanol (EtOH) were provided from Sinopharm Chemical Reagent Co., Ltd. All reagents were used as received without further purification.

Preparation of xerogel

First, the 2.5 wt% NFC solution was diluted to a concentration of 1 wt% (total weight: 10 g). Specific amounts of crosslinker KH560 (the ratio to cellulose solution is 1%, 2%, 3%, 4%, and 5%, respectively) were then added to the cellulose solution and thoroughly mixed. Next, 1 g PEI was introduced into the resulting suspension and homogenized at high speed for 10 min using a high-speed homogenizer. The mixture was then poured into a mold and allowed to stand at room temperature for 10 min to form a hydrogel. Following this, the hydrogel was frozen at -20 °C for 1 h. Subsequently, the frozen precursor was immersed in ethanol to completely replace the water content. Finally, the samples were air-dried at ambient temperature to produce xerogels. Based on the varying concentrations of crosslinker, the samples were designated as CNPK-1, CNPK-2, CNPK-3, CNPK-4 and CNPK-5. For large-scale samples, the process parameters were scaled up using the same ratio. Furthermore, CNK and CNP samples were synthesized without PEI and KH560, while all other experimental parameters remained unchanged.

Characterization

The morphologies and elemental distributions of the samples were obtained using scanning electron microscope (SEM, Zeiss Gemini 300) equipped with an energydispersive spectroscopy (EDS). The information of functional groups of xerogel during preparation and adsorption was obtained by Fourier transform infrared spectrometer (FTIR, Hyperion 3000) in ATR mode. The chemical composition of the xerogel before and after adsorption were analyzed by X-ray photoelectron spectroscopy (XPS, Thermo ESCALAB 250XI) with an Al-K α X-ray source. Raman mapping was conducted using Visible and near-infrared fast imaging confocal Raman spectrometer (Alpha300R) with a 532 nm wavelength of the excitation laser and a 10 μ m scan range (7.0 mW of laser power, 0.1 s of the exposure time, 40 of the number of scans). The hydrophilicity of the adsorbent before and after adsorption was determined by the dynamic contact angle of pure water droplets on the solid surface with the contact angle meter (Dataphysics OCA20). X-ray CT (micro-CT, Xradia 620) was used to visualize and reconstruct the three-dimensional structure of CNPK, with a light source-RA distance of 12 mm, a detector-RA distance of 15 mm, a voltage of 50 kV, and a power of 4 W, and 1008 SEM images were obtained. Wide-angle dynamic (static) light scattering (DLS&SLS)/Zeta potential analyzer was used to reflect the effect of solution pH on the surface charge characteristics of CNPK adsorbent, and each pH point was measured 3 times. Mechanical properties were tested using a single-column mechanical testing system (INSTRON 5982) equipped with a 1kN load cell and two flat-surface steel compression stages.

Batch Adsorption Experiments

Equilibrium PFAS removal

Experiments to investigate the removal of six PFAS using xerogel were conducted in polypropylene conical flasks at ambient temperature (25 °C) on a shaker set at 180 rpm. Control experiments, performed under

identical conditions, evaluated the removal efficiency for xerogels. Kinetic studies were carried out at a dosage of 1 g/L to adsorb single/multi- PFAS concentrations of 100 µg/L, with supernatant samples collected at intervals of 0, 10, 30, 60 and 120 min. Note that the concentration of each PFAS is equal in a multicomponent PFAS system. Isothermal adsorption experiments were conducted over a 6-hour period using initial PFAS concentrations ranging from 0.1 to 350 mg/L for HFPO-TrA; 0.1 to 300 mg/L for PFOA and HFPO-DA; and 0.1 to 200 mg/L for PFBA and PFPrA. The influence of pH was examined by adjusting the pH within the range of 3 to 7 using 1 M HCl and NaOH solutions. The concentration of PFAS in water after adsorption was measured using UPLC-MS/MS (ACQUILITY UPLC I-Class PLUS/XevoTQ-S). The chromatography and ion source instrument parameters can be found in the supporting information in **Table S1** and the MRM transitions can be found in **Table S2**.

The removal efficiency of PFAS at different experimental times was calculated by Eq. S1:

$$Removal = (C_0 - C_e) / C_0 \times 100 \quad (1)$$

The adsorption capacity was determined by Eq. S2:

$$q_e = (C_0 - C_e)V / m \quad (2)$$

Where, C_0 represents the initial and residual concentration of PFAS (mg/L), respectively. V represents the volume of the adsorbate solution (mL), and m represents the mass of the adsorbent (mg).

Sorption kinetic models of PFAS

The pseudo-first-order (PFO) and pseudo-second-order (PSO) models were employed to study the adsorption kinetics of the xerogel on PFAS. The kinetic models are represented by equations Eq. S3, S4, respectively.

Pseudo-first-order model:

$$q_t = q_e (1 - e^{-k_1 t}) \quad (3)$$

Pseudo-second-order model:

$$q_t = t(k_2 q_e^2) / (1 + k_2 q_e t) \quad (4)$$

Where, q_t (mg/g) represents the adsorption capacity at time t (min). q_e (mg/g) represents the equilibrium adsorption capacity. k_1 (min^{-1}) and k_2 ($\text{g}/(\text{mg} \cdot \text{min})$) are the rate constants for the two kinetic models.

Sorption isotherm models of PFAS

the Langmuir and Freundlich models were used to describe the adsorption equilibrium isotherm models. The isotherm models are represented by Eq. S5, S6, respectively.

$$\text{Langmuir model: } q_e = q_m k_L C_e / (1 + C_e k_L) \quad (5)$$

$$\text{Freundlich model: } q_e = k_f C_e^{1/n} \quad (6)$$

$$\text{Dimensionless separation factor: } R_L = \frac{1}{1 + k_L C_0} \quad (7)$$

Where, q_e (mg/g) and q_m (mg/g) represent the equilibrium adsorption capacity and maximum adsorption capacity, respectively. k_L (L/mg) is the Langmuir adsorption isotherm constant, k_f ($(\text{mg/g})/(\text{mg/L})^{1/n}$) and n are the Freundlich constants, C_e (mg P/L) represents the equilibrium concentration of the pollutant in the solution. R_L is the separation factor, in which $R_L = 0$ implies the adsorption is irreversible; $0 < R_L < 1$ indicates that it is favorable for adsorption, while $R_L > 1$ implies the opposite.

Calculation of the proportion of electrostatic interactions

Based on the results shown in Fig. 2b and using PFPrA as a reference, the adsorption capacity remains constant when the pH exceeds 6, indicating that electrostatic interactions are negligible under these conditions. This suggests that the amino groups in the xerogel are predominantly deprotonated at higher pH, thereby

minimizing electrostatic attraction. From this, the contribution of electrostatic interactions at lower pH (e.g., pH 3) can be estimated by comparing the increase in adsorption capacity. Using this approach, the electrostatic contribution for the remaining five PFAS compounds was inferred accordingly.

Recycling experiment

The regeneration experiments were evaluated through the adsorption/desorption experiments for five consecutive cycles. The regeneration performance of the xerogel was evaluated at a dosage of 5 g/L, with initial PFAS concentrations of 1 mg/L. In a typical procedure, PFAS-loaded CNPK xerogel was picked up from the aqueous phase after adsorption and then immersed into 50 mL MeOH for 6 h, followed by simultaneously achieving PFAS concentration and methanol recyclability through the rotary evaporation process (30 °C, 0.05 atm). This closed-loop solvent management system significantly reduces chemical consumption in scaled operations. Finally, the regenerated xerogel was further used for another cycle.

Reconstruction experiment

The discarded xerogel was immersed in 50 mL of 0.5 M NaOH and stirred at room temperature for 6 h. The original NFC gel was then collected by centrifugation and reconstructed into new xerogel using the same preparation process.

Computational details

Classical molecular dynamics (MD) simulations were performed using the AMBER99SB-ILDN force field by the Gromacs 2018.8 package¹. The simulation boxes were initially built by randomly distributing the chemical species (50 mol, 50 pollutant molecules, and 100 Cl⁻ ions and a varying number of H₂O molecules as solvate), with an initial size of 8*8*8 nm³. To mimic the situation of acidic solution in experiment, the mol molecule was protonated at two -NH₃ sites. The chemical structures of all species were relaxed based on density functional theory (DFT) at the B3LYP/6-311G(d) level with the GD3BJ correction using the Gaussian 16 package^{2,3}. The Sobtop package was used to generate the topology information of mol and the pollutants⁴. After energy minimization, the equilibration runs were successively conducted by a series of NVT/NPT processes at 1 atm and 297 K, with a total simulation time of 120 ps. The production run was conducted for 30 ps and used for the final analysis. During each simulation, the time step was set to be 0.5 fs, and the trajectory information was saved every 250 fs. The cutoff for the van der Waals forces was 12 Å, and the particle mesh Ewald (PME) was used to describe the Coulomb interactions, with dispersion correction considered.

Modeling the deprotonated form of PFAS at pH 3 would introduce an artificial net negative charge, leading to unrealistic electrostatic interactions and potentially misrepresenting key aspects of PFAS behavior. In this study, the specific PFAS molecules containing -COOH were modeled in its protonated form, assuming that the acidic functional groups remain predominantly protonated under the simulated conditions (pH 3), reflecting the expected dominant chemical species under the simulated acidic pH. Future studies employing constant-pH MD or explicit consideration of multiple protonation states could address these aspects more comprehensively.

Life Cycle Assessment (LCA)

The environmental sustainability of xerogel is systematically evaluated using a life cycle assessment approach. The functional unit of this study is defined as the production of 1 kg of xerogel, and the resource consumption and environmental emissions during the xerogel production life cycle are quantified. Detailed inventory data for xerogel production are listed in Table S16. In addition, the preparation process of xerogel involves the input of KH560 and PEI, which play a key role in the gelation process. The relevant inventory data are based on the research results⁵⁻⁸. Among them, the process-scale simulation method of the Aspen Plus tool supports the production data of KH560 silane coupling agent, which is shown in **Table S17**. The power consumption

data of the stirring and freezing stages during the gelation process were calibrated with reference to the energy specifications to ensure the accuracy and reliability of the data⁹. To reduce the environmental impact of ethanol and water produced in the solvent exchange stage, this study used distillation separation and molecular sieve adsorption processes to recover the solvent. The relevant process parameters were optimized based on the National Renewable Energy Laboratory (NREL) report and verified by Aspen Plus simulation to minimize the potential burden of ethanol and water emissions on the environment. SimaproTM (V9.5) was applied to the environmental impact assessment of the gel, and the material and energy background data were based on the Ecoinvent database v 3.9.1. LCIA is based on the CML-IA baseline V3.09/EU25 assessment method, and the environmental impact indicators considered include abiotic depletion (ADP), fossil fuel depletion (ADP fossil fuels, MJ), global warming potential (GWP 100a), ozone depletion potential (ODP), human toxicity (HTP), freshwater aquatic ecotoxicity (FAETP), marine aquatic ecotoxicity (MAETP), terrestrial ecotoxicity (TEP), photochemical oxidation potential (POCP), acidification (AP), and eutrophication (EP). In order to meet the policy needs of renewable energy, this study additionally explored renewable energy scenarios represented by photovoltaic power generation and biomass heat to explore the future environmental sustainability potential of xerogel. This paper selected gel materials for wastewater treatment applications and xerogel prepared at room temperature for comparative analysis, for example, chitin cryogel¹⁰, chitosan cryogel¹⁰, hybrid aerogel in powder form¹¹, amidoxime functionalized¹², schiff base functionalized silica aerogel¹³, mercapto functionalized aerogel¹⁴, polyvinyl alcohol aerogels¹⁵, hybrid aerogel in monolithic form¹¹, Inorganic aerogel¹¹.

