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# Supporting Information

## Constructing “breathing” dynamic skeletons with extra π-conjugated adsorption sites for iodine capture

*Lixin Xia,[a] Dongqi Yang,[a] Hongcui Zhang,[a] Qian Zhang,[a] Naishun Bu,[b] Peng Song,[c] Zhuojun Yan,*[a] and Ye Yuan*[d]*

a. College of Chemistry, Liaoning University, Shenyang 110036, P. R. China.
E-mail: zjyan@lnu.edu.cn
b. School of Environmental Science, Liaoning University, Shenyang 110036, P. R. China.
c. Department of Physics, Liaoning University, Shenyang 110036, P. R. China.
d. Key Laboratory of Polyoxometalate Science of the Ministry of Education, Faculty of Chemistry, Northeast Normal University, Changchun 130024, P. R. China.
E-mail: Yuany101@nenu.edu.cn

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## Experiment section:

*Materials*: 9,10-Dibromoanthracene was received from Alfa. 2,6-Dibromonaphthalene and 2,7-dibromofluorene were received from Energy Chemical. 1,4-Dibromonaphthalene and 4-(tetramethyl-1,3,2-dioxaborolan-2-yl)-N,N-bis-[4-(tetramethyl-1,3,2-dioxaborolan-2-yl) phenyl]aniline (BBA) were purchased from J&K Chemical. Tetrakis(triphenylphophine)palladium was got from Sigma-Aldrich. Other chemicals and solvents were purchased from commercial suppliers and used without further purification unless otherwise noted. All reactions were performed under a purified nitrogen atmosphere.

*Preparation of PAF samples*: 311 mg (0.96 mmol) of 2,7-dibromofluorene and 399 mg (0.64 mmol) of BBA were added to 60 mL THF and degassed by three freeze–pump–thaw cycles. Then 5 mL of potassium carbonate solution (2 M) and 40 mg of tetrakis(triphenylphosphine)palladium were followed by degassing for three freeze–pump–thaw cycles. After the mixture was heated to 80 °C under $N_2$ for 72 h, the resulting mixture was cooled to room temperature. The powder was filtered and washed with THF, water and acetone to remove the unreacted monomers or catalyst residues. The crude product was further purified by Soxhlet extractions with THF, DCM and methanol for 24 h each. The product was dried under vacuum for 10 h at 75 °C as a fine yellow powder, named as LNU-1.

LNU-2, LNU-3, and LNU-4 were synthesized through identical procedure of LNU-1 by replacing 2,7-dibromofluorene with 275 mg (0.96 mmol) of 1,4-dibromonaphthalene for LNU-2, 275 mg (0.96 mmol) of 2,6-dibromonaphthalene for LNU-3, and 323 mg (0.96 mmol) of 9,10-dibromoanthracene for LNU-4.

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*Characterization*: Fourier transform infrared spectroscopy (FTIR) spectra (film) was measured using a Shimadzn-prestige 21 transform infrared spectrometer. The solid-state $^{13}C$ cross polarization magic angle spinning nuclear magnetic resonance (CP MAS NMR) spectra was recorded on a Bruker AVANCE III model 400 MHz spectrometer. Thermogravimetric analysis (TGA) analysis was performed using a TGA/DSC 2 thermal analyzer system at the heating rate of 10 $^{o}C$ $min^{-1}$ in air atmosphere. Power X-ray diffraction (PXRD) measurement was performed by a Bruker D8 ADVANCE diffractometer using Cu-Ka radiation, 35 kV, 25 mA. Scanning electron microscope (SEM) images were obtained from a Su8010 cold field emission scanning microscopes. Transmission electron microscopy (TEM) was performed on a JEM-2100. The $N_2$ adsorption isotherm was measured on a Quantachrome AsiQ-C. Raman spectra was measured by using Renishaw inVia Raman spectrometer.

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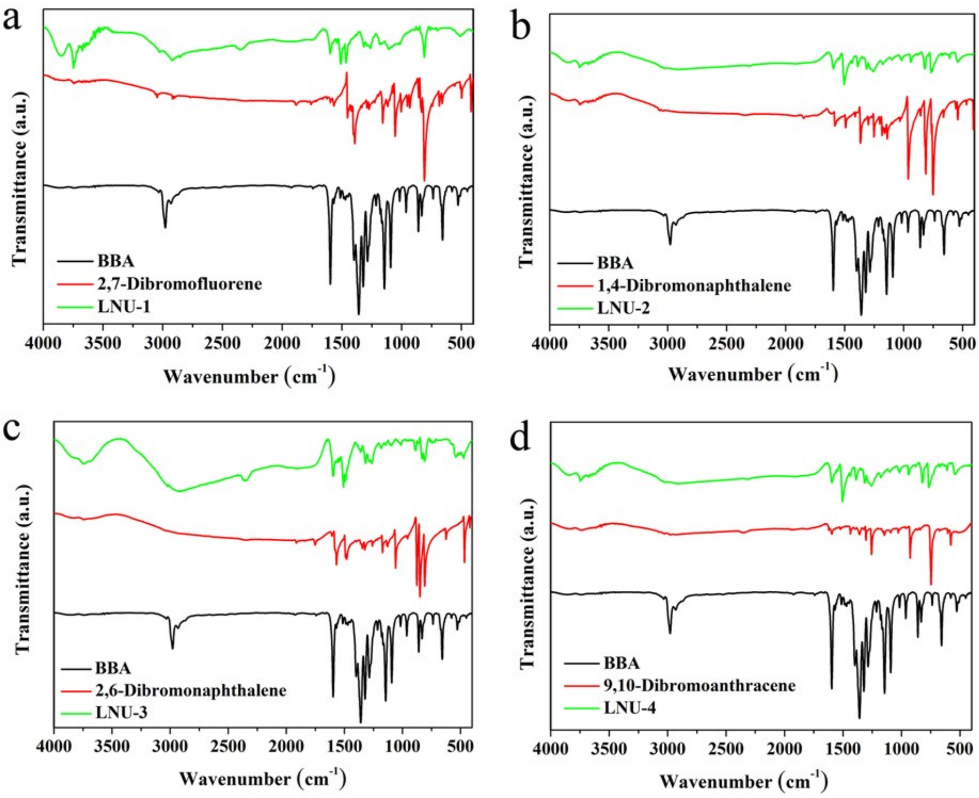

