Supplementary Information

Two Biocompatible Iron-based CPMs for High-Capacity Adsorption and pH-responsive Sustained Release of Diclofenac Sodium

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S1. The synthesis of materials

Synthesis of Fe-CPM-1 and Fe-CPM-2

According to the method provided in the literature, the tris(pyrazolyl)triazine ligand (TPT), different length linear dicarboxylic acid ligands (H_2BDC, H_2BPDC), and $Fe(ClO_4)_3 \cdot H_2O$ were mixed in a molar ratio of 2:1:1, and Fe-CPM-1 and Fe-CPM-2 were synthesized by hydrothermal method. Then, the samples were activated with methanol solvent and dried in a vacuum oven at 80℃ for 12 hours.

S2 Experimental detailed information

S2.1 Drug loading of DS

To investigate the loading capacity of Fe-CPM-1 and Fe-CPM-2 for DS molecules, MOF and 5-Fu were mixed in a mass ratio of 1:1 to 1:7 in a 20 mL solvent to determine the optimal mass ratio. The selected solvents for Fe-CPM-1 and Fe-CPM-2 were PBS solution (pH=7.4) and ethanol solution, respectively. The drug loading amount of MOF at different times was determined by measuring the absorbance of the supernatant (diluted to 100 times) using a UV-visible spectrophotometer.

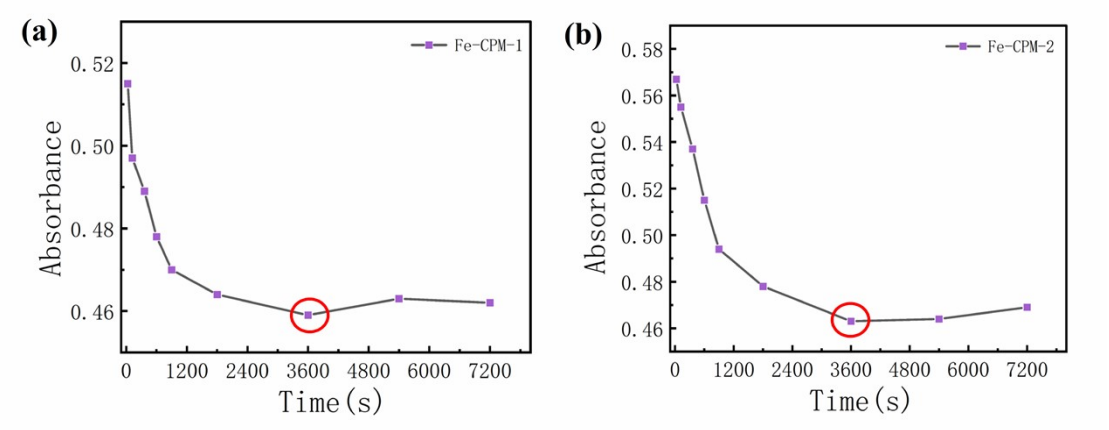

Figure S1 Plot of absorbance of DS versus drug loading time

S2.2 Sustained-release

The dialysis permeation method was used to simulate the pharmacokinetic behavior. In order to simulate the gastric, body fluid and blood environments of the human body, 100 mL PBS solutions with pH values of 1.5, 6.8, and 7.4 were used as the dialysis solution. Under the conditions of 37±0.5℃, appropriate samples were taken from the

dialysis bag at regular intervals, and the absorbance at 266 nm was measured to monitor the release rate of DS. The entire process lasted for 96 hours.