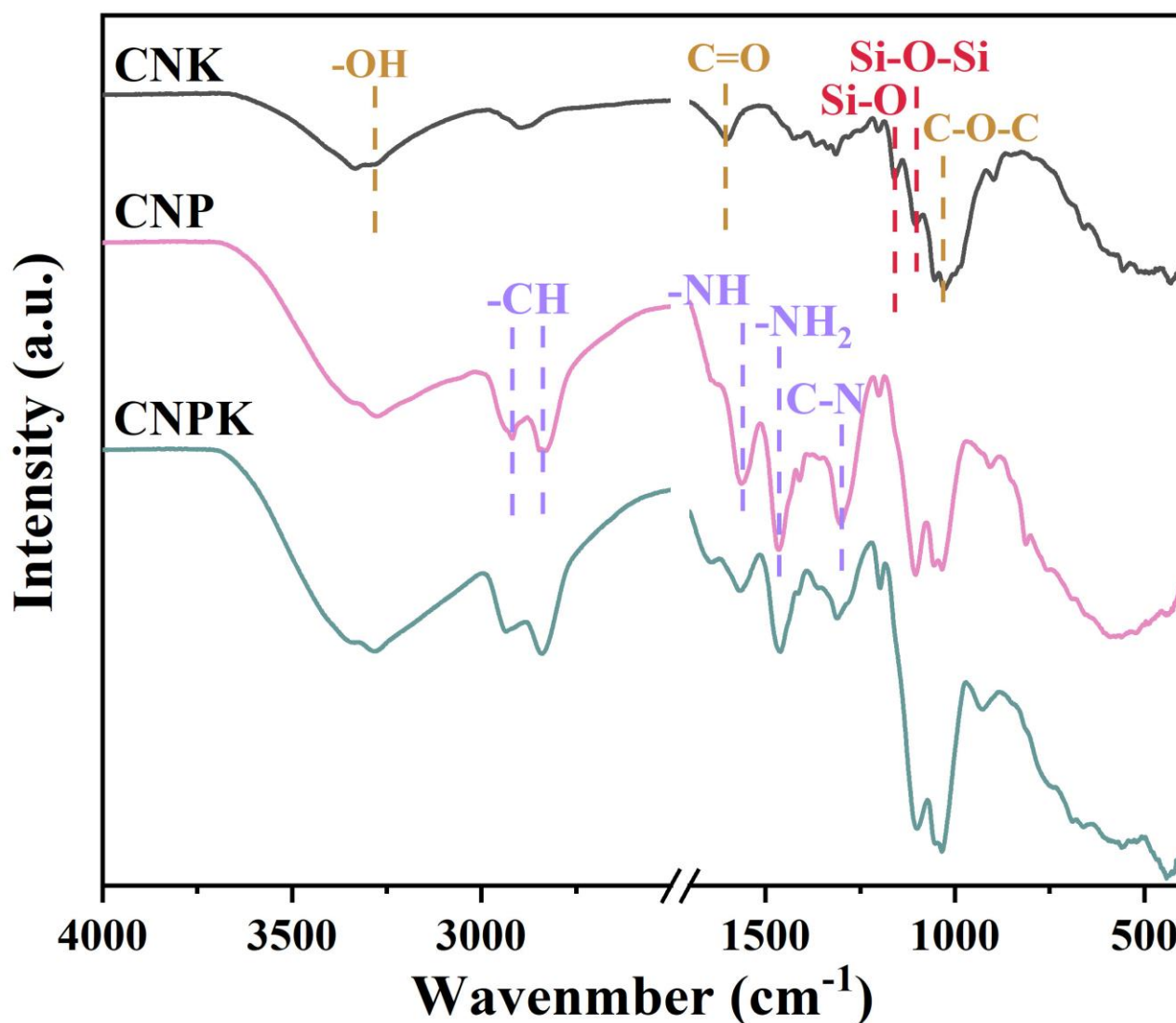


Fig. S1 FTIR spectra of CNK, CNP, CNPK.

To gain a more comprehensive understanding of the relationships among the components of xerogel, FTIR spectroscopy is performed on CNK, CNP and CNPK (Fig. S1). The spectra of various crosslinking modes exhibit a prominent peak at 3300 cm^{-1} , corresponding to the stretching vibration of the -OH groups within the NFC matrix. Additionally, NFC also exhibits characteristic bands around 1023 cm^{-1} (C-O-C) and 1609 cm^{-1} (C-O)¹⁶. In the CNK spectrum, the characteristic peak of the epoxy group from KH560 appears at 902 cm^{-1} , while the absorption peaks at 1106 cm^{-1} and 1157 cm^{-1} are attributed to the stretching vibrations of the Si-O and Si-O-Si bonds, respectively, which confirm the incorporation of KH560 into the xerogel structure^{17,18}. The peak observed at 1300 cm^{-1} in the CNP spectrum is assigned to the stretching vibrations of the C-N associated with the amide III group¹⁹. The peaks at 1458 cm^{-1} and 1560 cm^{-1} correspond to the bending vibrations of the -NH- and -NH_2 , respectively, both of which are characteristic of the amide II group²⁰. The C-H symmetric and asymmetric stretching vibration peaks of PEI are clearly observed within the range of 2931 to 2839 cm^{-1} ²¹.

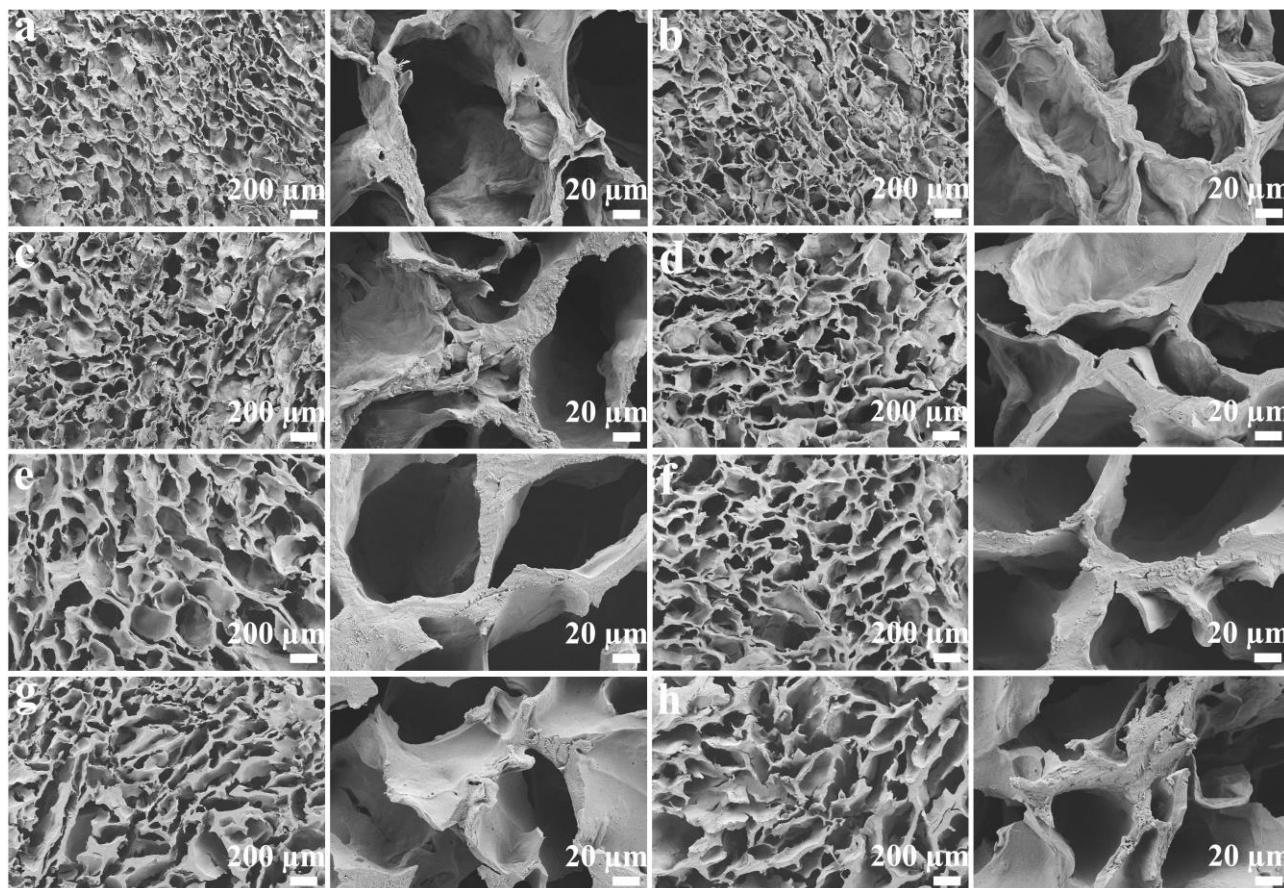


Fig. S2 Longitudinal and transverse SEM images of xerogel at different cross-linker contents: (a, b) 1%, (c, d) 2%, (e, f) 3%, (g, h) 5%.

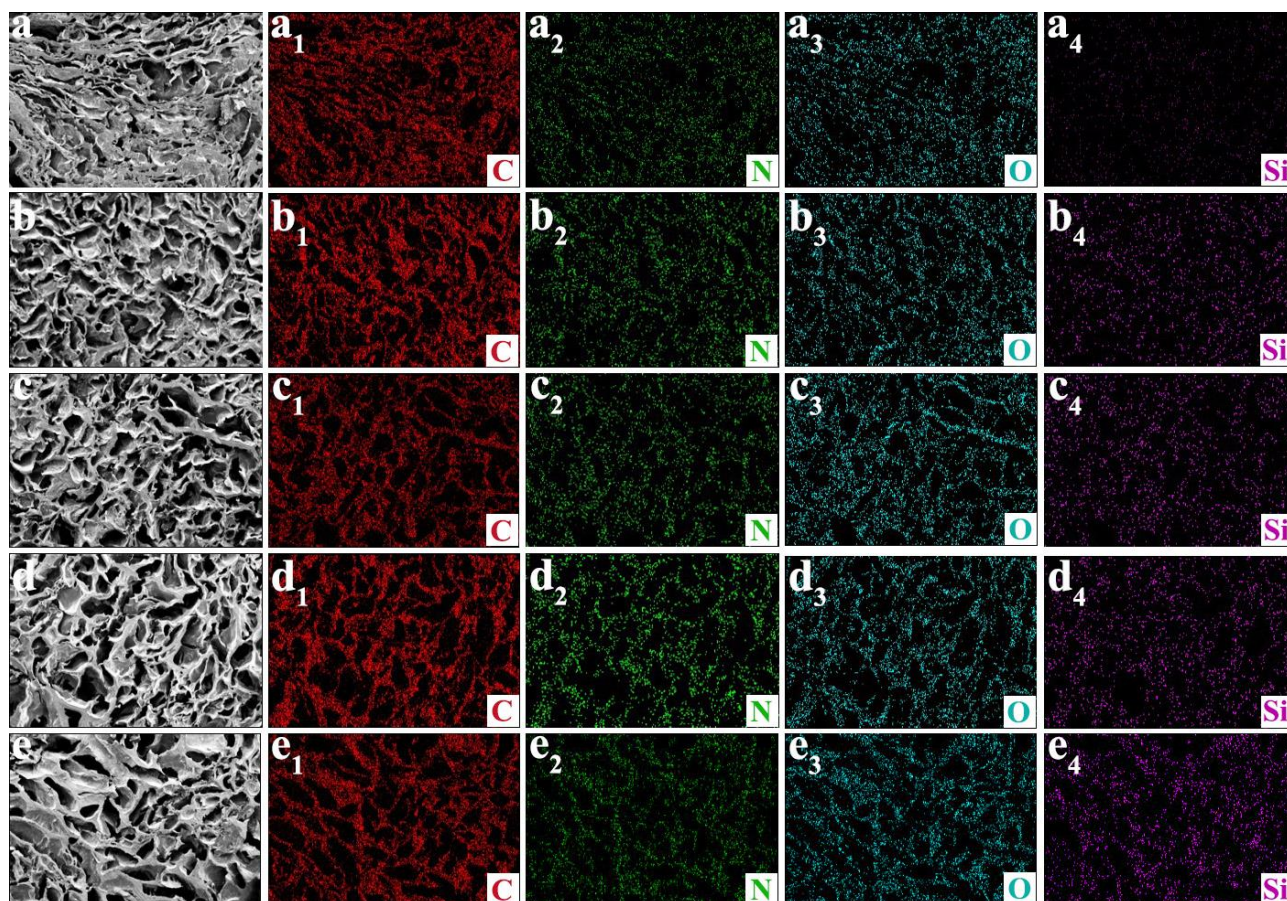


Fig. S3 Element distribution mapping of (a) CNPK-1, (b) CNPK-2, (c) CNPK-3, (d) CNPK-4, (e) CNPK-5.

Energy-dispersive X-ray spectroscopy (EDS) is employed to further quantify the elemental composition of various xerogels. As illustrated in **Fig. S3**, C, N, O and Si elements are uniformly distributed throughout the xerogel network skeleton. The N-element ratio decreases progressively with increasing Si contents in the xerogel (**Table S4**), confirming the findings from FTIR analysis.