**Fig. S1** FT-IR spectra of LNU-1 (a), LNU-2 (b), LNU-3 (c), and LNU-4 (d).

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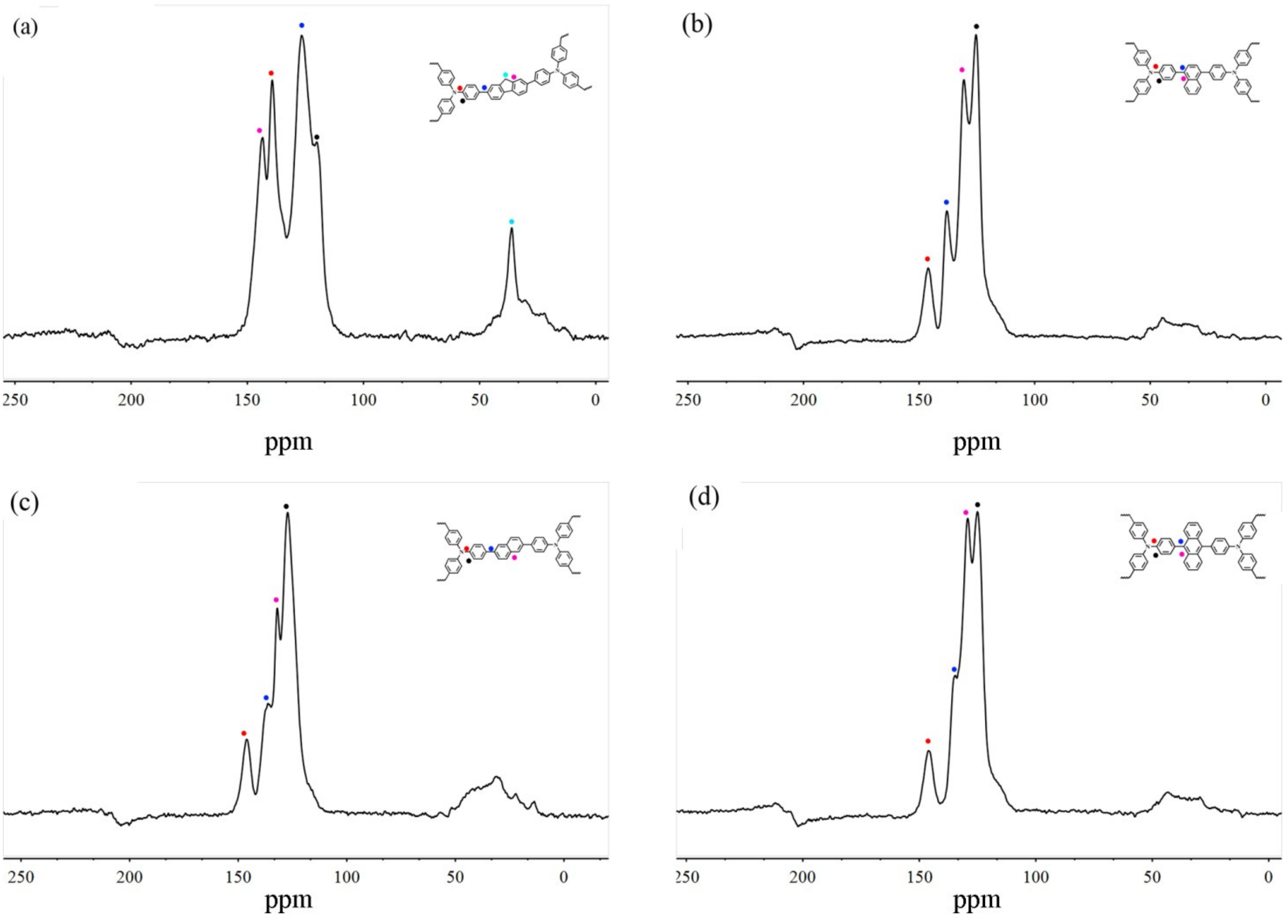