S3 X-ray powder diffraction

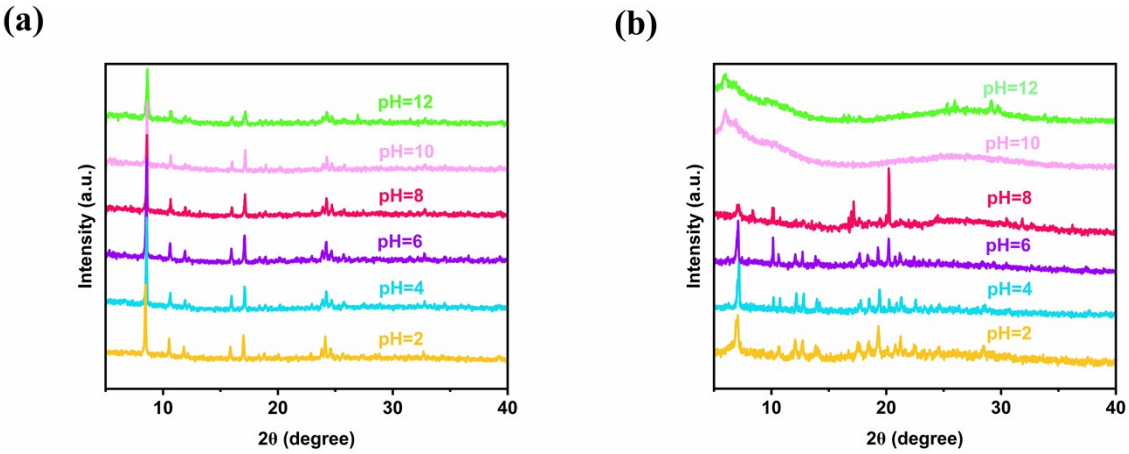

Figure S2 X-ray powder diffraction of Fe-CPM-1 in different pH solutions

S4 BET experiment

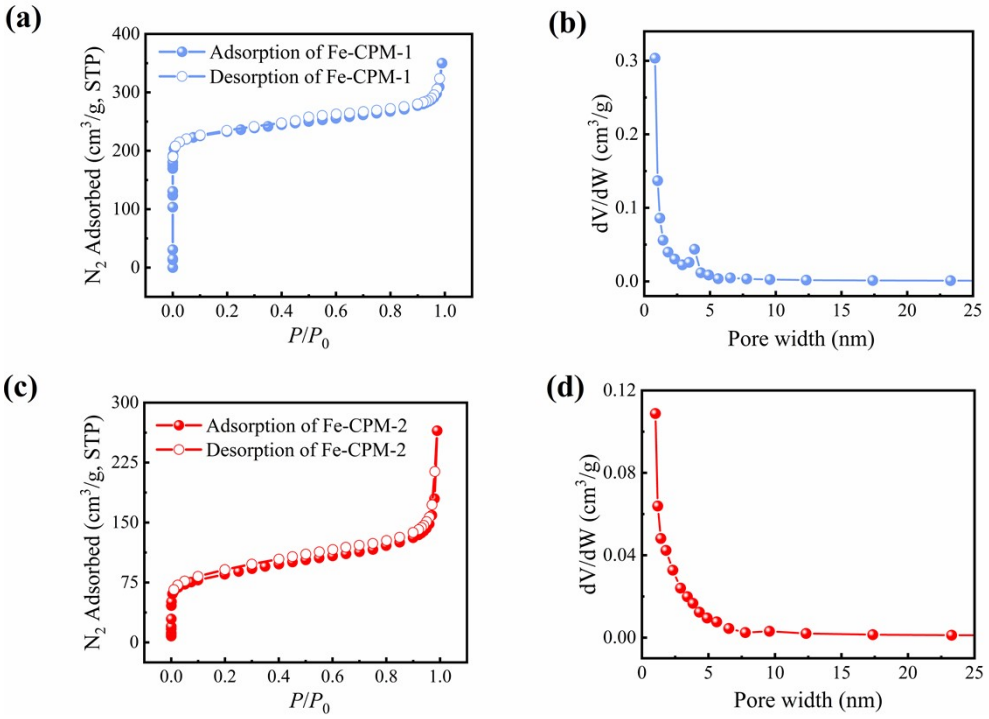

Figure S3 the N_2 adsorption/desorption isotherms of Fe-CPM-1 and 2 at 77K

S5 Thermogravimetric analysis

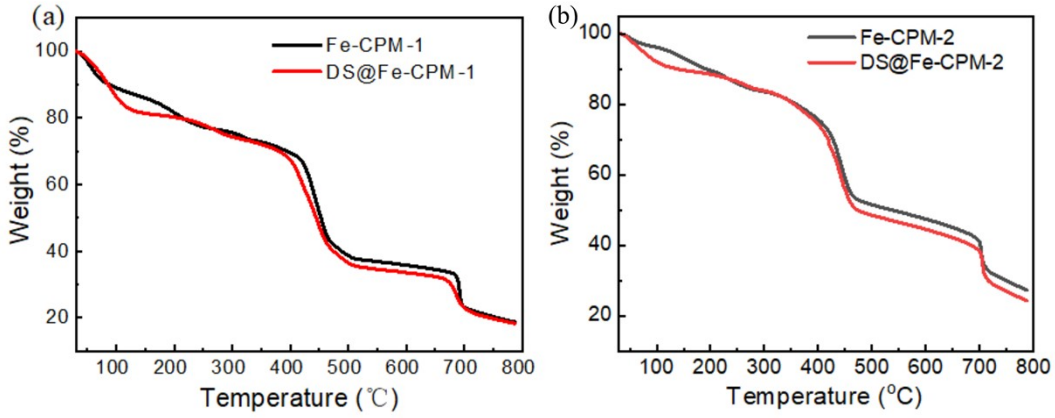

Figure S4 Thermogravimetric analysis of (a) Fe-CPM-1 and (b) DS@Fe-CPM-2

S6 Infrared spectra characterization