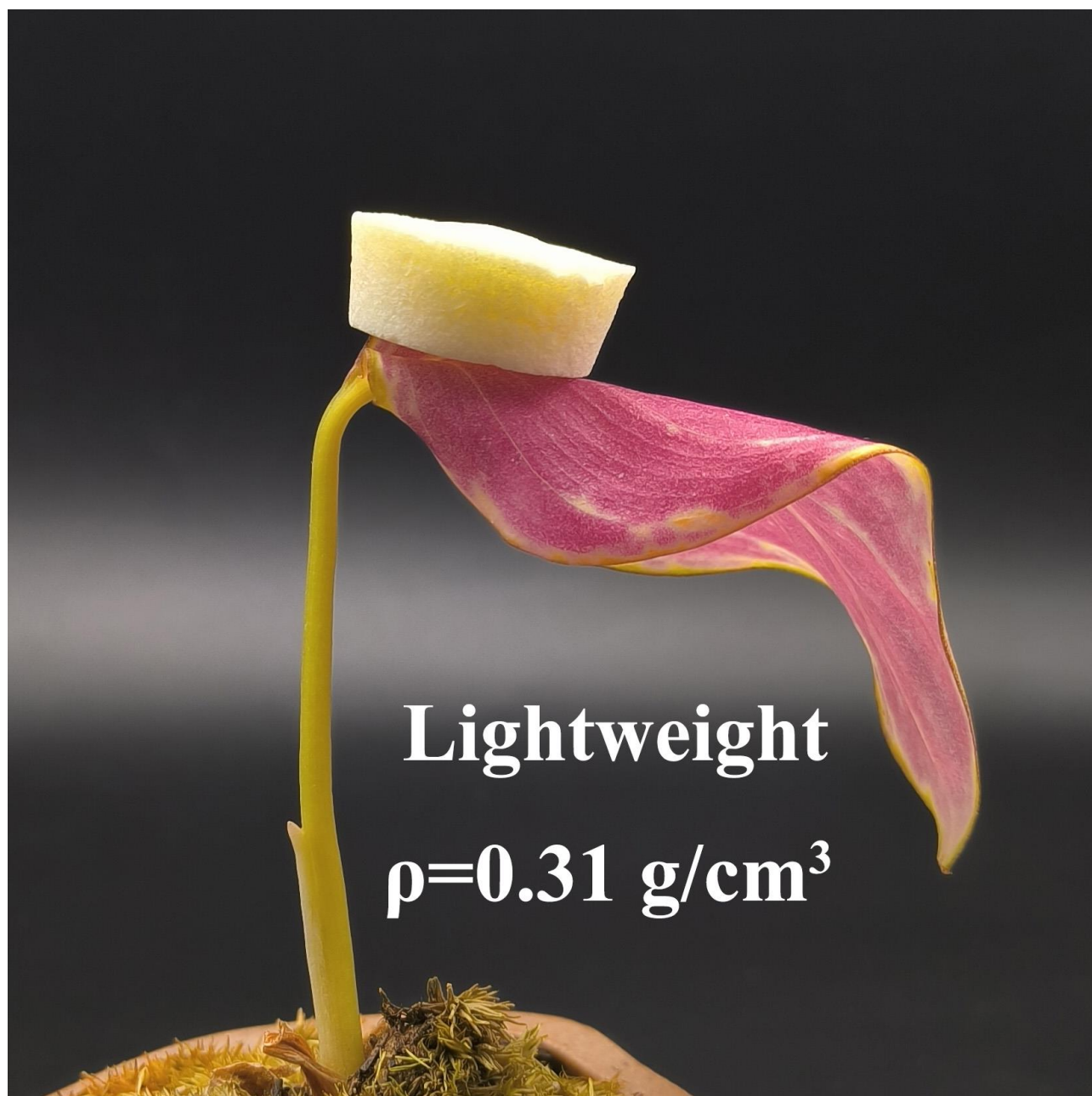


Fig. S4 Lightweight CNPK xerogel supported by soft flower stem.

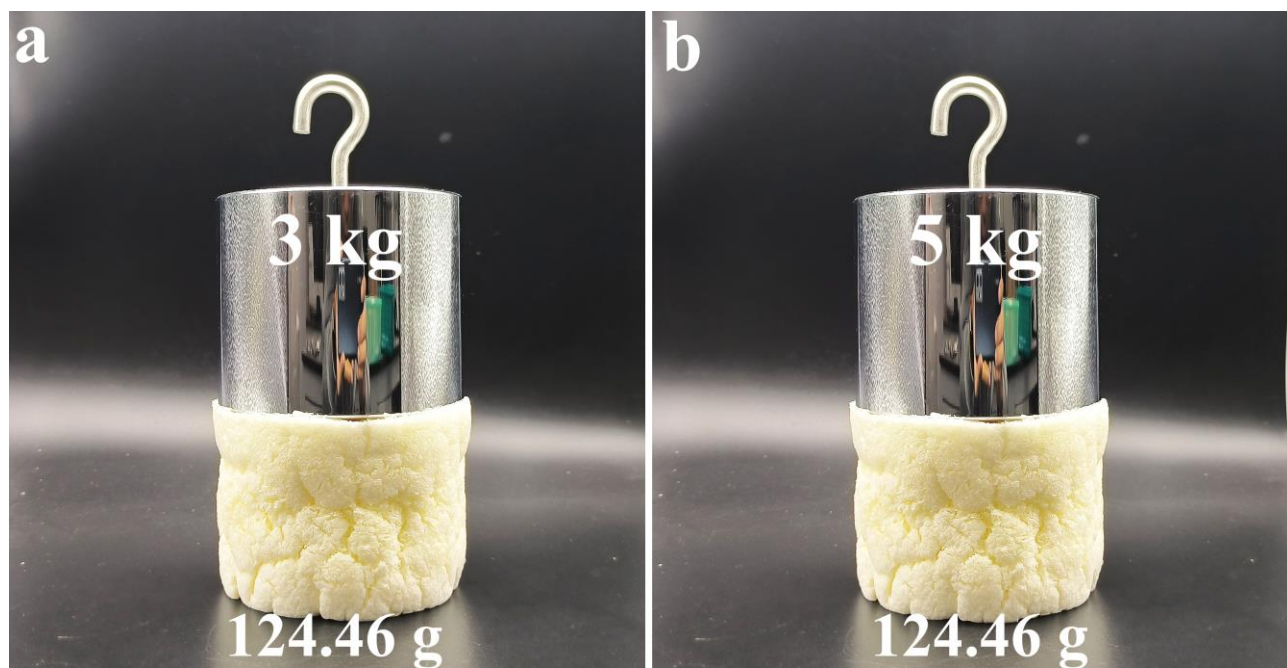


Fig. S5 CNPK xerogel can support loads up to 24 times (a) and 40 times (b) its own weight.

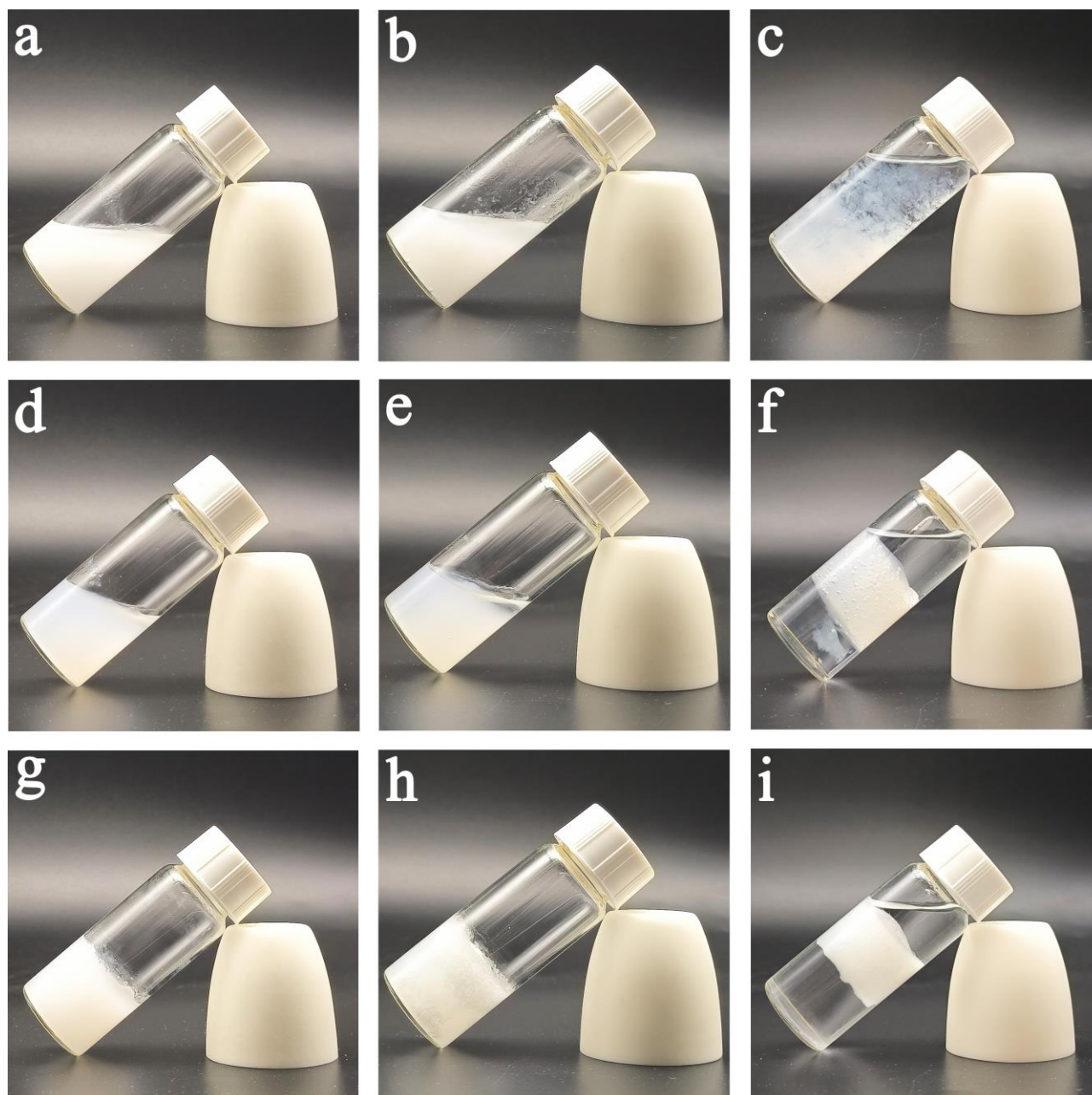


Fig. S6 CNK (a), CNP (d), CNPK (g) after homogenization and shearing; CNK (b), CNP (e), CNPK (h) after freeze-thaw; CNK (c), CNP (f), CNPK (i) after solvent exchange.

Fig. S6 highlights the essential role of cross-linking among the three polymers for xerogel formation. As seen in **Figs. S6a, b, c**, the KH560/NFC mixture fails to form a stable hydrogel following high-speed shearing without PEI, suggesting that the weak crosslinking between KH560 and NFC to form Si-O-C is insufficient to establish a robust 3D network structure. When KH560 is omitted (**Figs. S6d, e, f**), the dendritic structure of PEI becomes more entangled with the NFC chains, enhancing the tendency to form a xerogel precursor²². However, the internal stress generated by strong intramolecular and intermolecular hydrogen bonds cause severe structural collapse during ambient drying²³. This explains the formation of well-defined xerogels in systems where all three components coexist (**Figs. S6g, h, i**). The crosslinking processes occur through the following multi-step pathways: i) silane groups of KH560 react with hydroxyl groups on the NFC surface to form Si-O-C bonds; ii) amino groups of PEI interact with the epoxy groups of KH560, producing silicon-amino compounds; iii) the amino groups of PEI also form hydrogen bonds with the hydroxyl groups on NFC. These reactions lead to the creation of a three-dimensional crosslinked network between the NFC substrate, KH560 and PEI, enhancing the xerogel's mechanical strength and microstructure. Therefore, upcoming studies will conduct a comprehensive exploration of the properties and applications of CNPK xerogel.

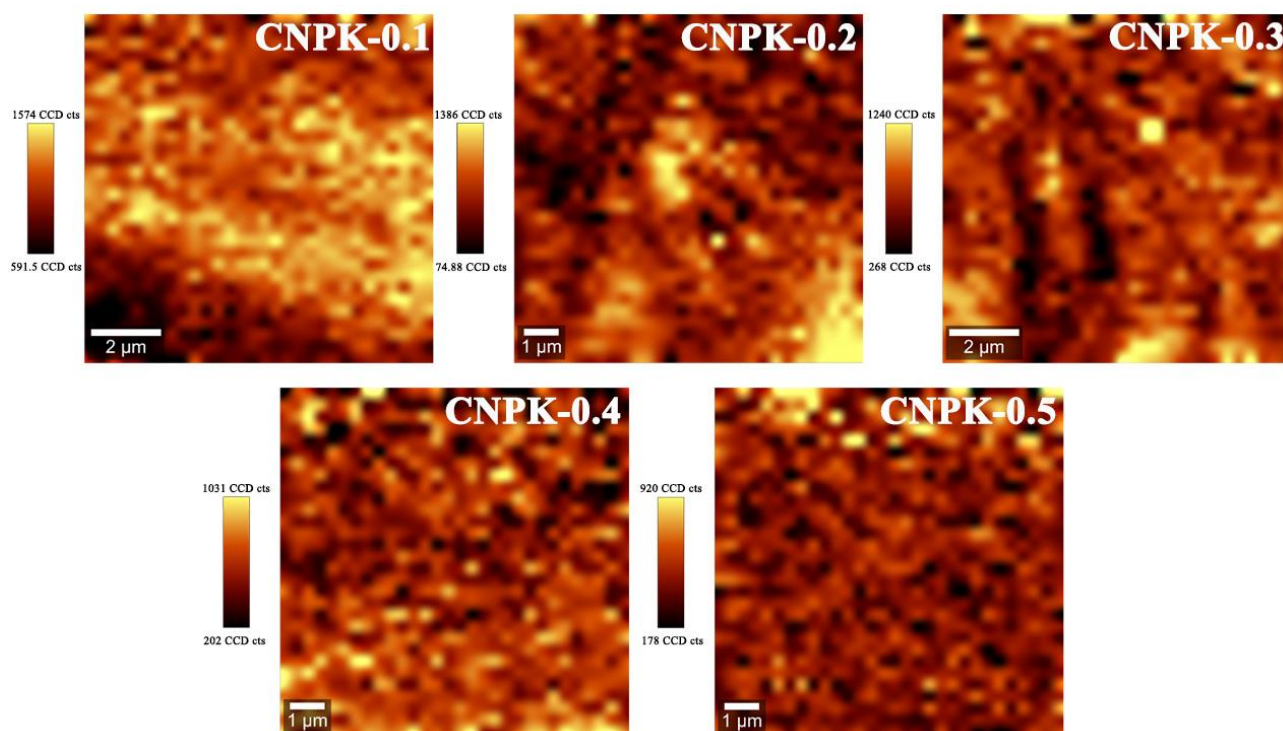


Fig. S7 2D Raman spectra of CNPK-1, CNPK-2, CNPK-3, CNPK-4, and CNPK-5.

