Electronic Supporting Information

for

Enhanced Removal of Diclofenac from Water using Zeolitic Imidazole Framework functionalized with Cetyltrimethylammonium Bromide (CTAB)

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Table S1. Modeling parameters for the diclofenac adsorption to CTAB-ZIF-67 at different temperatures derived from the intraparticle diffusion model.

Conditions	Boundary Layer diffusion		Intraparticle diffusion	
Temp. (°C)	$k_{P,1}$ (mg g^{-1} min$^{-0.5}$)	$R_{P,1}^2$	$k_{P,2}$ (mg g^{-1} min$^{-0.5}$)	$R_{P,2}^2$
20	4.74	0.986	0.97	0.988
30	5.49	0.978	0.76	0.960
40	7.57	0.963	0.75	0.988

Table S2. Element analyses of ZIF-67, CTAB-ZIF-67 before and after the diclofenac adsorption

	C (%)	N (%)	H (%)
ZIF-67 w/o CTAB	43.50	25.19	4.35
CTAB*	62.60	3.80	11.6
CTAB-ZIF-67-L	44.58	18.98	6.37
CTAB-ZIF-67-M	44.95	17.68	5.88
CTAB-ZIF-67-H	45.85	17.40	5.79
diclofenac*	52.80	4.40	3.16
CTAB-ZIF-67-L + diclofenac	43.62	17.60	6.02
CTAB-ZIF-67-M + diclofenac	43.80	16.54	5.90
CTAB-ZIF-67-H + diclofenac	43.94	16.49	5.82

*Estimated element analyses based on chemical formulas

Table S3. Surface areas and pore volumes of the pristine ZIF-67 and CTAB-ZIF-67

	BET surface area (m^2 g^{-1})	Pore volume (cm^3 g^{-1})
ZIF-67 (w/o CTAB)	1710	0.42
CTAB-ZIF-67-L	1103	0.34
CTAB-ZIF-67-M	817	0.23
CTAB-ZIF-67-H	709	0.20

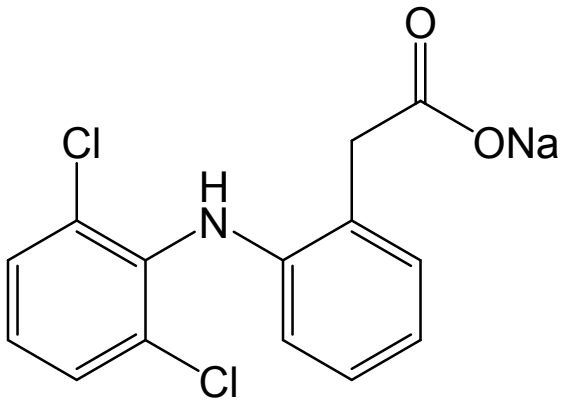

Fig. S1. Chemical structure of diclofenac (sodium salt) and chemical formula is $C_{14}H_{10}Cl_2NNaO_2$.

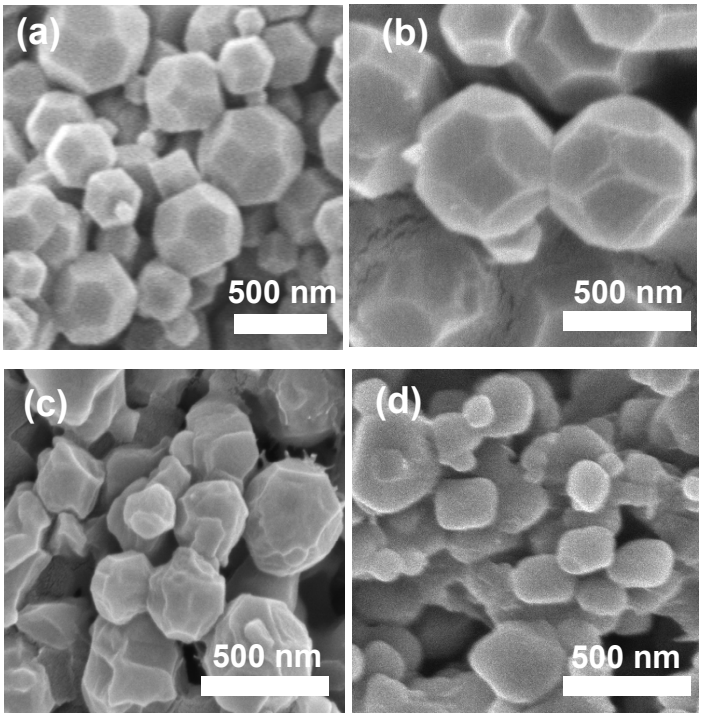

Fig. S2. SEM images of (a) pristine ZIF-67 (w/o CTAB) and CTAB-ZIF-67 with different CTAB loadings: (b) CTAB-ZIF-67-L, (c) CTAB-ZIF-67-M and (d) CTAB-ZIF-67-H.