**Fig. S2** $^{13}$C CP MAS NMR spectra of LNU-1 (a), LNU-2 (b), LNU-3 (c), and LNU-4 (d).

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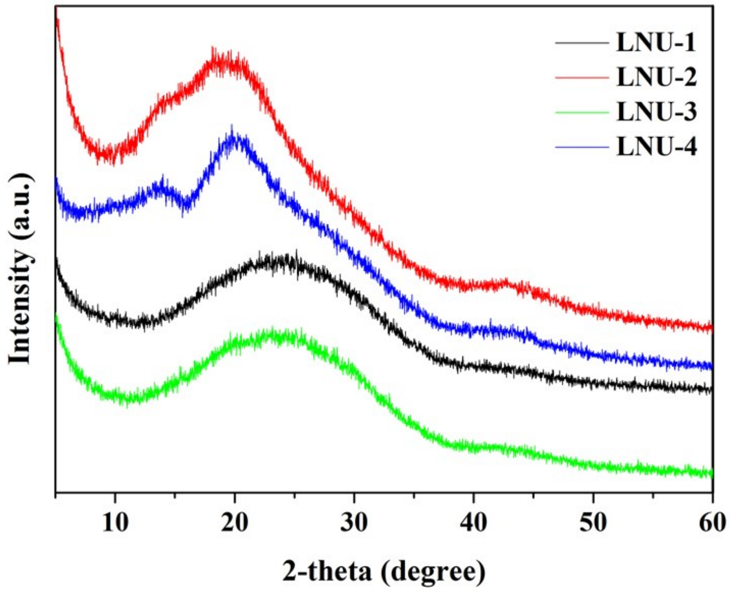

**Fig. S3** Powder X-ray diffraction patterns of LNU-1, LNU-2, LNU-3, and LNU-4.

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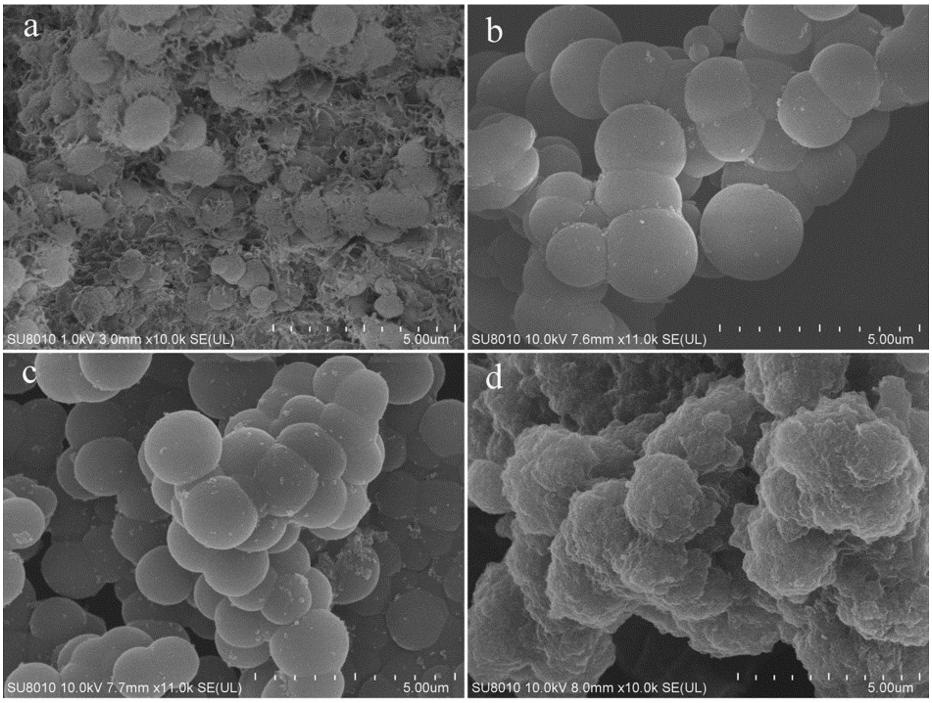

**Fig. S4** SEM images of LNU-1 (a), LNU-2 (b), LNU-3 (c), and LNU-4 (d), respectively.

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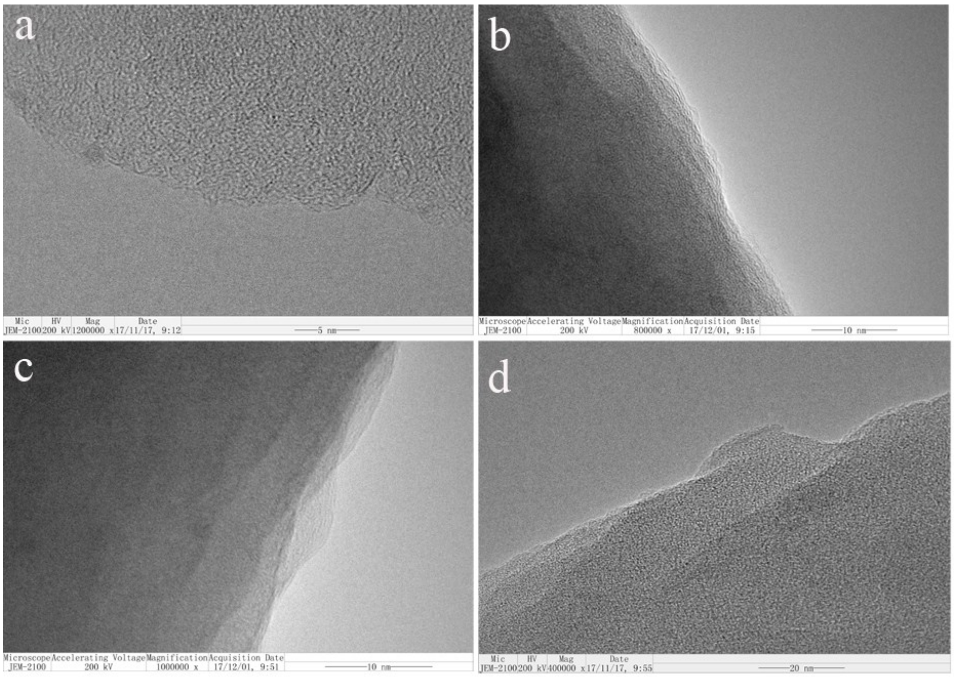