The corresponding 2D Raman spectra presented in **Fig. S7** (where bright yellow indicates higher absorption intensity) further elucidate the varying PEI content on the xerogel.

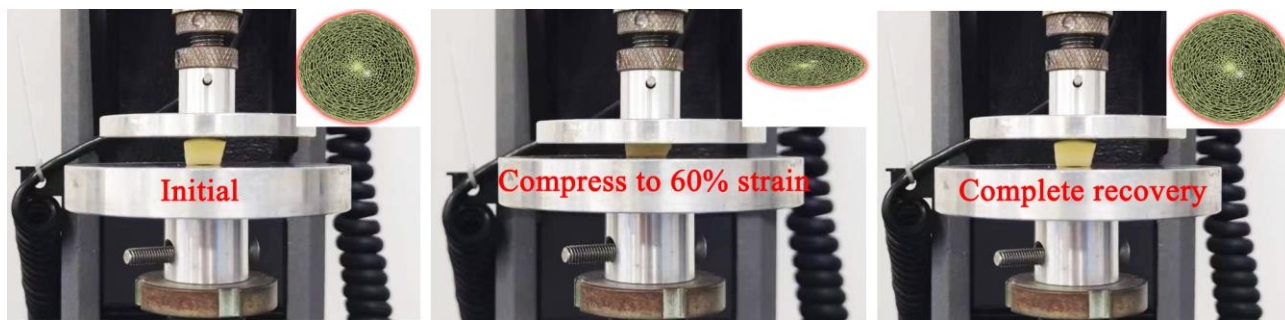


Fig. S8 Compression and recovery performance of CNPK-4 xerogel.

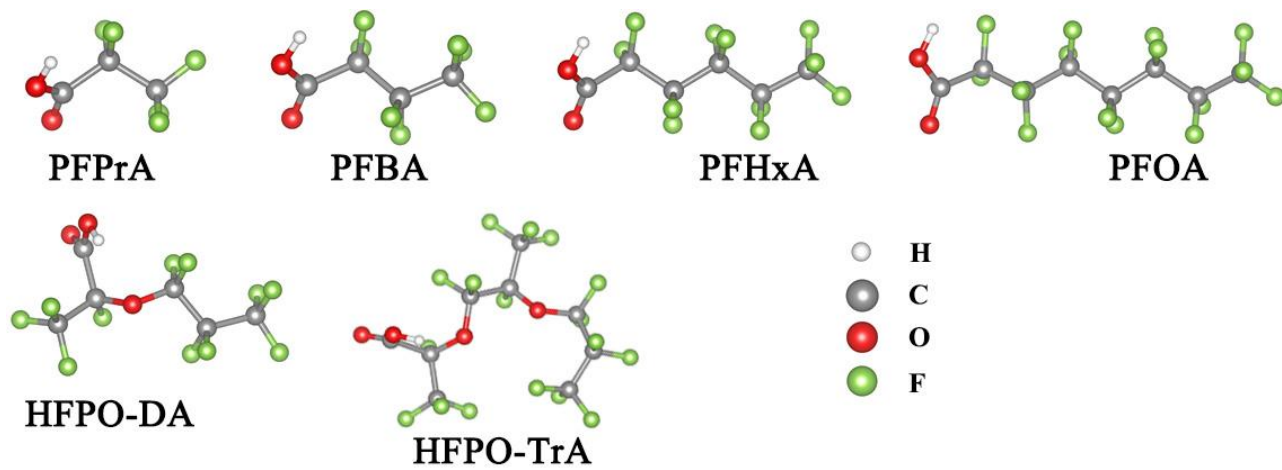


Fig. S9 Optimized molecular structures of six PFAS.

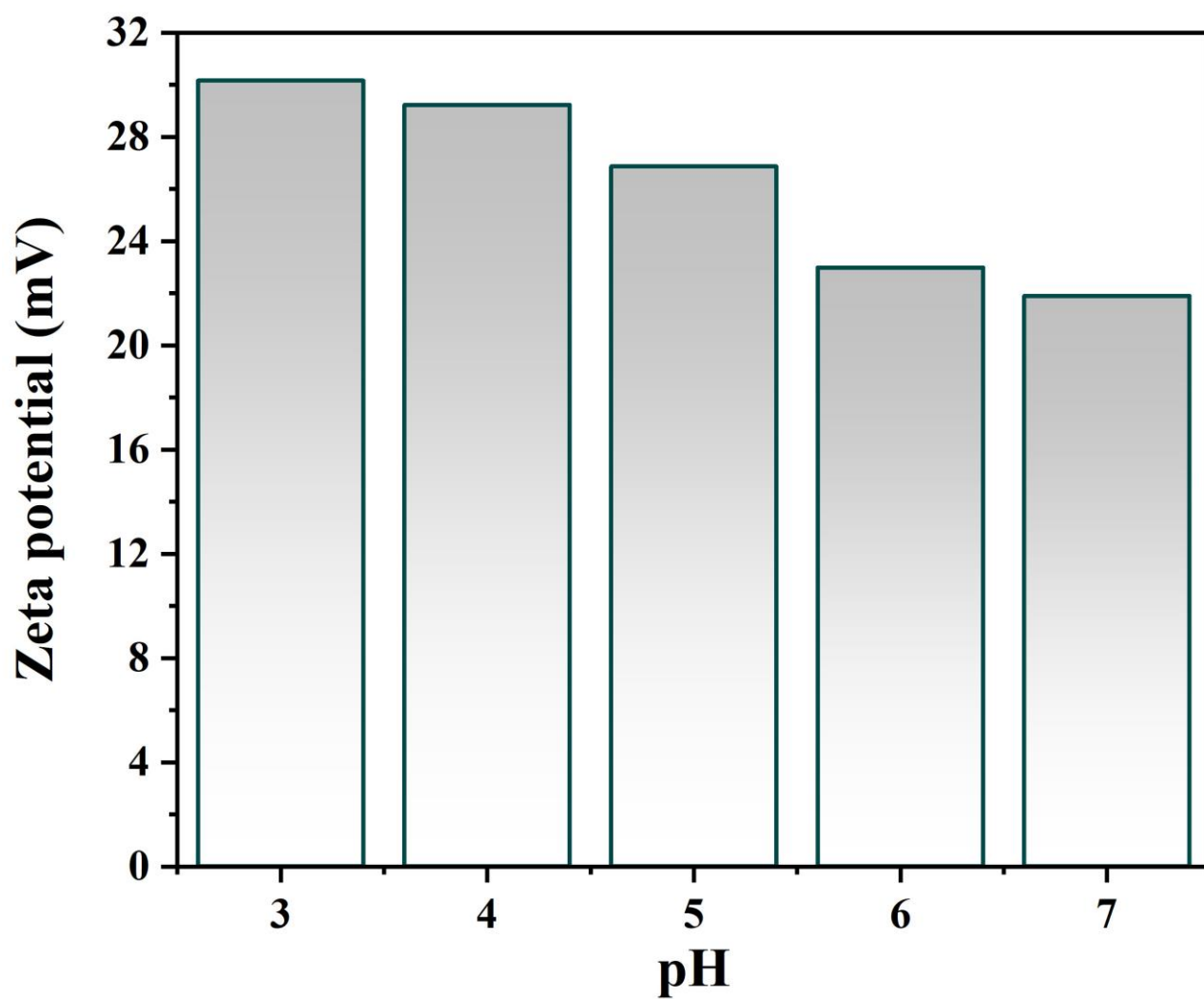


Fig. S10 Zeta potential of CNPK-4 under different pH conditions.

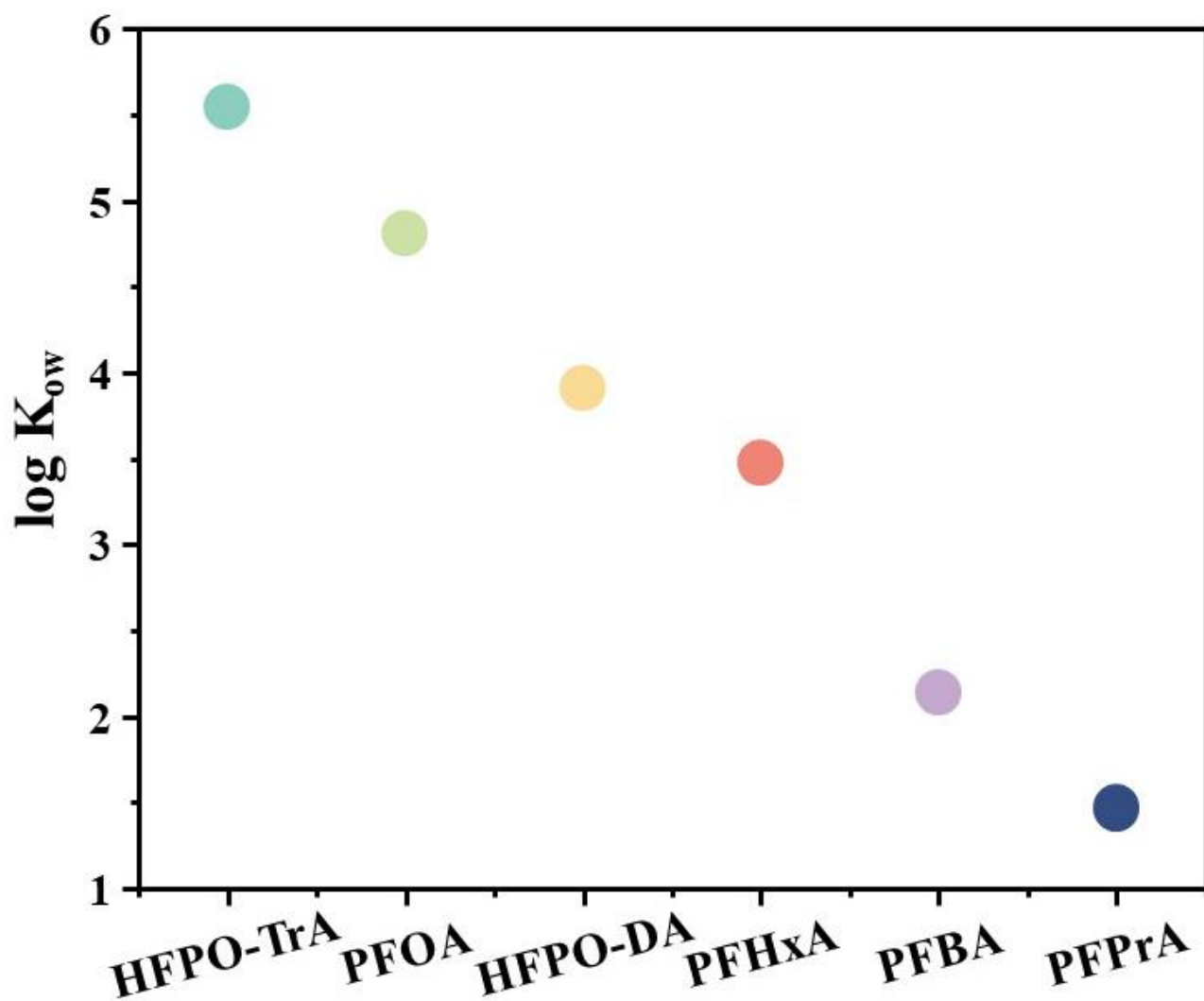


Fig. S11 Log K_{ow} of six PFAS.

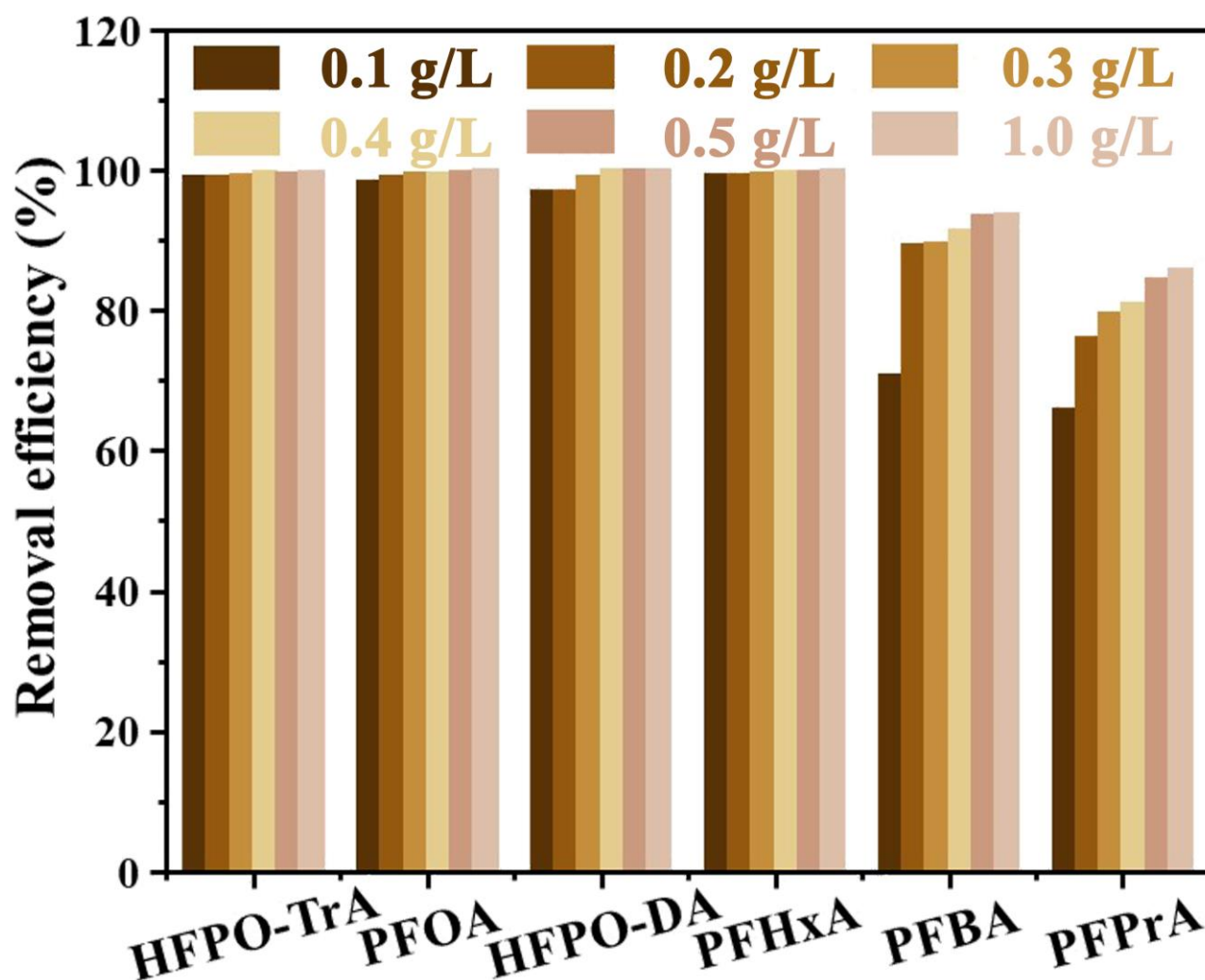


Fig. S12 Adsorbent dose-dependent removal efficiency of six PFAS (pH: 3; PFAS: 100 μ g/L).

