Electronic Supplementary Material (ESI) for Environmental Science: Nano.

Electronic Supplementary Information

Self-indicating and high-capacity mesoporous aerogel-based biosorbent fabricated from cellulose and chitosan via co-dissolution and regeneration for removing formaldehyde from indoor air

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The Electronic Supplementary Information file has 6 pages (including this cover page), including 7 figures and 1 table (Figure S1, Figure S2, Figure S3, Figure S4, Figure S5, Figure S6, Figure S7, and Table S1 and Table S2).

Stability and leaking of the experiment setup in Figure 2 for formaldehyde adsorption

The reproducibility of the aldehyde adsorption experiment setup shown in **Figure S1** was tested. Triplicate baseline experiments were conducted without adding aerogel. After the gasification of 5 mg paraformaldehyde, the formaldehyde concentration in the chamber was monitored throughout 40 h. The concentration and its degradation percent average and standard deviation at every time points were calculated. The formaldehyde loss due to sampling was compensated in the calculation. The data obtained is also used as a control group for the following experiments.

As shown in **Figure S1**, the starting formaldehyde concentration was 41.3 ± 0.2 mg/m^3. The small standard deviations from 3 independent experiments indicated that the reproducibility of the gas chamber was good. The formaldehyde concentration decreased with the time linearly with a high R^2 value. The concentration declining might be from the slow adsorption on the apparatus surface, natural formaldehyde decay, and the leakage at valves and joints. The formaldehyde concentration decreased by about 12% from 41.3 to 36.5 mg/m^3 in 40 h and dropped only 2% in the first 4 h. Since the adsorption experiment with aerogels was run for 2 h, the degradation and leaking of formaldehyde were almost negligible in our experiments.

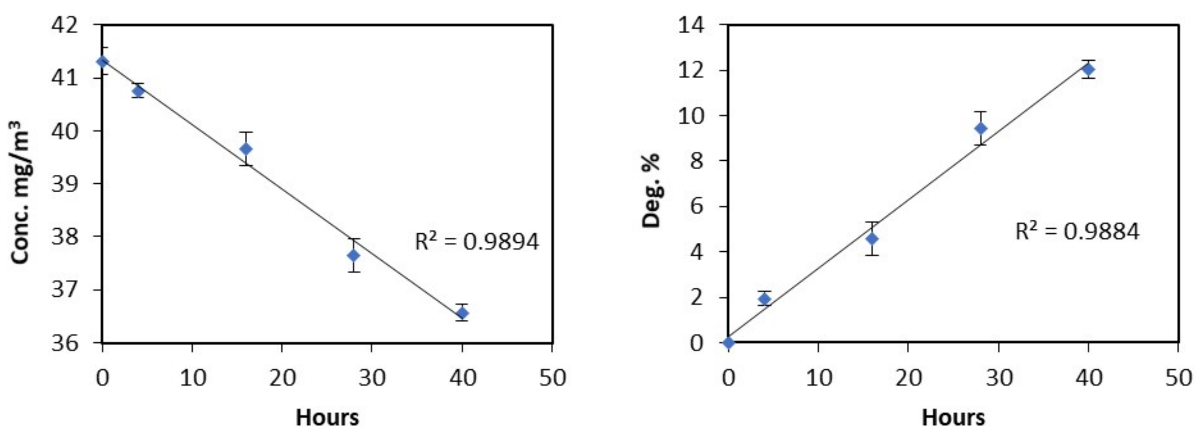

Figure S1. Change of formaldehyde concentration and degradation over time in the chamber.

Table S1. Characteristic FTIR bands and assignments of chitosan

Band, cm^{-1}	Assignment
3450	O-H of chitosan
3350	N-H and O-H stretching
2934	Asymmetrical stretching vibration of the C–H in CH_2 and CH_3 groups
1655	N-H (amide I)
1580-1600	Angular deformation of N–H bonds
1540	Amide II
1530	C-N and C-N-H bending
1420	C-N axial deformation; C-O stretching (amide I)

References:

1. Osman, Z.; Arof, A.K. FTIR studies of chitosan acetate based polymer electrolytes. Electrochimica, 2003, 48, 993-999.
2. Díaz-Visurraga, J.; Meléndrez, M.F.; García, A.; Paulraj, M.; Cárdenas, G. Semitransparent chitosan-TiO_2 nanotubes composite film for food package applications. J. Appl. Polym. Sci. 2009, 116, 3503–3515.
3. Alagumuthu, G.; Kumar, A. Synthesis and characterization of chitosan/TiO2 nanocomposites using liquid phase deposition technique. Int. J. Nanosci. Nanotechnol. 2013, 4, 105–111.
4. Kavitha, K.; Sutha, S.; Prabhu, M.; Rajendran, V.; Jayakumar, T. In situ synthesized novel biocompatible titania–chitosan nanocomposites with high surface area and antibacterial activity. Carbohydr. Polym. 2013, 93, 731–739.
5. Lustriane, C.; Dwivany, F.M., Suendo, V.; Reza, M.. Effect of chitosan and chitosan-nanoparticles on post harvest quality of banana fruits. J Plant Biotechnol. 2018, 45, 36–44.