**Fig. S5** TEM images of LNU-1 (a), LNU-2 (b), LNU-3 (c), and LNU-4 (d), respectively.

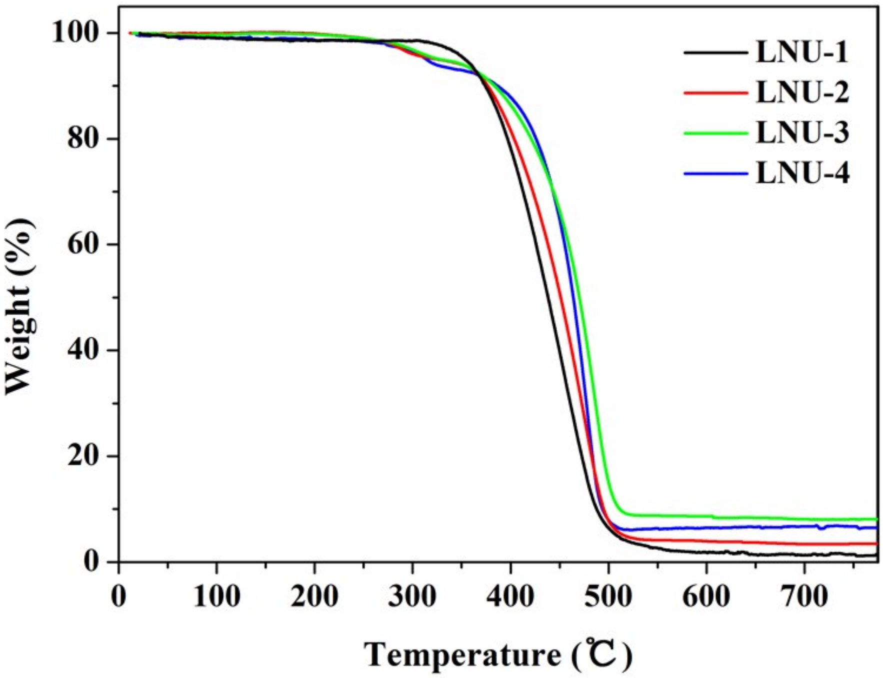

**Fig. S6** TGA plots for PAFs at air condition with the rate of 10 °C min$^{-1}$.

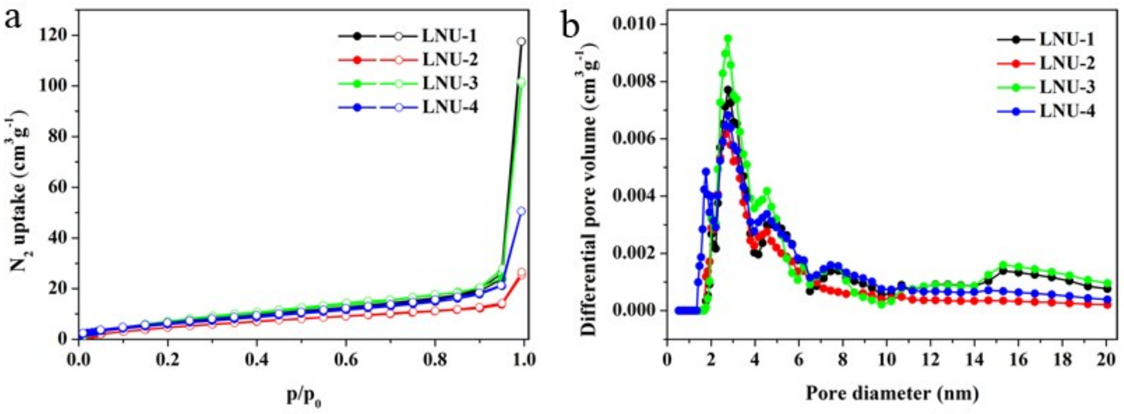

**Fig. S7** Nitrogen gas adsorption and desorption curves (a) and DFT pore size distributions (b) of LNU-1, LNU-2, LNU-3, and LNU-4, respectively.