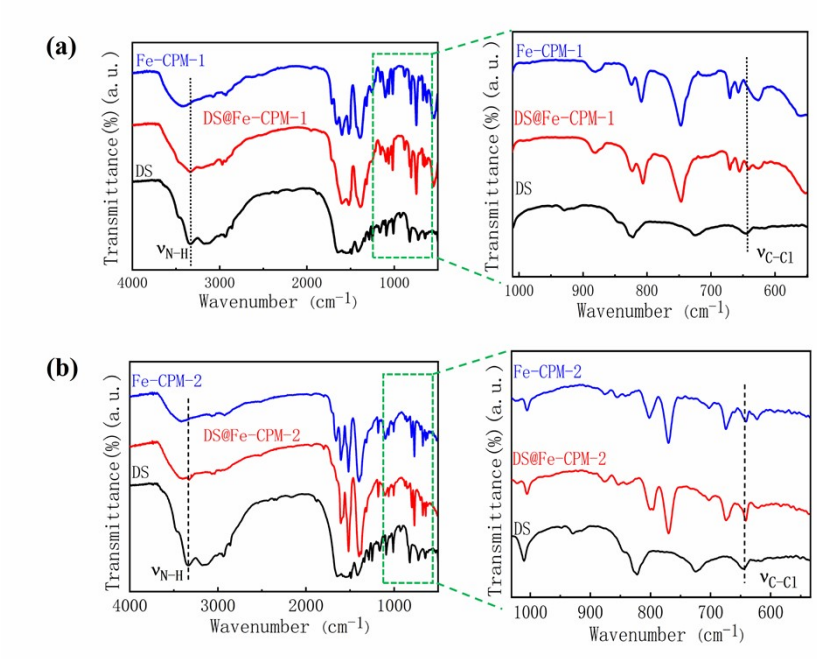

Figure S5 Infrared characterization diagram of (a) Fe-CPM-1 and (b) Fe-CPM-2. (black line: DS; blue line: Fe-CPMs; red line: DS@CPMs)

S7 Standard curve of DS

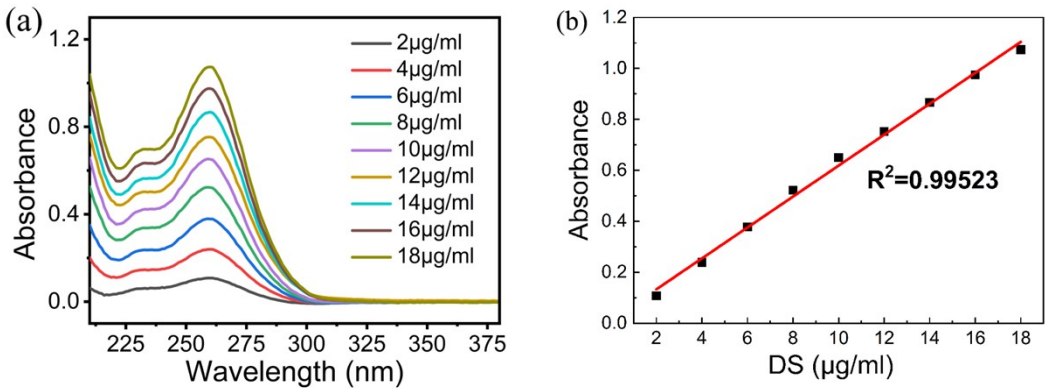

Figure S6 (a) Absorbance curve of DS in ethanol solution. (b) the standard curve of DS in ethanol solution

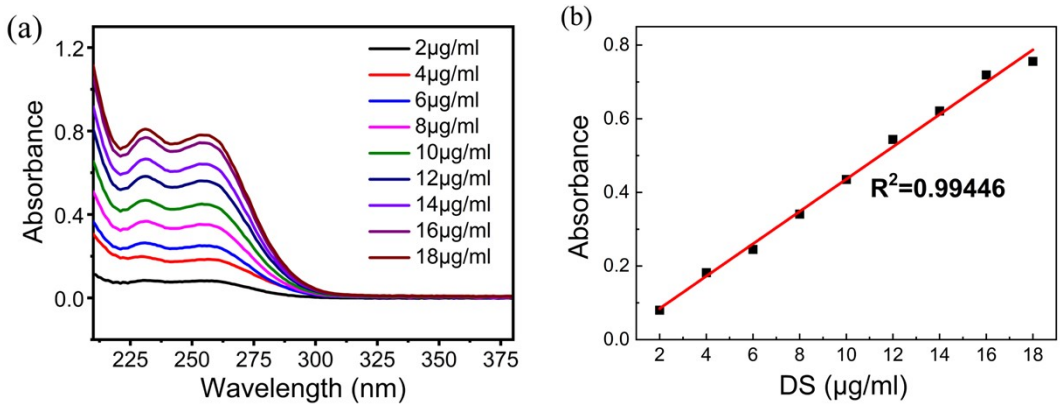

Figure S7 (a) Absorbance curve of DS in PBS solution. (b) the standard curve of DS in PBS solution