In addition, the effect of varying adsorbent dosage on the PFAS adsorption performance is also evaluated. As illustrated in **Fig. S12**, PFAS with $C \geq 6$ exhibit negligible variation in removal efficiency with increasing adsorbent loading, while PFBA and PFPrA demonstrate dose-dependent adsorption behavior, with removal efficiencies increasing from 70.8% and 65.8% at 0.1 g/L dosage to 93.7% and 86.0% at 1.0 g/L dosage within 2 h, respectively. This can be attributed to the increase in active binding sites and enhanced molecular interactions between functional groups and short chain PFAS species due to increased xerogel availability. CNPK-4 outperforms previous adsorbents in short-chain PFAS capture. For instance, poly(FVD)-TMA⁺ and PFPE-IEX⁺ required 5 g/L to remove 92.8% and 98.0% of PFBA at the same initial concentration with 24 h treatment period²⁴, highlighting the superior efficiency of CNPK-4 at lower dosage.

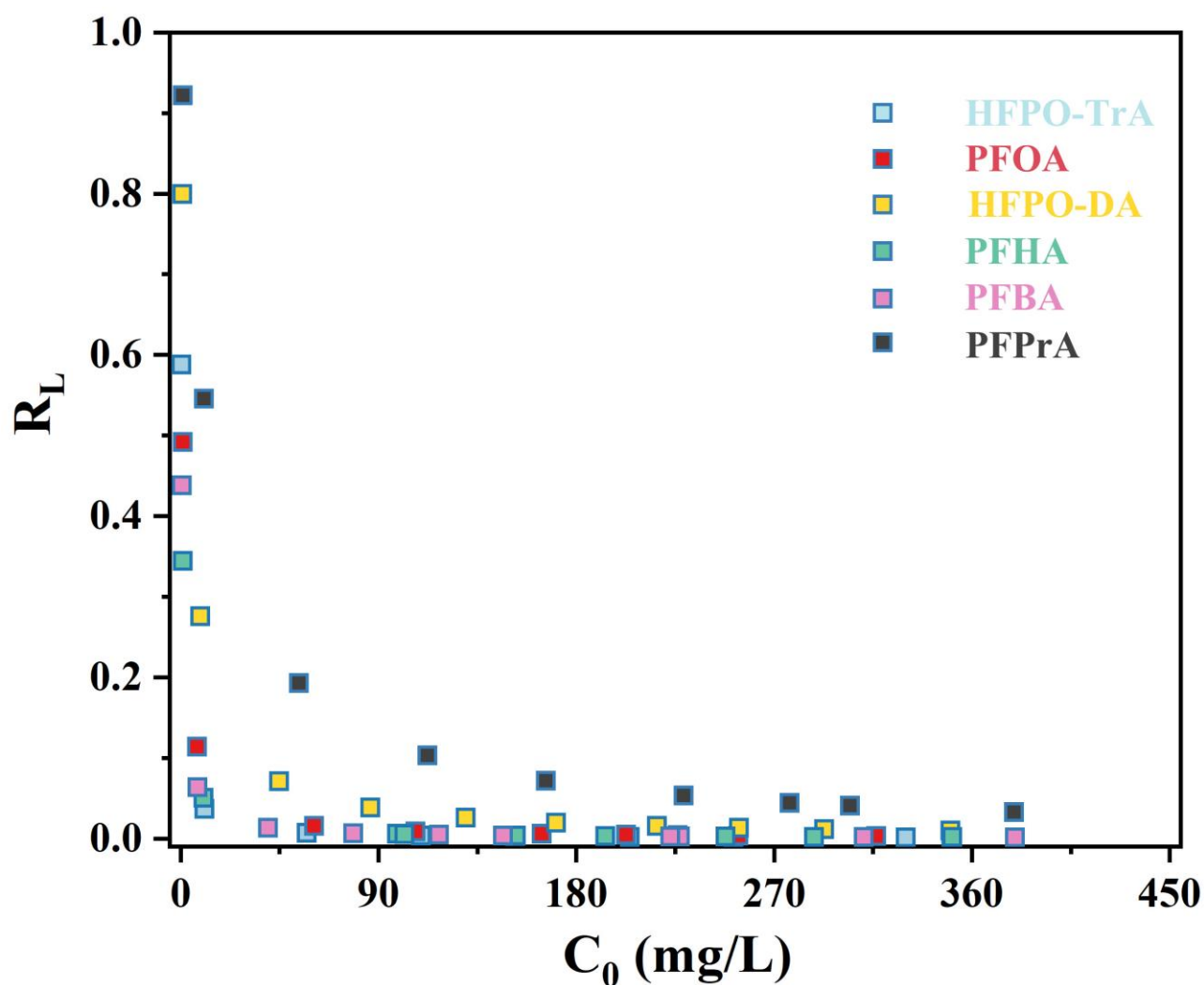


Fig. S13 Dimensionless separation factor (R_L) calculation.

The dimensionless separation factor (R_L) derived from Langmuir isotherm analysis ($0 < R_L < 1$) confirms thermodynamically favorable adsorption across tested PFAS concentrations²⁵⁻²⁸.

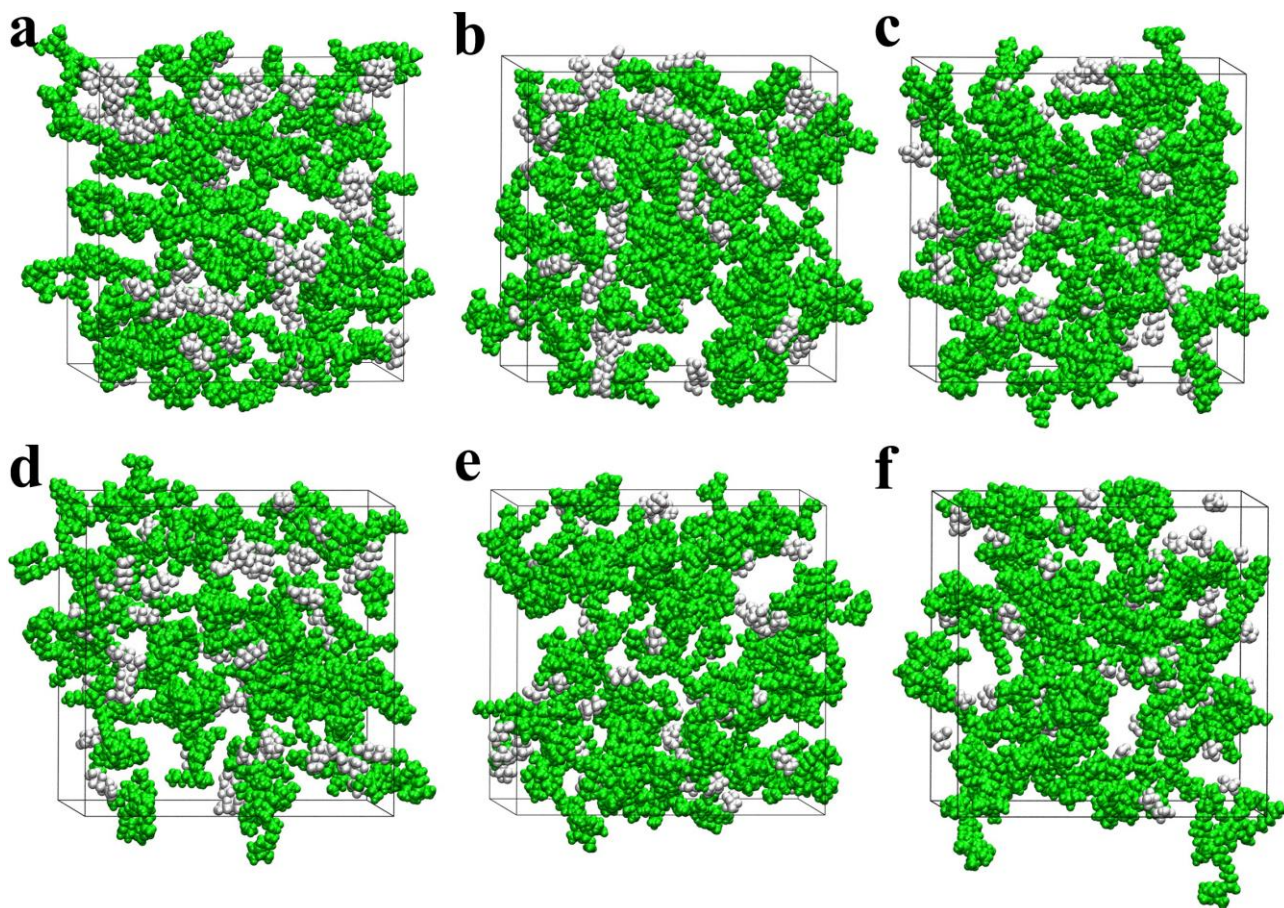


Fig. S14 Results of the (a) HFPO-TrA, (b) PFOA, (c) HFPO-DA, (d) PFHxA, (e) PFBA and (f) PFPrA systems at the final step of MD simulation in presentation mode (For clarity, the solvate H_2O molecules and the Cl^- ions were omitted in the figure; Green represents xerogel, and gray represents PFAS contaminants).

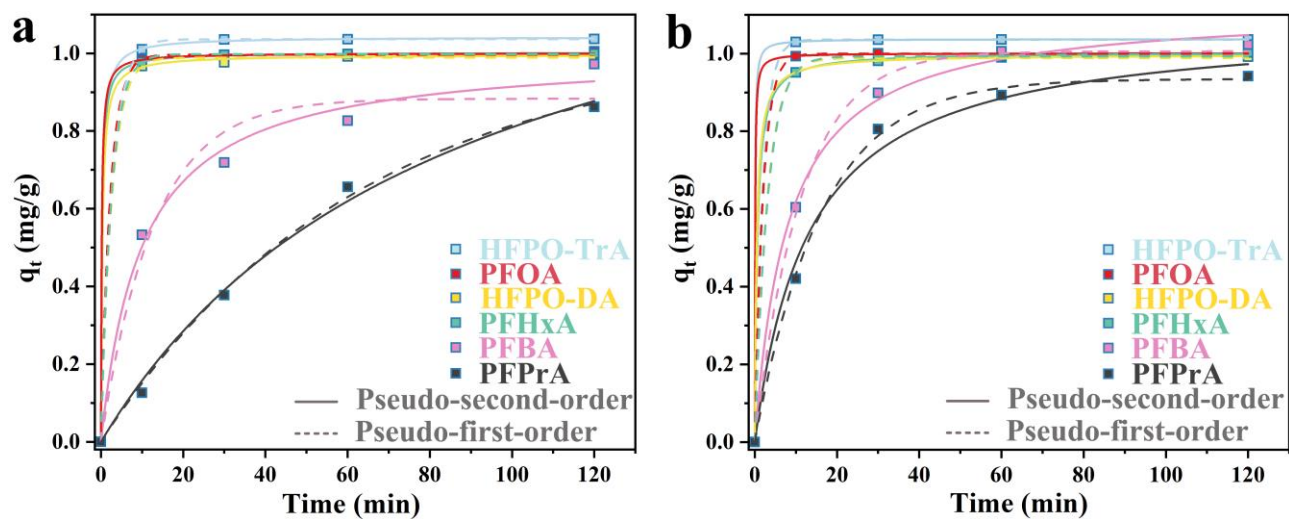


Fig. S15 (a) Pseudo first-order and pseudo second-order for CNPK-4 adsorption of single-PFAS; (b) Pseudo first-order and pseudo second-order for CNPK-4 adsorption of mixed-PFAS. (pH: 3; PFAS: 100 $\mu\text{g/L}$; adsorbent: 1 g/L).

