Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Combined Experimental and Simulation Study of Nanoporous Metal-Organic Frameworks as Materials for Drug Delivery

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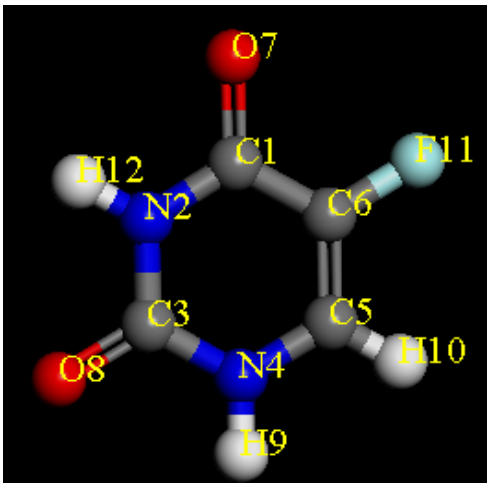

Fig. S1 Atomic types for 5-FU.

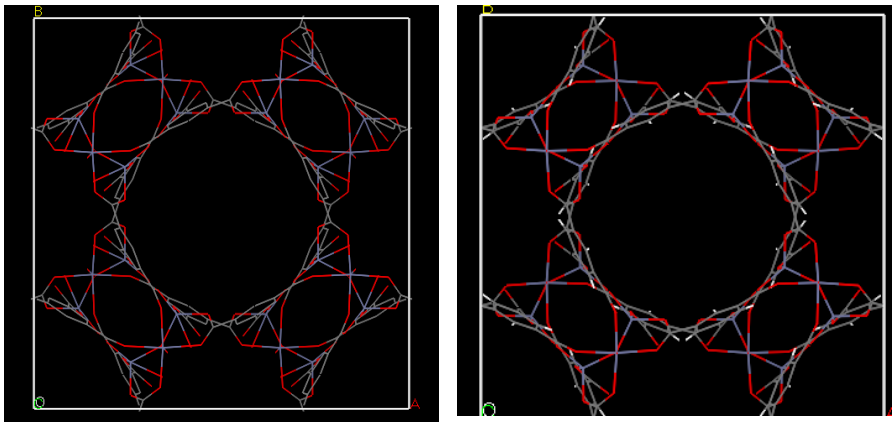

Fig. S2 The structure of GDMU (left) and NTU-Z11(right)

Force field parameters:

Table S1 Lennard-Jones parameters for 5-FU.

Molecule	Atoms	$\varepsilon / k_b(K)$	$\sigma(\mathring{A})$
5-FU	N	85.578	3.250
	C	43.292	3.340
	O	105.714	3.340
	H_N	7.903	1.069
	H_A	7.551	2.511
	F	30.707	3.118

*H_N denotes the hydrogen atom bonding to nitrogen atom, H_A is the hydrogen atoms bonding to carbon atom of the ring.

Table S2 Lennard-Jones parameters NTU-Z11 and GDMU

Atoms	$\varepsilon / k_b(K)$	$\sigma(\mathring{A})$
C	52.836	3.431
H	22.141	2.572
O	30.192	3.119
Zn	62.399	2.462

Table S3 Atomic charges for 5-FU

Atom	C1	N2	C3	N4	C5	C6
Charges	0.708465	-0.648790	0.821119	-0.521854	0.012750	0.057248
Atom	O7	O8	H9	H10	F11	H12
Charge	-0.545470	-0.603685	0.362918	0.174767	-0.190623	0.373155

Structural information for MOFs studied in this work:

Table S4 Details of the different MOFs simulation boxes used in the simulations.