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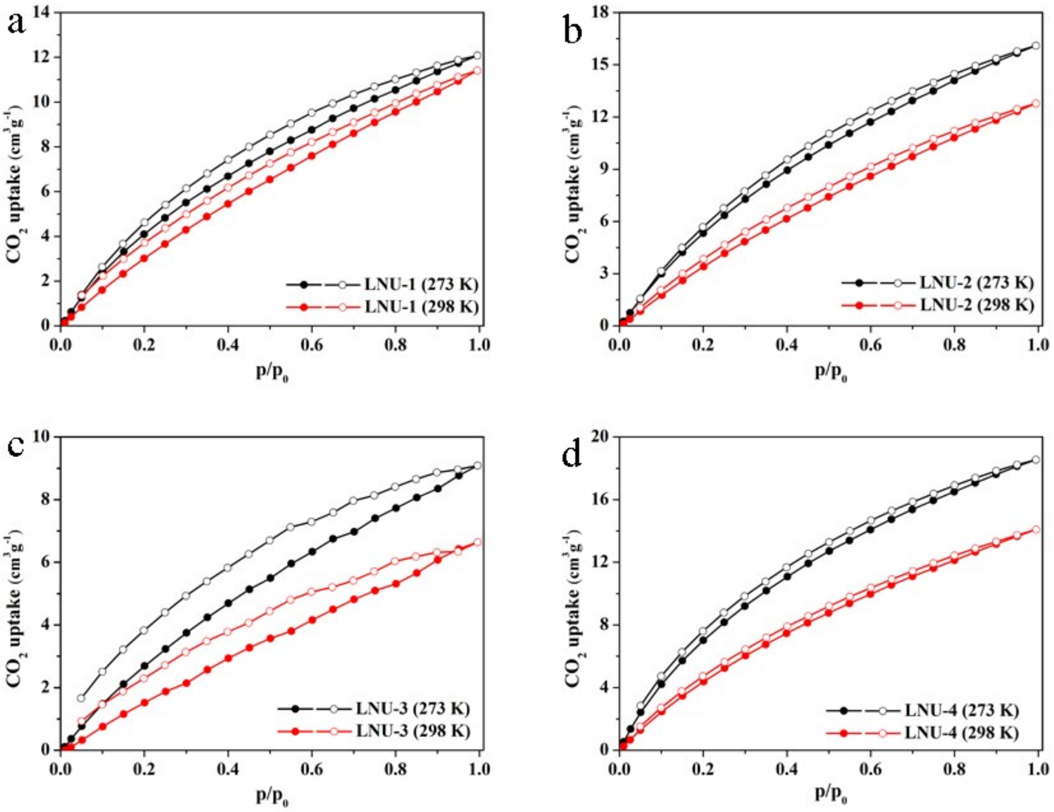

**Fig.S8** Carbon dioxide adsorption of LNU-1 (a), LNU-2 (b), LNU-3 (c), and LNU-4 (d), respectively.

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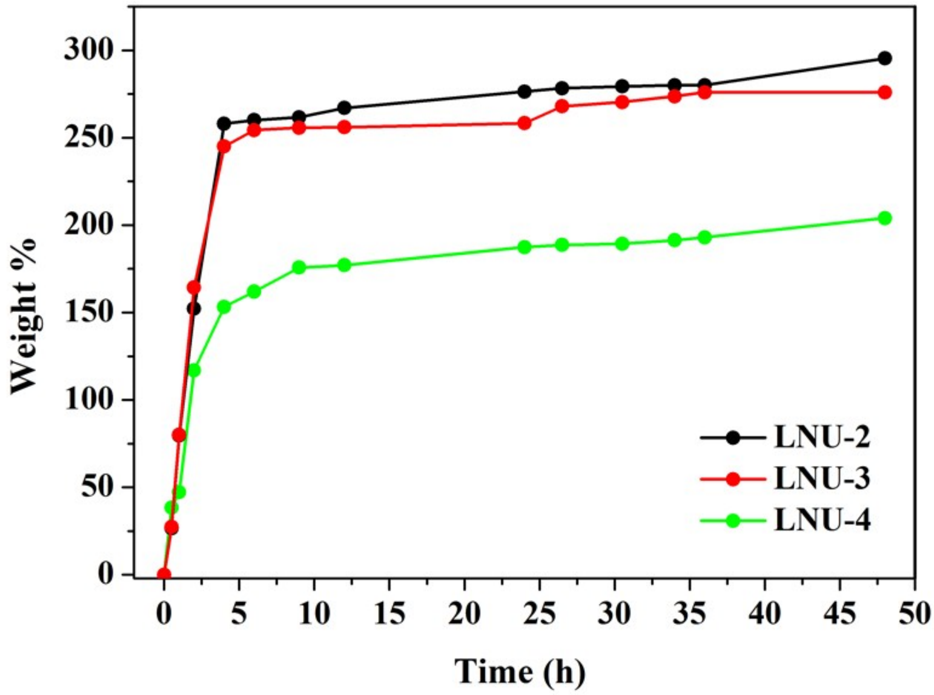