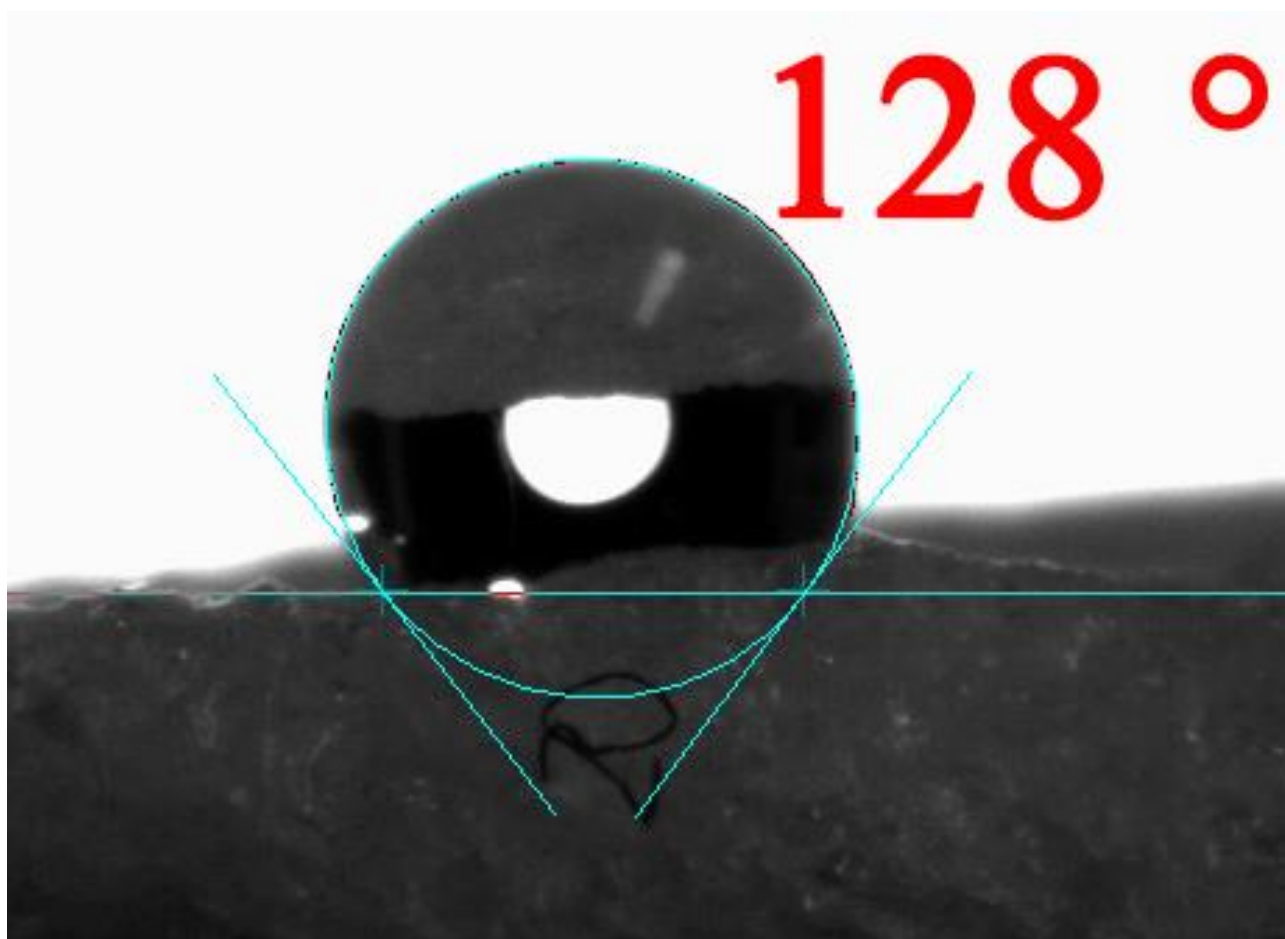


Fig. S16 Surface wettability of CNPK-4 after adsorption of mixed-PFAS.

As shown in **Fig. S16** and **Video S5**, the contact angle increases from 0° to 128° after adsorption process, further confirming the successful immobilization of PFAS onto the xerogel framework.

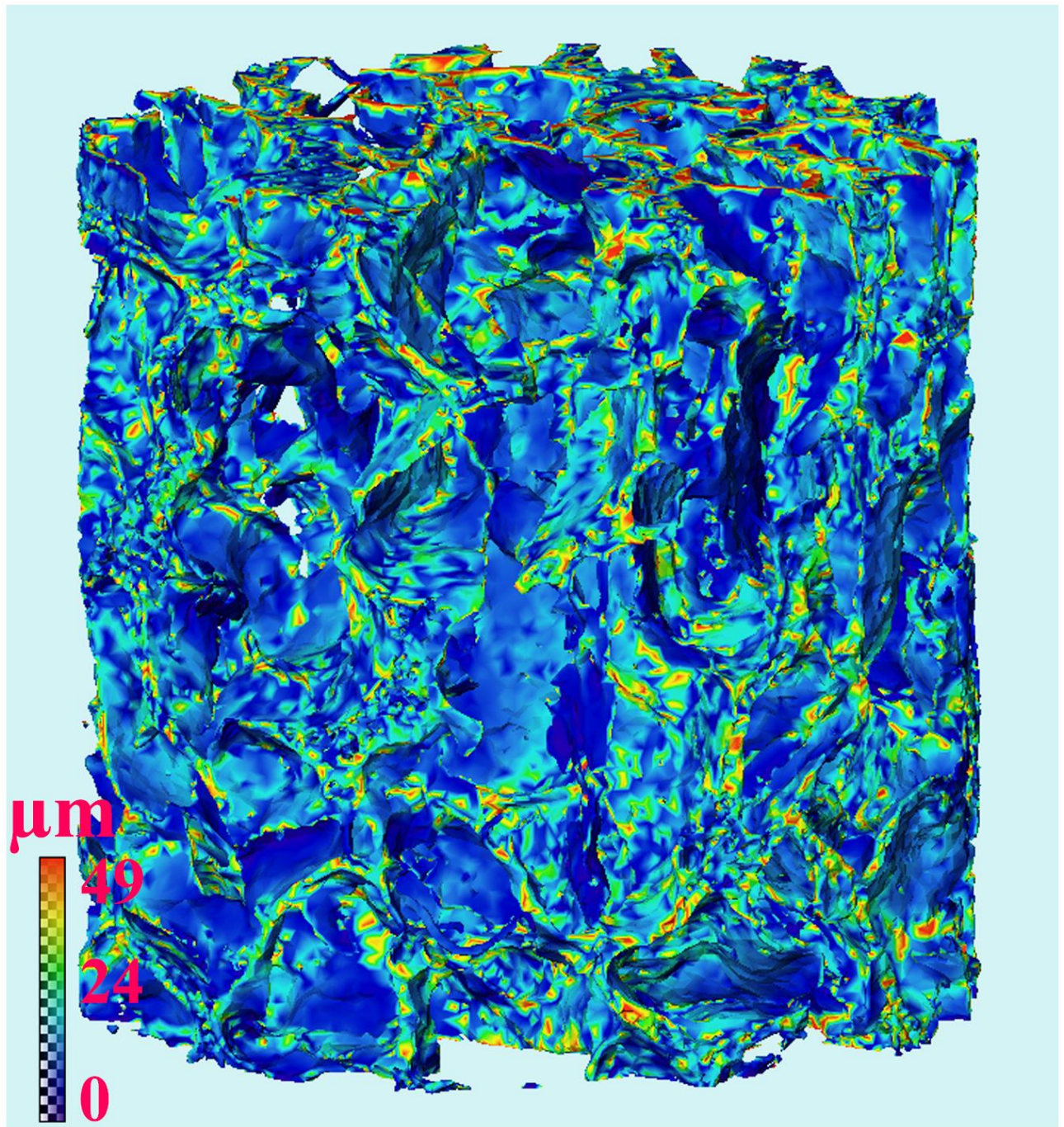


Fig. S17 The wall thickness distribution of CNPK-4 derived from 3D reconstruction.

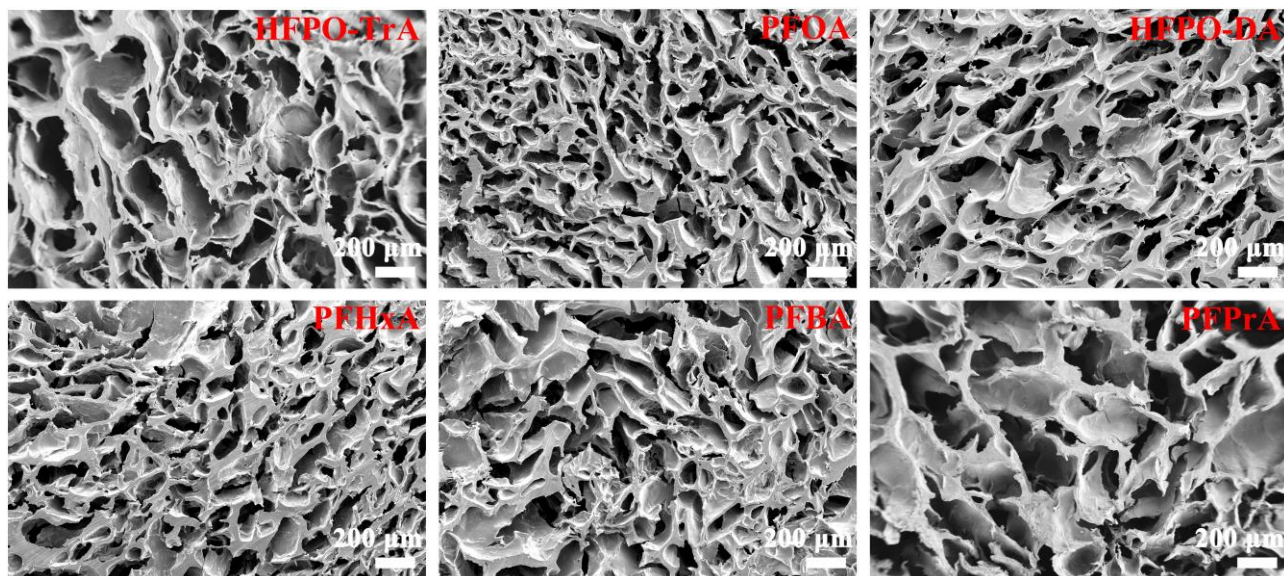


Fig. S18 Microstructure of CNPK-4 after 5 cycles of adsorption of different PFAS.

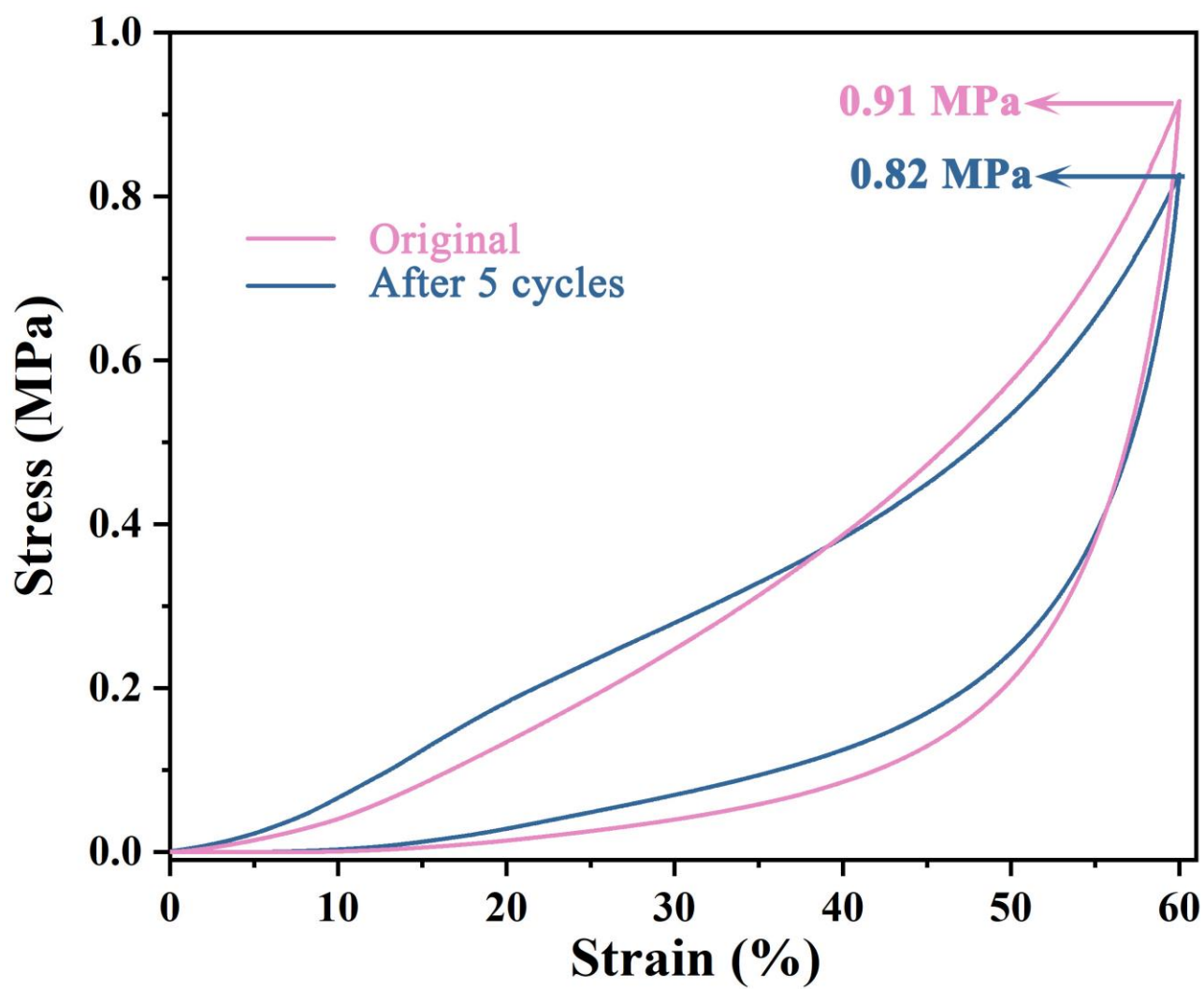


Fig. S19 Changes in mechanical properties of CNPK-4 after 5 cycles.