MOFs	Number of cells	Simulation box sizes (Å)
GDMC	2×2×2	41.027×41.027×35.62

NTU-Z11	2×2×2	41.56×41.56×35.354

Drug Loading

To load 5-fluorouracil (5-FU) into the pores of **NTU-Z11** and **GDMU**, dehydrated samples were dispersed in a 5-FU containing methanol solution (25 mL) and stirred for different days. The adsorbed amount of 5-FU into the porous solids was estimated by UV–Vis absorption spectroscopy at 265 nm. Experiments were performed in quadruplicate and drug payloads 5-FU was calculated according to the following formula:

5-FU =5-FU(mg)/hydrated materials(mg)

Optimization of 5-FU adsorption

Table S5

Impregnation parameters	g 5-FU/g dehydrated **NTU-Z11**		
5-FU/ material weight ratio (in ethanol)	1:1	1day	0.184
		2 day	**0.382**
		3 day	0.171
		5 day	0.191
	1:2	1 day	0.185
		2 day	0.200
		3 day	0.198
		5 day	0.180
	1:3	1 day	0.185
		2 day	0.190
		3 day	0.188
		5 day	0.182

Impregnation parameters of drug loading experiments in title compounds

Impregnation parameters	g 5-FU/g dehydrated **GDMU**		
5-FU/ material weight ratio (in ethanol)	1:1	1day	0.166
		2 day	0.161
		3 day	0.125
	1:2	1day	0.165
		2 day	0.189
		3 day	0.123
	1:3	1day	0.200
		2 day	0.123
		3 day	**0.206**

Drug Release

Amount of inclusions were loaded into a dialysis bag (MWCO = 1000), which were dialyzed against 500 mL of PBS buffer solution at room temperature. During each time interval, 1 mL of solution was taken out, and 1 mL of fresh PBS buffer was added. The content of 5-FU in the samples taken out was determined by UV–Vis at 265 nm.

