

Supporting Information

Mesoporous silica functionalized with AIE luminogen for drug delivery

Dongdong Li, Jihong Yu* and Ruren Xu

State Key Laboratory of Inorganic Synthesis and Preparative Chemistry, College of
Chemistry, Jilin University, Changchun 130012, PR China

Experimental procedure

Starting materials

3-Aminopropyltriethoxysilane (APTS, Sigma-Aldrich), tetraethoxysilane (TEOS, Beijing Beihua Chemical Co., Ltd.), ibuprofen (IBU, Wuhan Fortuna Chemical Co., Ltd.), dimethyl sulfoxide (DMSO, Beijing Chemical Regent Co., Ltd.). All the initial chemicals in this work were used without further purification except toluene were distilled from sodium with benzophenone as color reagent.

Synthesis of -NH₂ modified SBA-15 (SN)

1 g SBA-15 was dehydrated under vacuum at 120 °C and loaded into a three-neck flask sealed with rubber septums, then 20 ml anhydrous toluene and 3 ml APTS were mixed and injected into the bottle at room temperature. The slurry was refluxed with stirring under N₂ atmosphere for 6 h and filtered, washed with ethanol, and dried at 60 °C for 24 h, marked as SN.

Drug loading and in vitro release

0.1 g SNF sample was added into 15 ml of hexane solution containing 60 mg/ml ibuprofen, which was stirred in a vial for 24 h and sealed to prevent the evaporation of organic vapor. The SNF sample loaded with IBU was separated by centrifugation, dried at 60 °C in air. UV-vis at 263 nm was used to determine the amount of IBU adsorbed. 50mg of the solid was immersed into the simulated body fluid (SBF) with pH 7.4 at 37 °C under slow stirring. The volume of SBF was determined by IBU adsorbed to the materials with the ratio of 1 ml/mg. The ibuprofen release medium solution (0.5 ml) was taken out for UV-vis analysis at 220 nm at given time intervals and replaced with the same volume of fresh SBF. The release system of SN was prepared through the same process.

Physical measurements

Powder X-ray diffraction (XRD) patterns were recorded on a Rigaku D/MAX 2500/PC X-ray diffractometer with CuK α radiation ($\lambda=0.15405$ nm). N₂ adsorption-desorption isotherms were measured on a Micromeritics Gemini V at 77 K. Transmission-electron-microscopy (TEM) images were recorded with a Tecnai F20 electron microscope. Infrared (IR) measurements of the samples dispersed in KBr pellets were performed on a Perkin-Elmer spectrum 430 FT-IR spectrometer. UV-Vis adsorption spectra were obtained on a Shimadzu UV-2550 spectrophotometer. The UV/Vis excitation and emission spectra were obtained on a Shimadzu RF-5301PC spectrofluorometer. Thermogravimetric analysis (TGA) of SN was performed on TGA Q500 system in air with a heating rate of 10 K min⁻¹.

Table S1. Textural parameters of SN, SNF and SNF-IBU.

sample	$S_{\text{BET}}(\text{m}^2/\text{g})$	$D_{\text{BJH}}(\text{nm})$	$V(\text{cm}^3/\text{g})$	IBU loading (wt%)
SN	246	5.71	0.34	50.0
SNF	263	5.76	0.33	59.8
SNF-IBU	9	-	0.02	-

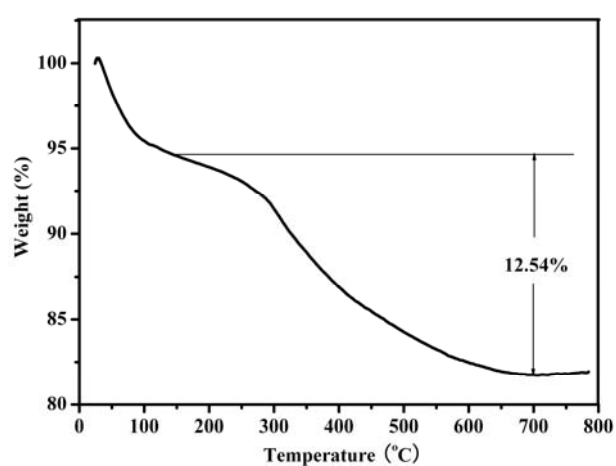


Figure S1. TG profile of SN.