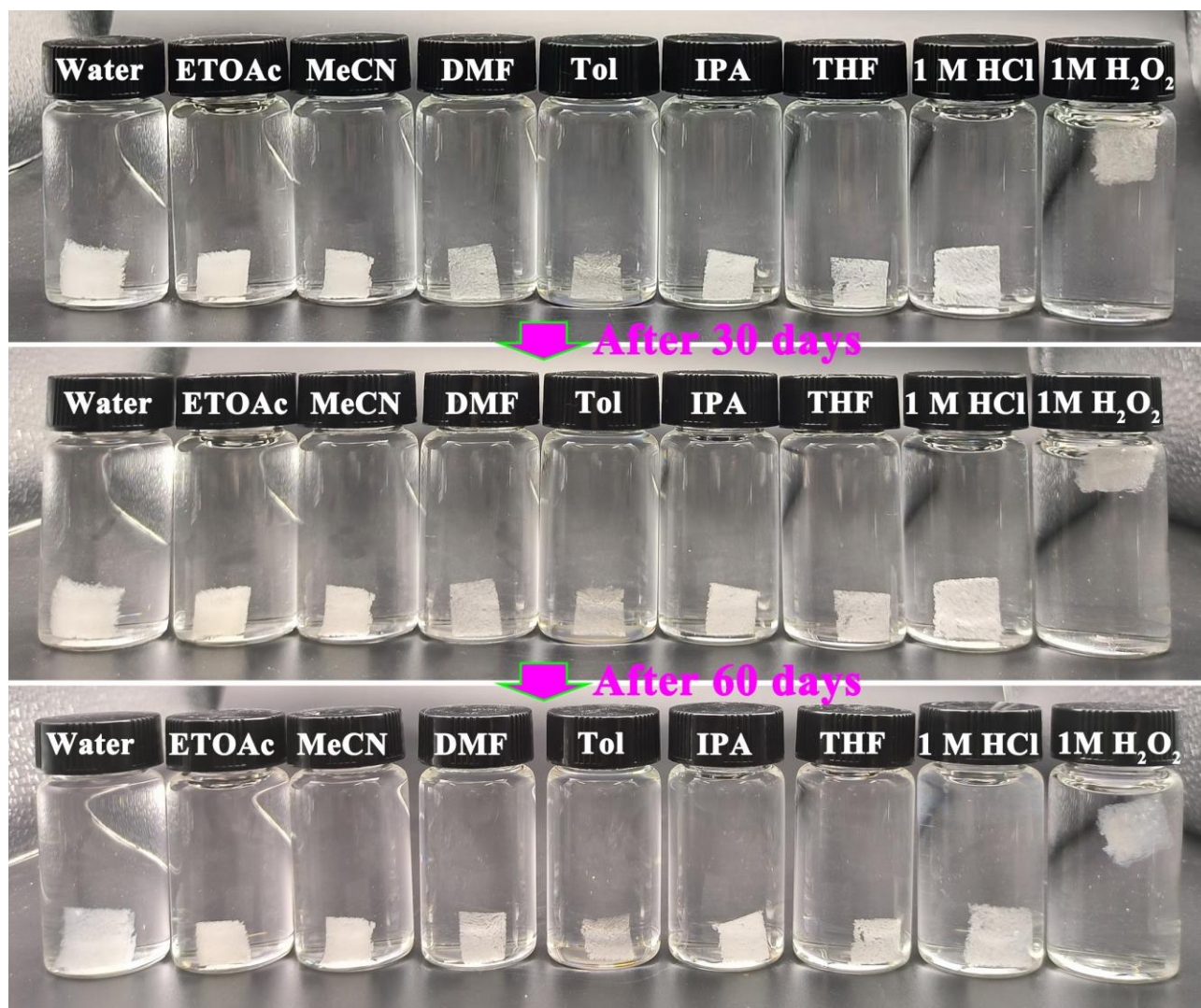


Fig. S20 Optical photos of xerogel after immersion in various solvents for 60 days.

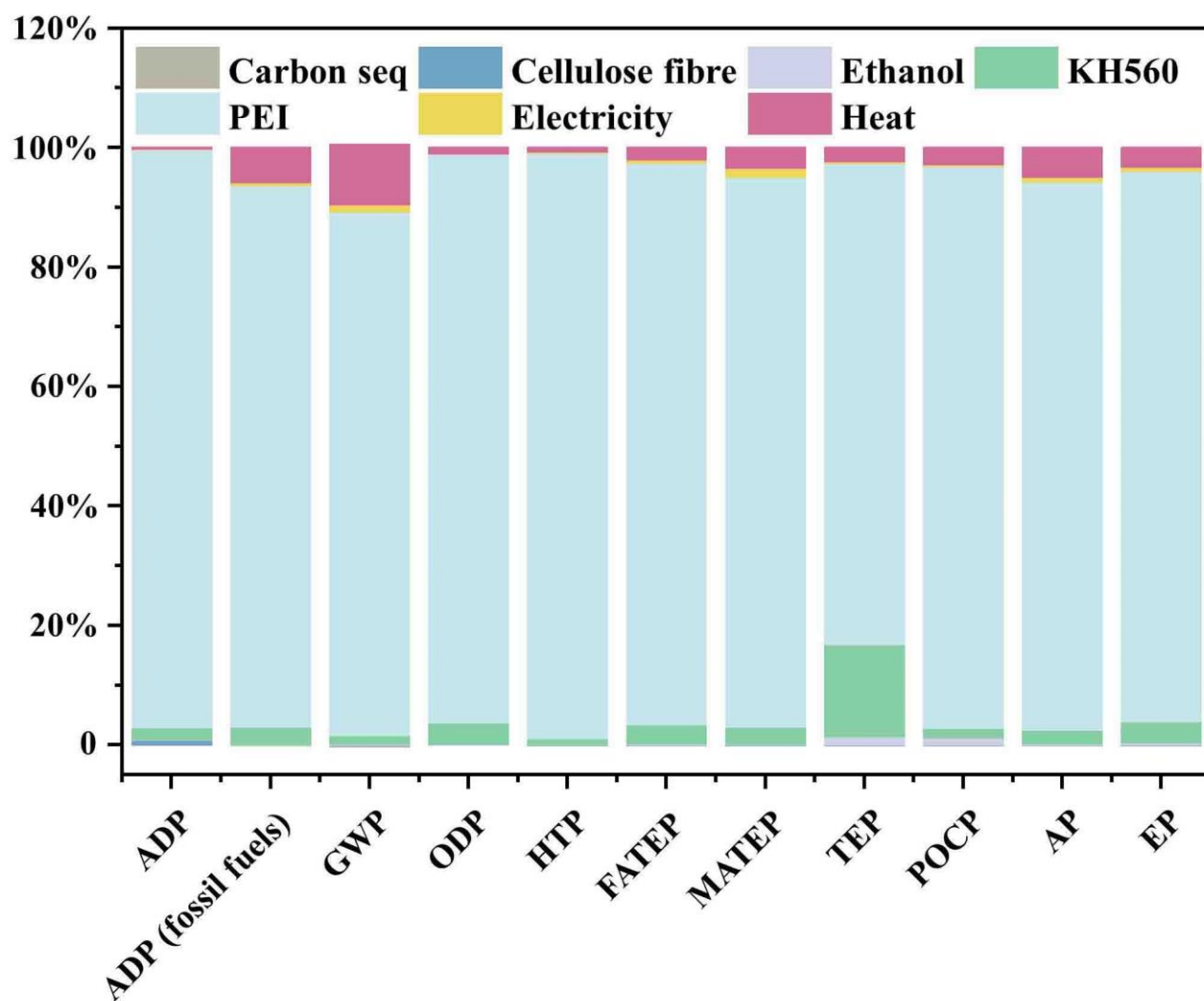


Fig. S21 Contribution analysis of the environmental impact of xerogel production.

276 **Table S1** Chromatography and Ion Source Parameters.

LC method	
Mobile phase A:	0.2 mM ammonium acetate in H ₂ O
Mobile phase B:	Acetonitrile
Column:	C18 (1.7 μm, 2.1×50 mm)
Column temperature (°C):	40
Injection volume (μL):	5
Flow rate (mL/min):	0.3
MS method	
Ion Source:	ESI
Polarity:	Negative
Gas temp (°C):	450
Gas flow (L/h):	900
Nebulizer (Bar):	7
Capillary voltage (kV):	0.5

277
278 **Table S2** Complete MRM parameters for each analyte measured in targeted analysis.

Compound	Parent (m/z)	Daughter (m/z)	Dwell (s)	Cone (V)	Collision (V)
HFPO-TrA	494.9	184.9	0.162	34	6
PFOA	413	169	0.162	15	18
HFPO-DA	328.9	168.9	0.162	36	12
PFHxA	313	119	0.163	15	20
PFBA	212.9	169	0.247	20	8
PFPrA	162.8	119	0.497	6	10

279
280 **Table S3** Performance comparison of cellulose-based aerogel.

Material	Preparation	Stress (Mpa)	Number of cycles	Ref.
Ct-Cel5	Freeze drying	< 0.025 (40%)	500 (40%)	26
X12.5	Ambient drying	0.782 (80%)	1 (80%)	29
Cellulose ethanol gels	Ambient drying	0.028 (70%)	1 (70%)	30
Cellulose aerogel	Ambient drying	< 0.080 (50%)	5 (50%)	31
BGP1.0 BGP1.5	Ambient drying	0.026 (50%) 0.017 (50%)	1 (50%)	32
BC aerogel IMr-BC aerogel	Ambient drying	0.194 (50%) 0.231 (50%)	150 (40%)	33
TCNF aerogel TD aerogel TDB aerogel	Freeze drying	0.020 (80%) 0.450 (80%) 0.370 (80%)	1 (80%)	16
CP-D CPM-D	Freeze drying	0.037 (80%) 0.043 (80%)	1 (80%)	34

CNPK	Ambient drying	0.24 (40%) 0.91 (60%) 1.96 (80%)	10 (60%)	This work
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Table S4 Atomic percentage of elements in EDS spectra with different crosslinking agent content.

Element Sample	C	N	O	Si
CNPK-1	65.00	21.08	12.91	1.01
CNPK-2	63.69	20.48	13.77	2.05
CNPK-3	63.04	17.50	16.67	2.78
CNPK-4	63.55	16.57	16.45	3.43
CNPK-5	63.31	15.98	16.78	3.93

Table S5 Summary of the Langmuir and Freundlich for PFAS adsorption onto CNPK-4 xerogel.

Sample	Langmuir Model			Freundlich Model		
	q_{max}	k_L	R²	K_f	n	R²
HFPO-TrA	3261.86	2.387	0.996	1643.14	5.283	0.854
PFOA	1827.13	1.045	0.983	727.58	4.374	0.900
HFPO-DA	2147.22	0.435	0.960	776.95	4.098	0.824
PFHxA	1270.69	1.785	0.983	563.80	5.134	0.836
PFBA	1017.16	0.190	0.995	231.05	3.094	0.924
PFPrA	1010.34	0.077	0.991	181.51	2.829	0.933

Table S6 Comparison of adsorption capacities for PFAS between CNPK and other adsorbents.

	pH	T (°C)	Adsorbent dosage (g/L)	Q_{max} (mg/g)						Ref.
				HFPO -TrA	PFOA	HFPO -DA	PFHxA	PFBA	PFPrA	
AC	n.a.	24	0.1	n.a.	n.a.	n.a.	n.a.	5.0	1.2	35
A900	n.a.	24	0.1	n.a.	n.a.	n.a.	n.a.	14.7	10.8	35
GAC	3	25	0.05	n.a.	161.4	n.a.	n.a.	n.a.	n.a.	25
AI400	3	25	0.05	n.a.	1209.1	n.a.	n.a.	n.a.	n.a.	25
A520E	7	22	0.22	n.a.	217.8	n.a.	n.a.	238	n.a.	36
PAC	7	22	0.22	n.a.	172.6	n.a.	n.a.	53.5	n.a.	36
PAM-PANI	6	25	1	n.a.	41.7	n.a.	n.a.	n.a.	n.a.	37
PEI-PVC NF	7	25	0.2	n.a.	234.8	n.a.	n.a.	98.7	n.a.	37
PMO-NH-0	7	22	0.5	n.a.	n.a.	n.a.	n.a.	303.0	n.a.	38
PMO-NH-CF-1								263.2		
PMO-NH-CF-2								227.3		
PMO-NH-CF-3								192.3		
QC-CMPS	4-10	25	0.5	n.a.	35	31	n.a.	n.a.	n.a.	39
RAPIMER	2	23	0.02	n.a.	3529	n.a.	n.a.	n.a.	n.a.	21
PCN-1003	1-12	25	1	n.a.	642	n.a.	n.a.	n.a.	n.a.	40
TG-PD COF	n.a	24	0.1	n.a	2600	n.a	n.a	n.a	n.a	41
PCN-1002	n.a	25	1	n.a	632	n.a	n.a	n.a	n.a	42
COFs	7	n.a	0.05	1.071	n.a	0.679	n.a	n.a	n.a	43

CNPK xerogel	3	25	0.1	3261.8 6	1827.13	2147.2 2	1270.69	1017.16	1010.34	This work
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Table S7 The kinetics parameters of pseudo-first-order, pseudo-second-order for PFAS adsorption onto CNPK-4 xerogel.