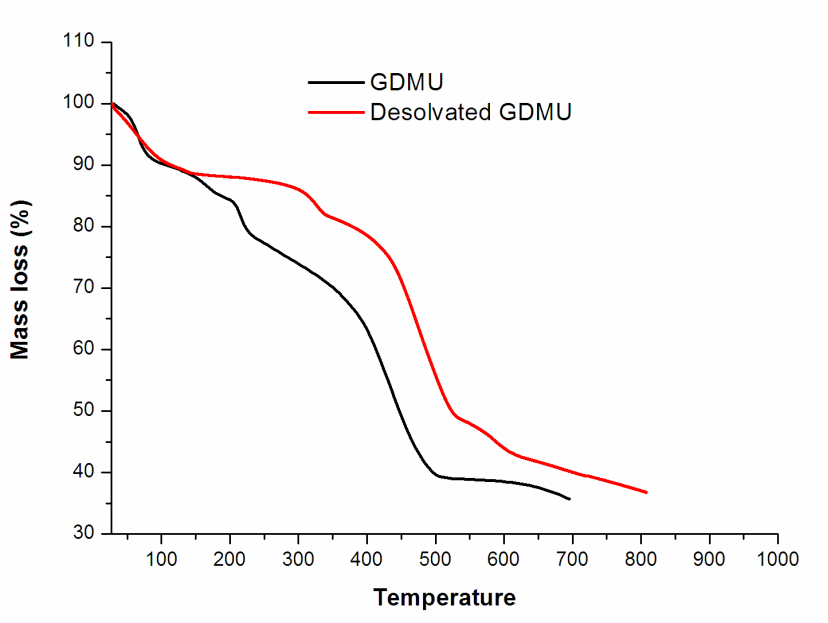

Fig. S3 The TGA curves of **GDMU** and **desolvated GDMU**

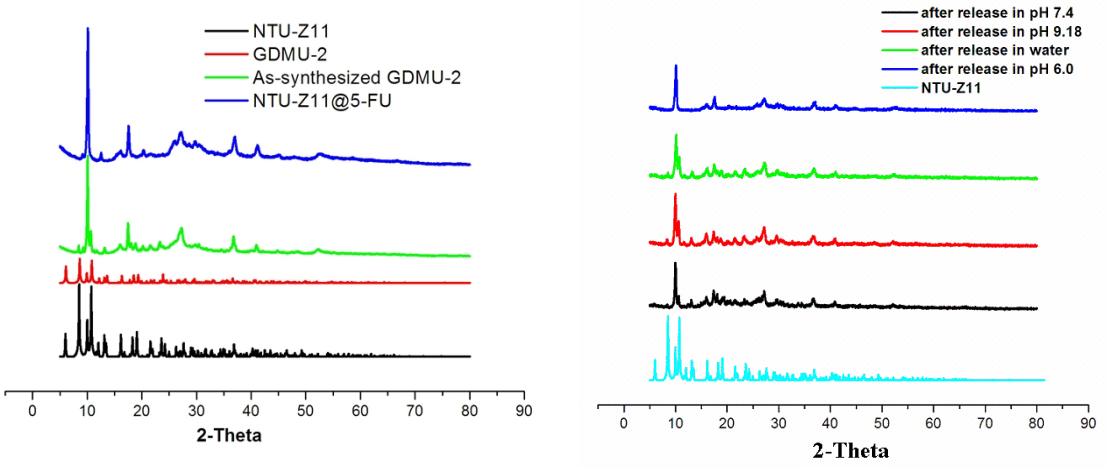

Fig. S4 (a) the PXRD pattern of NTU-Z11 and GDMU; and (b) the different PXRD pattern in released buffer solution.

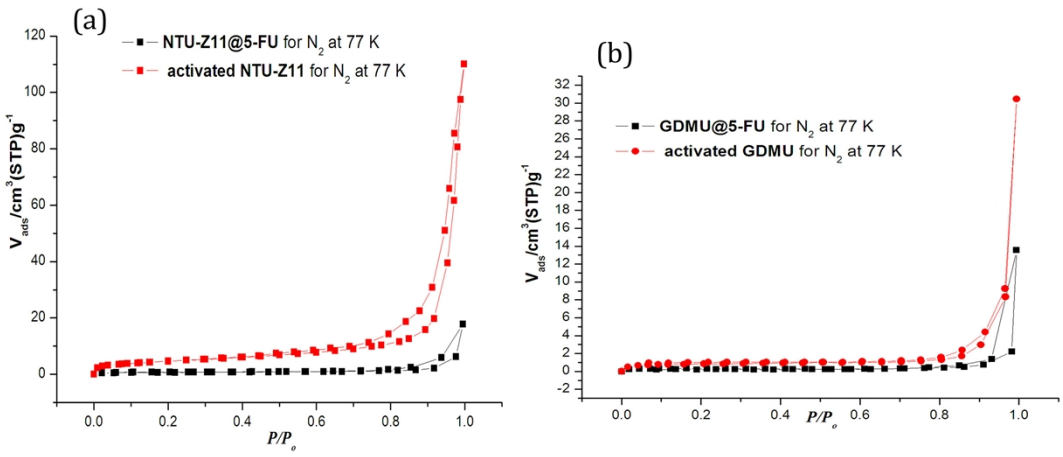

Fig. S5 view of the N_2 isotherms of two activated MOFs and 5-FU@MOFs materials

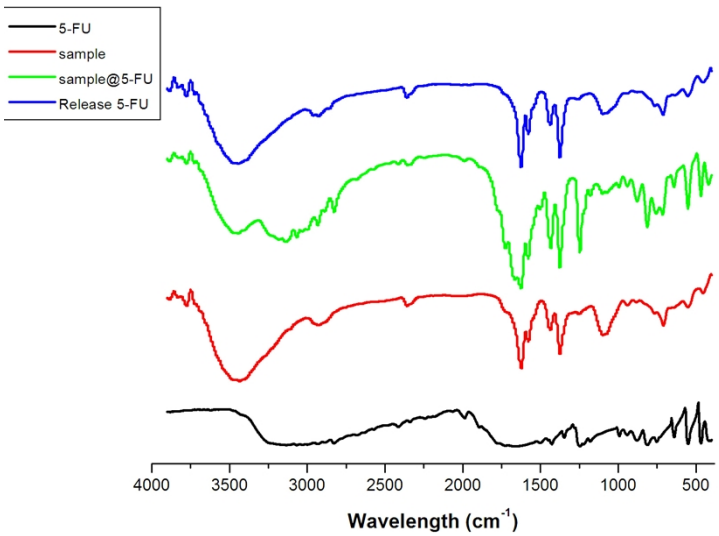

Fig. S6 IR spectra of 5-FU, sample, sample @5-FU, and after 5-FU released sample in **GDMU.**

Activated process for the samples

The activated samples were prepared by soaking the as-synthesized samples in CH_3OH for two days, then in CH_2Cl_2 for three days and subsequent heating at 120 °C in a quartz tube under high vacuum for 10 h to remove the free DMF and H_2O molecules prior to measurements.