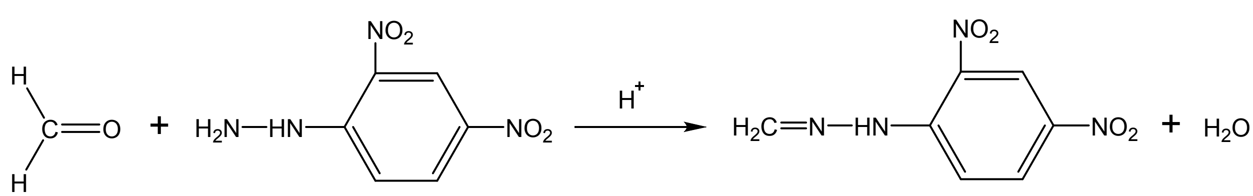

Figure S2. Reaction mechanism of 2,4 – DNPH with formaldehyde.

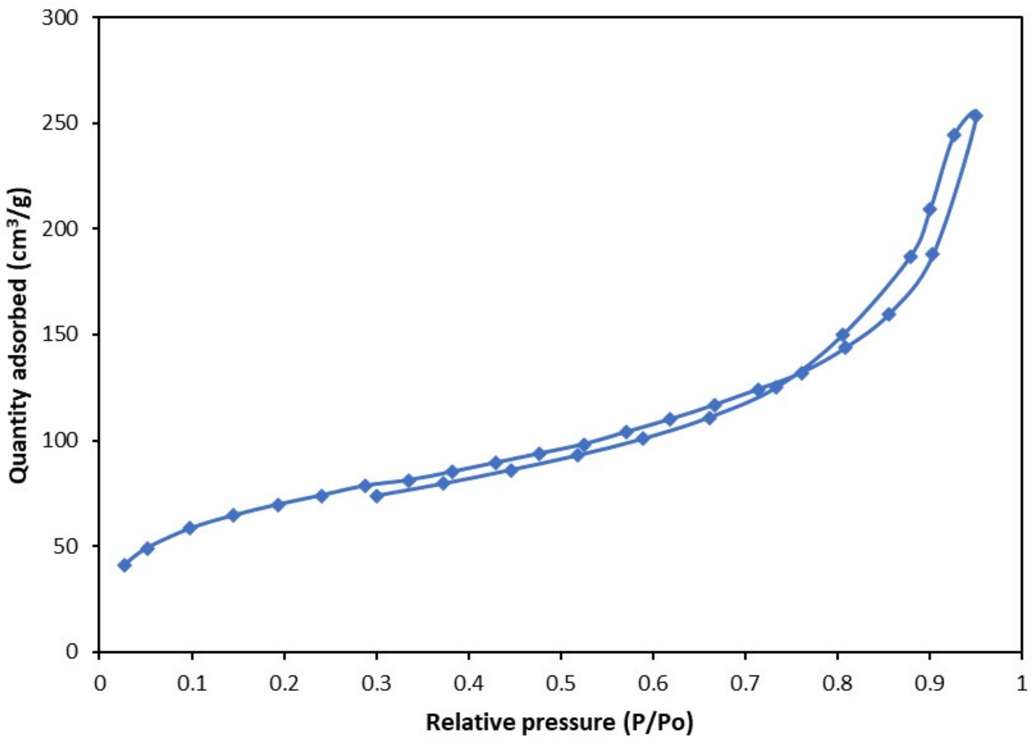

Figure S3. Nitrogen adsorption-desorption isotherm of 1.5% cellulose-chitosan 2:1 composite aerogel, indicating a typical type IV mesoporous material.

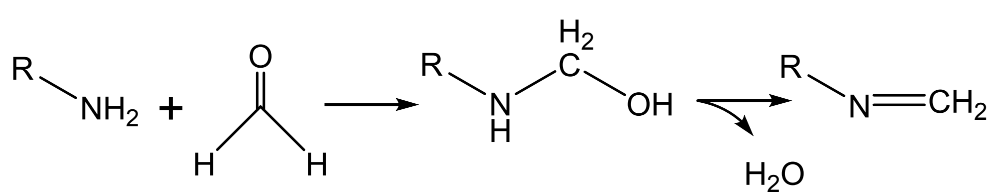

Figure S4. The mechanism of the free amino group reacts with formaldehyde.

