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Supporting Information

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Green Preparation of Shell-Based Biochar and Its Adsorption of Multi-Component Chlorinated Volatile Organic Compounds

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11 1、Materials characterization

12 The specific surface area and pore size distribution of the samples were

13 measured using the fully automated gas adsorption analyzer ASAP 2020 from

14 Micromeritics Instrument Corporation (USA). The pore structure was characterized

15 by N₂ adsorption-desorption isotherms, and the specific surface area was calculated

16 using the BET method (Testing Parameters:Sample mass: 0.1 g, Analysis adsorptive :

17 N₂, Analysis bath temp. : -195.640 °C, Equilibration interval: 10 to 15 s). The surface

18 morphology of the materials was examined using a field emission scanning electron

19 microscope (Regulus 8100) from Hitachi Ltd., Japan. The surface functional groups

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20 of the materials were determined using a Fourier transform infrared spectrometer
21 (Nicolet iS50 FT-IR) from Thermo Fisher Scientific (USA). The Raman spectra of the
22 materials were obtained using a laser Raman spectrometer (RM2000) from Renishaw
23 plc (UK), with an excitation wavelength of 532 nm and a scanning range between
24 500–3500 cm⁻¹. X-ray photoelectron spectroscopy (XPS) was performed using an
25 ESCALAB 250 system from Thermo Fisher Scientific (USA), with Al-K α radiation at
26 a power of 150 W. The elemental content of the materials was analyzed using an
27 elemental analyzer (Vario EL cube) from Elementar Analysensysteme GmbH
28 (Germany) via the combustion method. The thermal stability of the shell-derived
29 biochar adsorbent was evaluated using a thermogravimetric analyzer (TGA/DSC 3+)
30 from Mettler-Toledo Group (Switzerland).

31 2、Calculation of adsorption capacity

32 The adsorption capacities of VOCs were calculated by integrating the
33 breakthrough curve using the following equation. The breakthrough time was defined
34 as the time when the outlet concentration of VOCs was 5% of the inlet concentration,
35 and the equilibrium adsorption time was the time required for an equal concentration
36 of the VOC at the outlet and inlet.

$$37 q = \frac{FC_0 10^{-9}}{W} \left[t_s - \int_0^{t_s} \frac{C_i}{C_0} dt \right]$$

38 where q (g·g⁻¹) is the estimated maximum adsorption capacity, F (mL·min⁻¹) is
39 the total gas flow, C_0 and C_i (mg·m⁻³) is the inlet and outlet gas concentration,
40 respectively, W (g) is the mass of adsorbent, and t_s (min) is the adsorption time.