100 ppb (Single)	Experi mental $q_{e(exp)}$	Pseudo-first-order model			Pseudo-second-order model		
		q_e (mg·g ⁻¹)	k_1 (h ⁻¹)	R ²	q_e (mg·g ⁻¹)	k_2 (h ⁻¹)	R ²
HFPO-TrA	1.036	1.036	0.368	0.999	1.041	3.167	0.999
PFOA	1.005	0.996	0.440	0.999	1.000	5.654	0.999
HFPO-DA	0.998	0.989	0.379	0.999	0.996	3.078	0.999
PFHxA	0.999	0.997	0.390	0.999	1.002	4.051	0.999
PFBA	0.972	0.883	0.077	0.954	1.005	0.099	0.990
PFPrA	0.861	0.872	0.028	0.991	1.107	0.025	0.997
100 ppb (Mix)	Experi mental $q_{e(exp)}$	Pseudo-first-order model			Pseudo-second-order model		
		q_e (mg·g ⁻¹)	k_1 (h ⁻¹)	R ²	q_e (mg·g ⁻¹)	k_2 (h ⁻¹)	R ²
HFPO-TrA	1.036	1.036	0.516	1	1.037	13.904	1.000
PFOA	0.997	0.999	0.501	0.999	1.000	13.800	0.999
HFPO-DA	0.991	0.988	0.328	0.999	0.997	2.100	0.999
PFHxA	1.002	0.992	0.317	0.999	1.004	1.750	0.999
PFBA	1.022	1.005	0.087	0.997	1.118	0.111	0.997
PFPrA	0.941	0.934	0.062	0.998	1.080	0.069	0.990

Table S8 Detailed textural characteristics and porosimetry properties of CNPK-4 xerogel.

Total pore area (m ² /g)	Total pore volume (cm ³ /g)	Medianpore size A (nm)	Medianpore size V (nm)	Average pore size 4V/A (nm)	Porosity %	Bulk density g/mL
2.210	2.412	6.57	94039.23	4367.60	80.7751	0.3348

Table S9 The adsorption energy of xerogel for PFAS calculated by Molecular dynamics simulation.

PFAS	Adsorption energy (kJ/mol)		
	Coulomb Force	Van der Waals Force	Total
HFPO-TrA	-7.9	-31.26	-39.16
PFOA	-8.96	-21.62	-30.58
HFPO-DA	-9.48	-24.6	-34.08
PFHxA	-9.48	-23.42	-32.9
PFBA	-7.5	-14.72	-22.22
PFPrA	-4.78	-12.28	-17.06

Table S10 Parameters of the simulated wastewater.

TOC (mg/L)	BOD (mg/L)	TP (mg/L)	NH ⁺ ₄ -N (mg/L)	Fe (mg/L)	Cu (mg/L)	Ni (mg/L)	Cr (mg/L)	Ba (mg/L)	Pb (mg/L)
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440	22.6	0.79	2	3.6	4	0.5	1.5	0.37	0.25
Cd	Zn	Mn	Ca	Mg	Co	F	HA		
(mg/L)	(mg/L)	(mg/L)	(mg/L)	(mg/L)	(mg/L)	(mg/L)	(mg/L)		
0.15	0.22	0.23	59.3	53.6	0.56	10	10		

Table S11 Materials and energy inputs for xerogel.

Materials/energy	Account	Unit	Description
Inputs			
Nanocellulose dry	35.46	kg	Cellulose fibre ⁴⁴ market for cellulose fibre Cut-off, U
Water ^a	3.37	kg	Water, unspecified natural origin, CN
KH560 silane coupling agent	92.86	kg	-
PEI ^b	232.14	kg	-
Ethanol ^a	49.94	kg	Ethanol, without water, in 95% solution state, from fermentation ⁴⁴ market for ethanol, without water, in 95% solution state, from fermentation Cut-off, U
Electricity-stiring 500 rpm, 0.5 h ^c	256.97	kWh	Electricity, medium voltage ⁴⁵ market group for electricity, medium voltage Cut-off, U
Electricity 4-freezing, - 30 °C,1 h ^c	48.41	kWh	Electricity, medium voltage ⁴⁵ market group for electricity, medium voltage Cut-off, U
Electricity-ethanol/water separation ^d	0.99	kWh	Electricity, medium voltage ⁴⁵ market group for electricity, medium voltage Cut-off, U
Cooling water ^d	11928.19	kg	Water, cooling, unspecified natural origin, CN
Heat ^d	19292.84	MJ	Heat, from steam, in chemical industry ⁴⁴ market for heat, from steam, in chemical industry Cut-off, U
Output			
Xerogel	360.46	kg	-

a: Cyclic make-up is calculated using Aspen Plus; b: Inventory data was obtained from previous work⁸; c: The electricity consumption for the stirring and freezing processes was corrected according to previous work⁹; d: Data were obtained by Aspen Plus scale-up simulation.

Table S12 Materials and energy inputs for KH560^a.

Materials/energy	Account	Unit	Description
Inputs			
C ₃ H ₆ O ^b	559.65	kg	-
NaOH	385.97	kg	Sodium hydroxide, without water, in 50% solution state ⁴⁶ market for sodium hydroxide, without water, in 50% solution state Cut-off, U
C ₃ H ₅ ClO	901.48	kg	Epichlorohydrin ⁴⁶ market for epichlorohydrin Cut-off, U

Si	245.61	kg	Silicone product ⁴⁴ market for silicone product Cut-off, U
CH ₃ OH	1092.11	kg	Methanol ⁴⁶ market for methanol Cut-off, U
Heat	4212.32	MJ	Heat, from steam, in chemical industry ⁴⁴ market for heat, from steam, in chemical industry Cut-off, U
Electricity	20.74	kWh	Electricity, medium voltage ⁴⁵ market group for electricity, medium voltage Cut-off, U
Cooling water	1574.39	kg	Water, cooling, unspecified natural origin, CN
Output			
KH560	1765.55	kg	-
Wastewater	1228.04	kg	Waste water/m ³ ³
Water	173.69	kg	Water, decarbonised ⁴⁵ market for water, decarbonised Cut-off, U
H ₂	17.54	kg	Hydrogen, gaseous ⁴⁶ market for hydrogen, gaseous Cut-off, U

a: Inventory data was obtained from previous work⁵⁻⁷; b: Inventory data was obtained from previous work⁴⁷.

305 **Table S13** Full LCA results of xerogel.

Impact category	Unit	Total	Carbon seq.	Cellulose fibre	Ethanol	KH560	PEI	Electricity	Heat
ADP	kg Sb eq	7.38E-04	0.00E+00	6.01E-06	1.08E-06	1.49E-05	7.13E-04	5.18E-07	1.73E-06
ADP (fossil fuels)	MJ	1.40E+03	0.00E+00	3.51E-01	7.37E-01	4.22E+01	1.27E+03	7.24E+00	8.11E+01
GWP	kg CO ₂ eq	6.78E+01	-1.60E-01	3.29E-02	1.19E-01	9.65E-01	5.93E+01	8.03E-01	6.76E+00
ODP	kg CFC-11 eq	7.01E-06	0.00E+00	4.29E-10	8.22E-09	2.53E-07	6.68E-06	1.45E-09	7.06E-08
HTP	kg 1,4-DB eq	1.81E+02	0.00E+00	4.45E-02	1.97E-01	1.83E+00	1.77E+02	3.13E-01	1.30E+00
FATEP	kg 1,4-DB eq	3.69E+01	0.00E+00	3.45E-02	7.89E-02	1.18E+00	3.47E+01	2.06E-01	7.34E-01
MATEP	kg 1,4-DB eq	8.08E+04	0.00E+00	6.52E+01	6.36E+01	2.33E+03	7.43E+04	1.21E+03	2.80E+03
TEP	kg 1,4-DB eq	5.35E-01	0.00E+00	4.50E-04	7.27E-03	8.25E-02	4.31E-01	1.83E-03	1.22E-02
POCP	kg C ₂ H ₄ eq	3.81E-02	0.00E+00	9.29E-06	4.85E-04	5.99E-04	3.58E-02	1.32E-04	1.06E-03
AP	kg SO ₂ eq	4.15E-01	0.00E+00	2.02E-04	9.05E-04	9.68E-03	3.80E-01	3.51E-03	2.01E-02
EP	kg PO ₄ ⁻ eq	1.15E-01	0.00E+00	6.80E-05	5.07E-04	3.97E-03	1.06E-01	7.63E-04	3.71E-03

306

307 **Table S14** Full LCA results of xerogel, chitin cryogel, chitosan cryogel, polyvinyl alcohol aerogels, amidoxime functionalized, schiff base functionalized silica
308 aerogel and mercapto functionalized aerogel.

Impact category	Xerogel	2wt% chitin cryogel	2wt% chitosan cryogel	Polyvinyl alcohol aerogels	Amidoxime functionalized	Schiff base functionalized silica aerogel	Mercapto functionalized aerogel
ADP	7.38E-04	4.82E-04	4.41E-04	2.74E-04	9.00E-03	1.00E-02	1.80E-02
ADP (fossil fuels)	1.40E+03	1.46E+03	1.33E+03	3.16E+03	NA	NA	NA
GWP	6.78E+01	1.41E+02	1.30E+02	3.43E+02	6.90E+01	7.63E+01	1.18E+02
ODP	7.01E-06	4.04E-06	1.01E-05	2.77E-06	9.53E-06	1.53E-04	1.90E-05
HTP	1.81E+02	8.75E+01	6.91E+01	1.38E+02	NA	NA	NA
FATEP	3.69E+01	5.85E+01	4.16E+01	9.05E+01	NA	NA	NA
MATEP	8.08E+04	2.02E+05	1.68E+05	5.16E+05	NA	NA	NA
TEP	5.35E-01	1.99E+00	6.00E-01	8.45E-01	NA	NA	NA
POCP	3.81E-02	4.04E-02	2.51E-02	5.84E-02	NA	NA	NA
AP	4.15E-01	6.59E-01	5.66E-01	1.50E+00	2.90E-01	3.20E-01	4.66E-01
EP	1.15E-01	2.33E-01	4.74E-01	3.31E-01	4.00E-02	4.00E-02	6.40E-02

309

310 **Table S15** Full LCA results of xerogel, GAC and PAC for PFOA.

Impact category	Xerogel	GAC	PAC
ADP	4.04E-04	9.85E-06	9.21E-06
ADP (fossil fuels)	765.54266	228.80723	213.95994
GWP	37.129906	20.501787	19.171428
ODP	3.84E-06	1.01E-07	9.47E-08
HTP	99.02023	8.5015247	7.9498615
FATEP	20.19798	6.0985365	5.7028029
MATEP	44211.099	22655.675	21185.55
TEP	0.29284297	0.05283493	0.04940647
POCP	0.02082997	0.00557926	0.00521722
AP	0.226943	0.12175803	0.11385716
EP	0.06284724	0.03302855	0.03088533

311
312 **Table S16** Full LCA results of xerogel, AC, GAC and PAC for PFBA.

Impact category	Xerogel	AC	GAC	PAC
ADP	7.25E-04	3.18E-04	2.37E-04	2.97E-05
ADP (fossil fuels)	1375.1484	7385.8972	5495.7864	690.27077
GWP	66.696651	661.79768	492.4383	61.850251
ODP	6.90E-06	3.27E-06	2.43E-06	3.06E-07
HTP	177.87057	274.42922	204.20056	25.647591
FATEP	36.281741	196.86076	146.4825	18.398202
MATEP	79416.637	731325.19	544173.16	68348.149
TEP	0.52603542	1.7055114	1.2690572	0.15939359
POCP	0.03741699	0.18009835	0.13400973	0.01683162
AP	0.40765894	3.9303492	2.9245411	0.36732236
EP	0.11289284	1.0661614	0.79332211	0.09964126

313
314 **Table S17** Full LCA results of xerogel and GAC for PFPrA.

Impact category	Xerogel	GAC
ADP	7.30E-04	0.0013249
ADP (fossil fuels)	1384.4309	30774.572
GWP	67.146867	2757.4904
ODP	6.94E-06	1.36E-05
HTP	179.07124	1143.4551
FATEP	36.52665	820.25316
MATEP	79952.715	3047188.3
TEP	0.52958626	7.1062975

POCP	0.03766956	0.75040979
AP	0.41041072	16.376455
EP	0.11365489	4.4423394

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Scalable and sustainable cellulose xerogels for high-capacity enrichment of per- and polyfluoroalkyl substances

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