**Fig. S9** Iodine uptakes of the LNU-2, LNU-3, and LNU-4.

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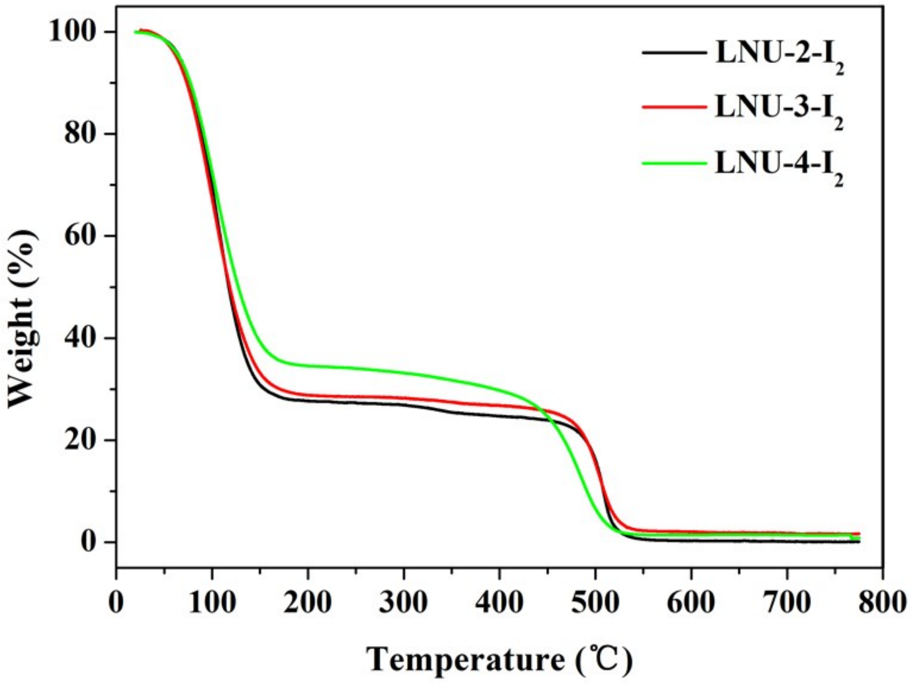

**Fig. S10** TGA plots for the iodine adsorbed LNU-2, LNU-3, and LNU-4 at air condition with the rate of 10 °C min$^{-1}$.