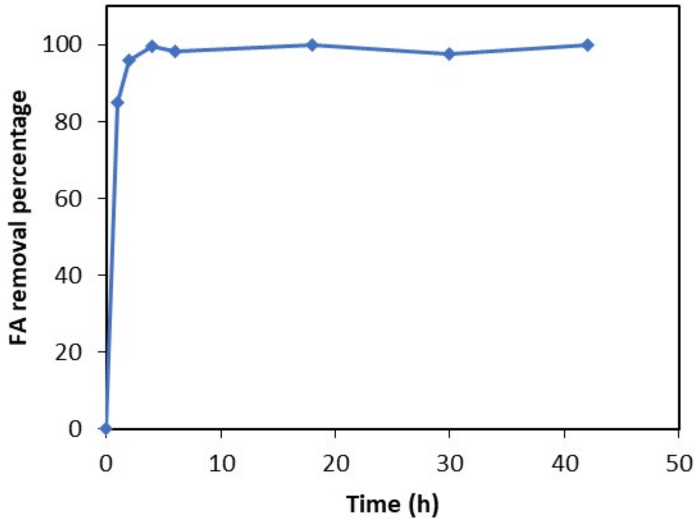

Figure S5. Formaldehyde removal percent over 42 h.

Langmuir and Freundlich isotherm model fitting of the aerogel formaldehyde adsorption

The linear form of Langmuir isotherm is expressed as:

$$\frac{C_e}{q_e} = \frac{1}{q_{max}K_L} + \frac{1}{q_{max}}C_e$$

Where, C_e is the concentration of formaldehyde at a certain time (ppm); q_e is the amount of formaldehyde gas adsorbed on aerogel (mg/g); q_{max} is the maximum amount of formaldehyde adsorbed on aerogel (mg/g); and K_L is the adsorption equilibrium constant (L/mg). By plotting C_e/q_e versus C_e, a straight line with slope $1/q_{max}$ and intercept $1/K_Lq_{max}$ is obtained.

The Freundlich isotherm is an empirical equation based on a heterogeneous surface. The isotherm is expressed by the following equation:

$$q_e = K_F C_e^{\frac{1}{n}}$$

In this equation, K_F ($mg^{(1-1/n)}L^{1/n}/g$) and n are the Freundlich constants, which represent the adsorption capacity and intensity, respectively. An n value larger than 1 means favorable adsorption.

Table S2. Langmuir and Freundlich isotherm model fitting parameters

	Langmuir parameters			Freundlich parameters		
	q_{max}	K_L	R^2	n	K_F	R^2
Cell 30 min	0.51	0.42	0.9672	1.03	2.35	0.9647
Comp 30 min	3.62	0.30	0.8916	1.31	0.64	0.9401
Comp 45 min	3.98	0.48	0.9761	1.30	0.51	0.9893
Comp 60 min	4.29	0.63	0.9730	1.31	0.46	0.9888
Comp 90 min	3.94	0.47	0.9431	1.26	0.32	0.9819

Note: Cell stands for cellulose aerogel; Comp stands for composite aerogel.

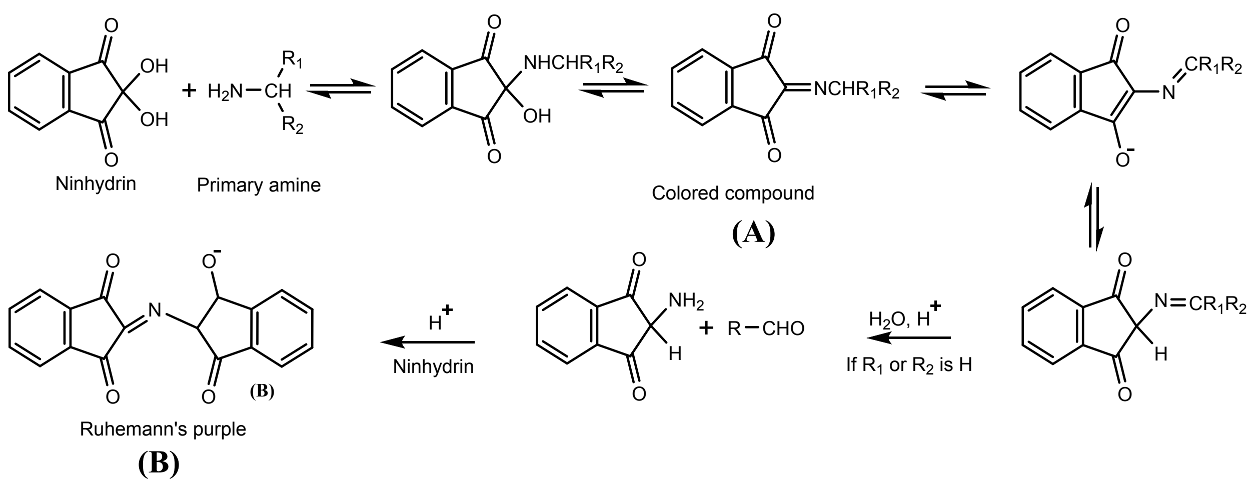

Figure S6. Reaction mechanism of ninhydrin with an amine to form Ruhemann's purple.