S8 Zeta potential under different concentrations of DS

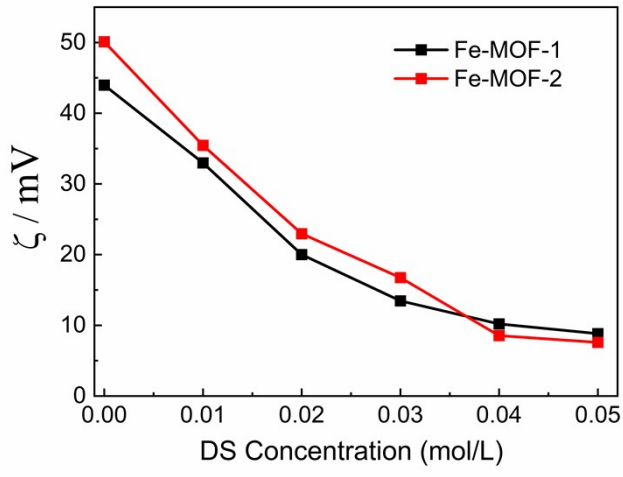

Figure S8 Zeta potential of Fe-CPM-1 and Fe-CPM-2 under different concentrations of DS

S9 Kinetic model fitting

Table S1 The fitting equation of the slow release process and each dynamic model of DS@Fe-

CPM-1

pH=7.4	Model	Fitted Equations	Correlation Coefficients(R^2)
First order		$y=0.56199\ (1-e^{-0.85799x})$	0.96332
Hill		$y=0.59062x^{0.01002}/(0.00754^{0.01002}+x^{0.01002})$	0.98680
Higuchi		$y=0.041049x^{0.5}+0.30543$	0.55370
Korsemeyer-peppas		$y=-0.015902+0.37991x^{0.12292}$	0.88510
pH=6.8	Model	Fitted Equations	Correlation Coefficients(R^2)
First order		$y=0.60039\ (1-e^{-0.64712x})$	0.98760
Hill		$y=0.61367x^{1.37558}/(0.010473^{1.37558}+x^{1.37558})$	0.99459
Higuchi		$y=0.047474x^{0.5}+0.29205$	0.55101
Korsemeyer-peppas		$y=-0.029989+0.38179x^{0.14134}$	0.82227
pH=1.5	Model	Fitted Equations	Correlation Coefficients(R^2)
First order		$y=0.70754\ (1-e^{-0.68587x})$	0.96753
Hill		$y=0.74680x^{0.99356}/(0.009629^{0.99356}+x^{0.99356})$	0.99498
Higuchi		$y=0.055438x^{0.5}+0.35389$	0.59376
Korsemeyer-peppas		$y=-0.027378+0.45377x^{0.1379}$	0.88249

Table S-2 The fitting equation of the slow release process and each dynamic model of DS@Fe-CPM-2

pH=7.4	Model	Fitted Equations	Correlation Coefficients(R^2)
First order		$y=0.74688\ (1-e^{-0.57722x})$	0.97044
Hill		$y=0.78588x^{1.08478}/(0.012284^{1.08478}+x^{1.08478})$	0.99208
Higuchi		$y=0.069016x^{0.5}+0.30302$	0.64906
Korsemeyer-peppas		$y=-0.064075+0.45038x^{0.1663}$	0.86099
pH=6.8	Model	Fitted Equations	Correlation Coefficients(R^2)
First order		$y=0.66441\ (1-e^{-0.53229x})$	0.95481
Hill		$y=0.71971x^{0.93307}/(0.043412^{0.93307}+x^{0.93307})$	0.98943

Higuchi		$y=0.063742x^{0.5}+0.25612$	0.69353
Korsemeyer-peppas		$y=-0.056612+0.38854x^{0.17474}$	0.88762
pH=1.5	Model	Fitted Equations	Correlation Coefficients(R^2)
First-order		$y=0.59193\ (1-e^{-0.89049x})$	0.91338
Hill		$y=0.64172x^{0.68865}/(0.28645^{0.68865}+x^{0.68865})$	0.99325
Higuchi		$y=0.035959x^{0.5}+0.38131$	0.45863
Korsemeyer-peppas		$y=-0.00901+0.4555x^{0.08944}$	0.92484