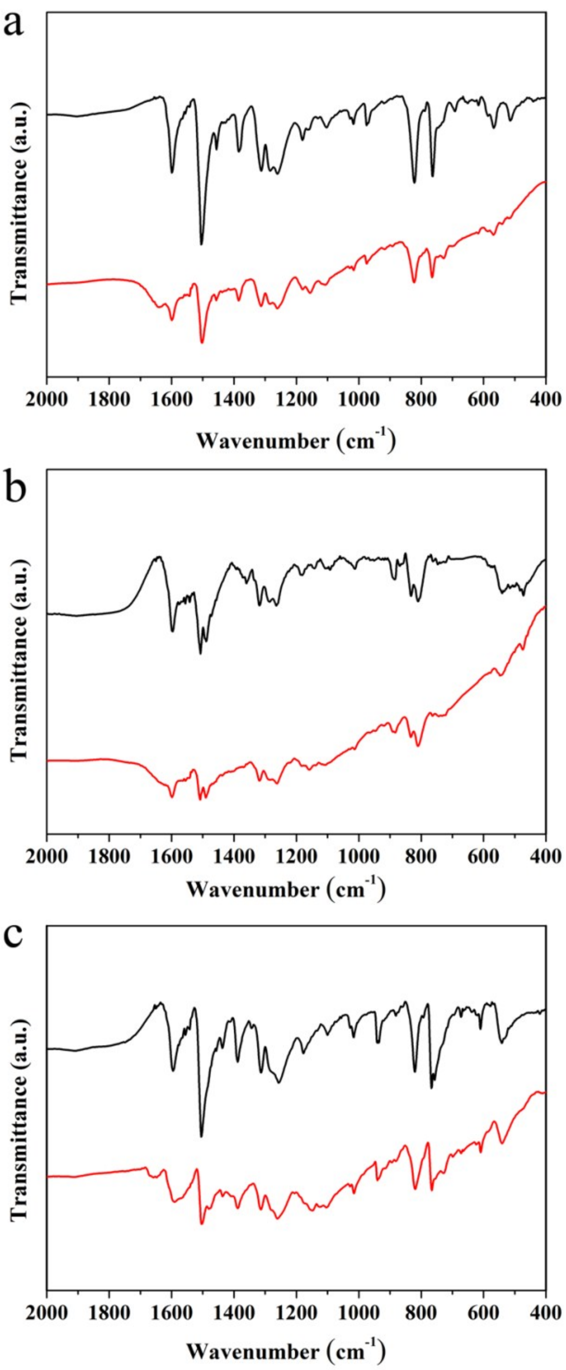

**Fig. S11** FT-IR spectra for before (black) and after (red) iodine adsorptions of LNU-2 (a), LNU-3 (b), and LNU-4 (c).

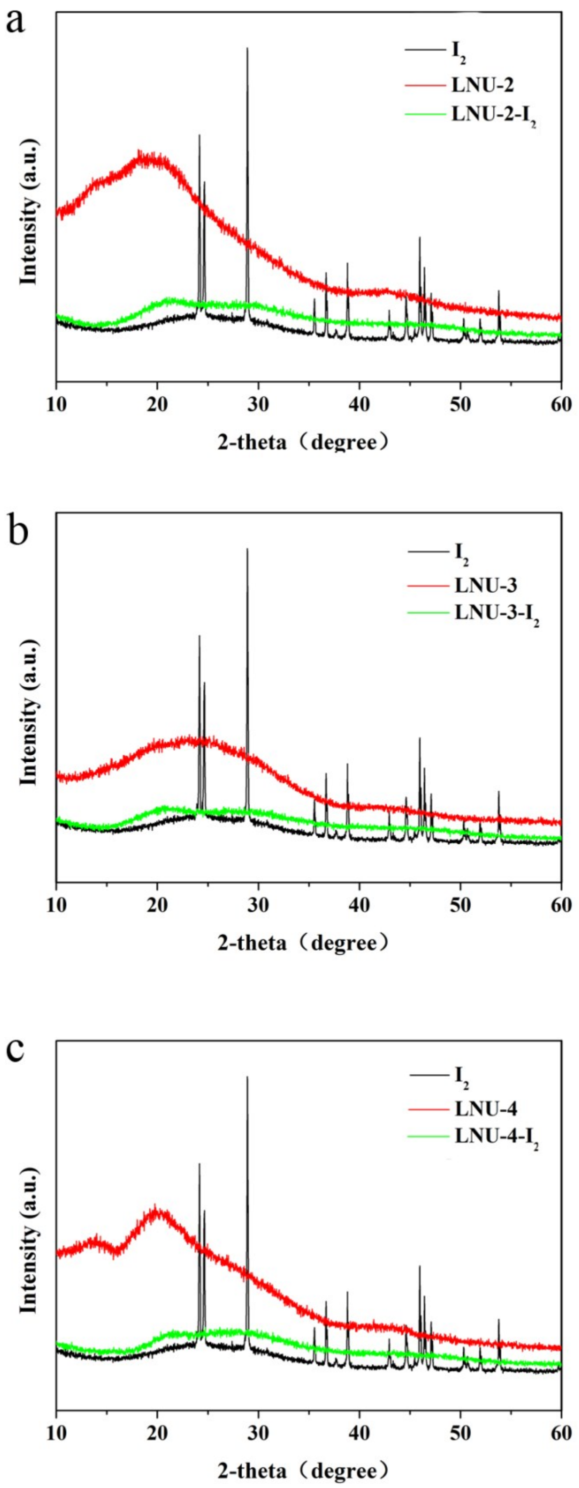

**Fig. S12** PXRD spectra for before and after iodine adsorptions of LNU-2 (a), LNU-3 (b), and LNU-4 (c).

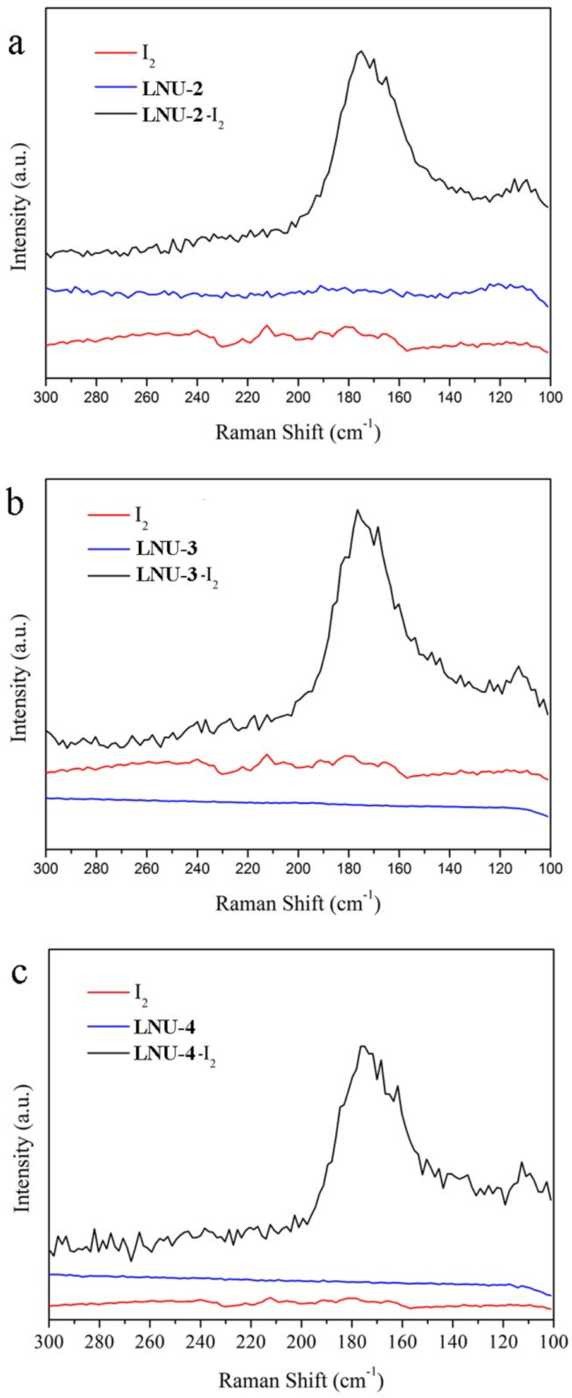

**Fig. S13** Raman spectra for before and after iodine adsorptions of LNU-2 (a), LNU-3 (b), and LNU-4 (c).

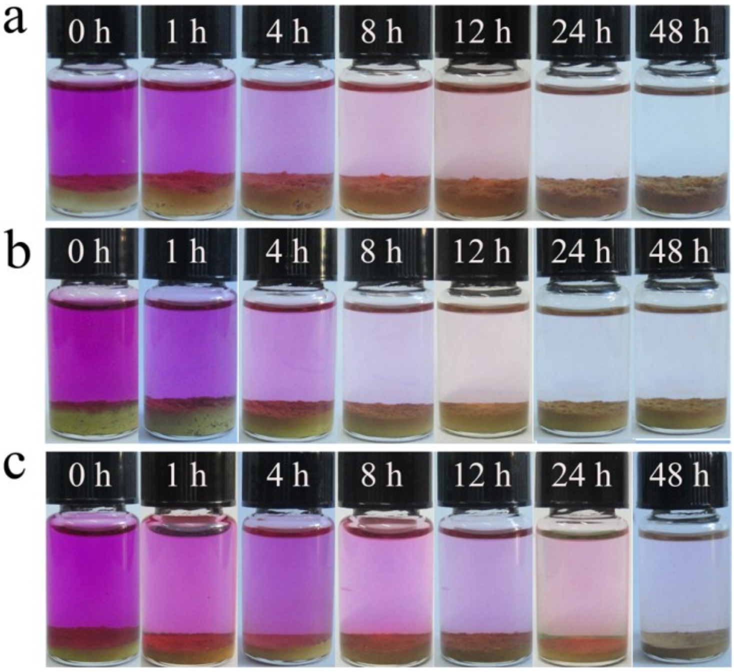