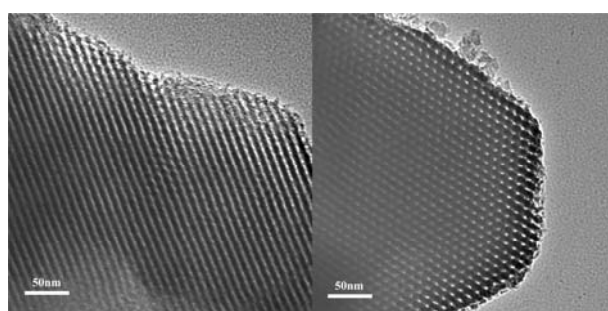


Figure S2. TEM images of SNF

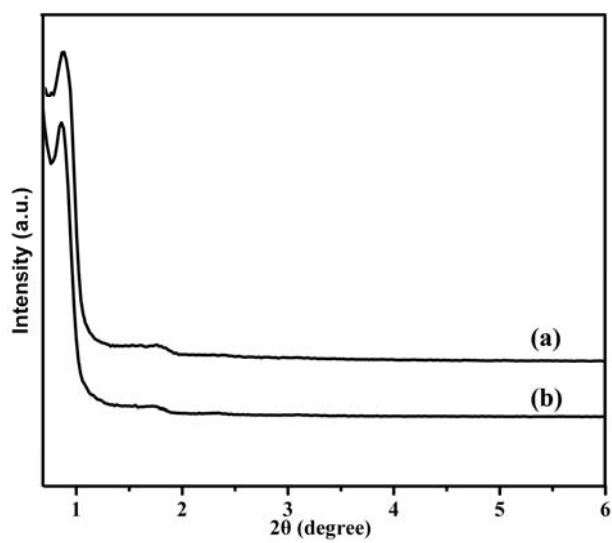


Figure S3. XRD patterns of SN (a), SNF (b).

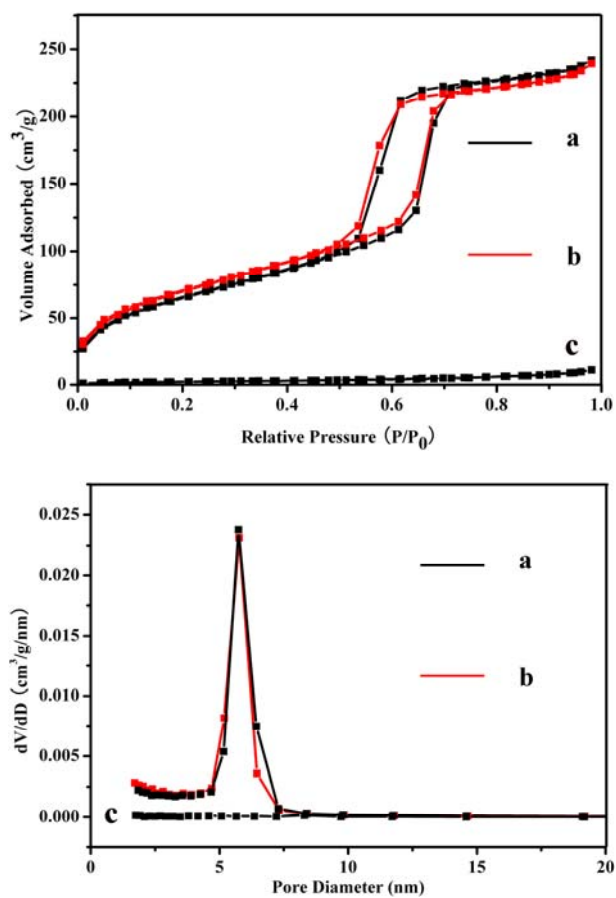


Figure S4. (A) N₂ adsorption-desorption isotherms of SN (a), SNF (b), SNF-IBU (c) and (B) corresponding pore size distribution.

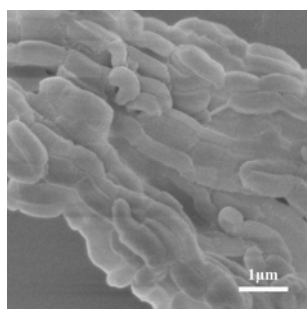


Figure S5. SEM image of SNF

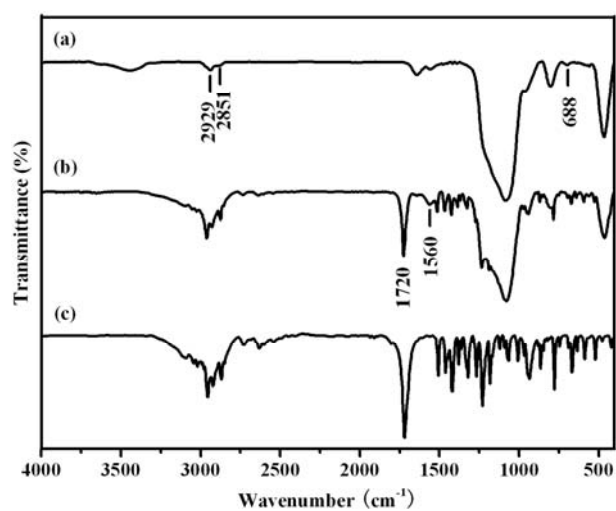


Figure S6. FT-IR spectra of SNF (a), SNF-IBU (b), and IBU (c).