**Fig. S14** Photographs showing the color change of $I_2$ enrichment progress when 30 mg of LNU-2 (a), LNU-3 (b), and LNU-4 (c) were immersed in a hexane solution of $I_2$ (1000 mg $L^{-1}$, 3 mL), respectively.

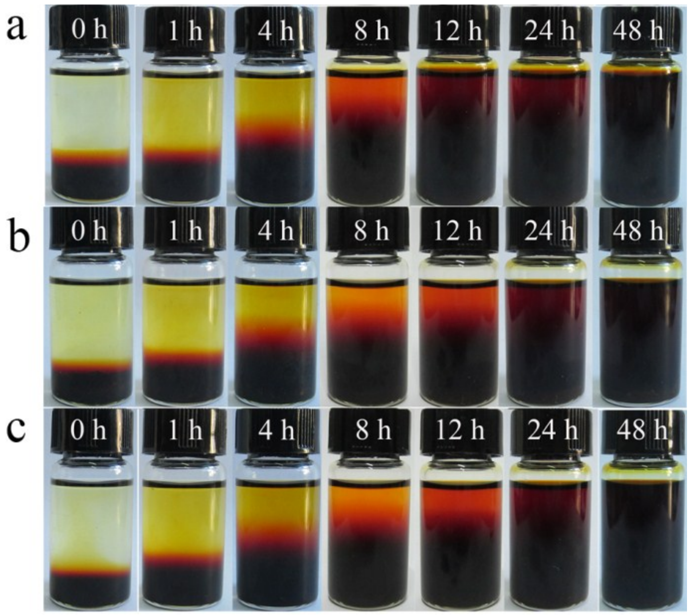

**Fig. S15** Photographs of the iodine release from LNU-2 (a), LNU-3 (b), and LNU-4 (c), when the iodine adsorbed polymer networks were immersed in ethanol.

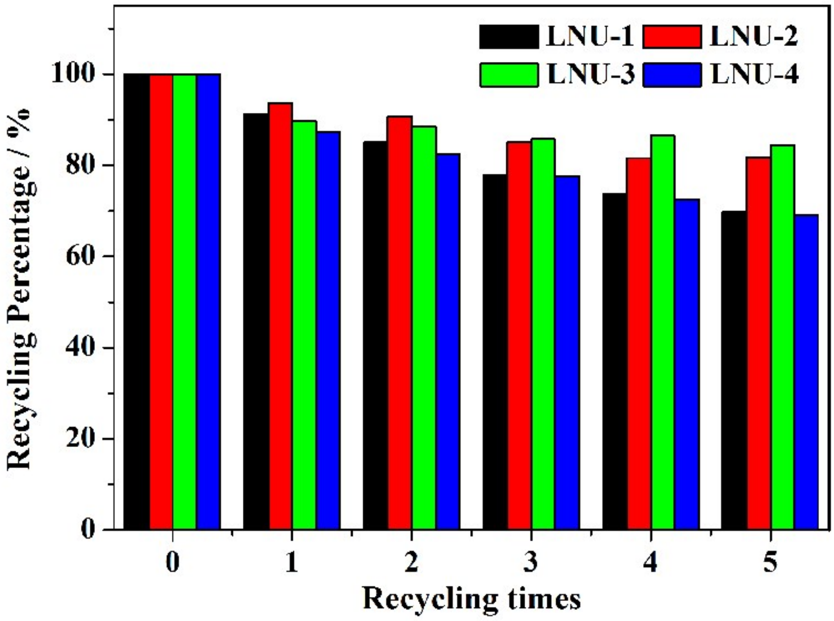

**Fig. S16** Cycle used PAF samples the: LNU-1, LNU-2, LNU-3, and LNU-4 in iodine vapor capture.