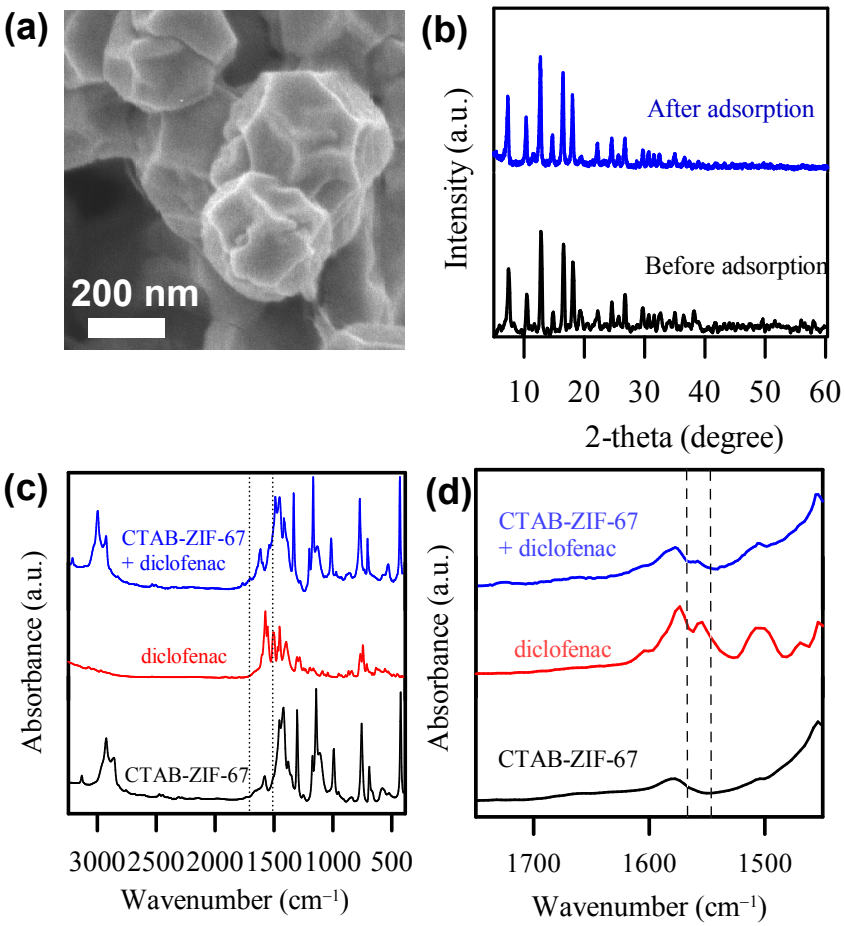

Fig. S3. Characterization of the post-adsorption CTAB-ZIF-67-M: (a) SEM image, (b) XRD pattern, (c) full-range IR spectrum and (d) selected-range IR spectrum.

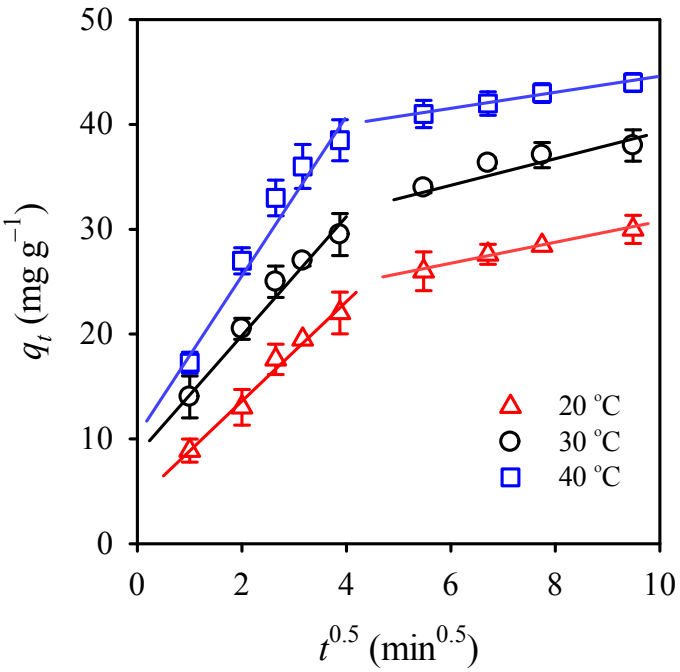

Fig. S4. Modeling of the kinetic data using Weber-Morris intraparticle diffusion model.

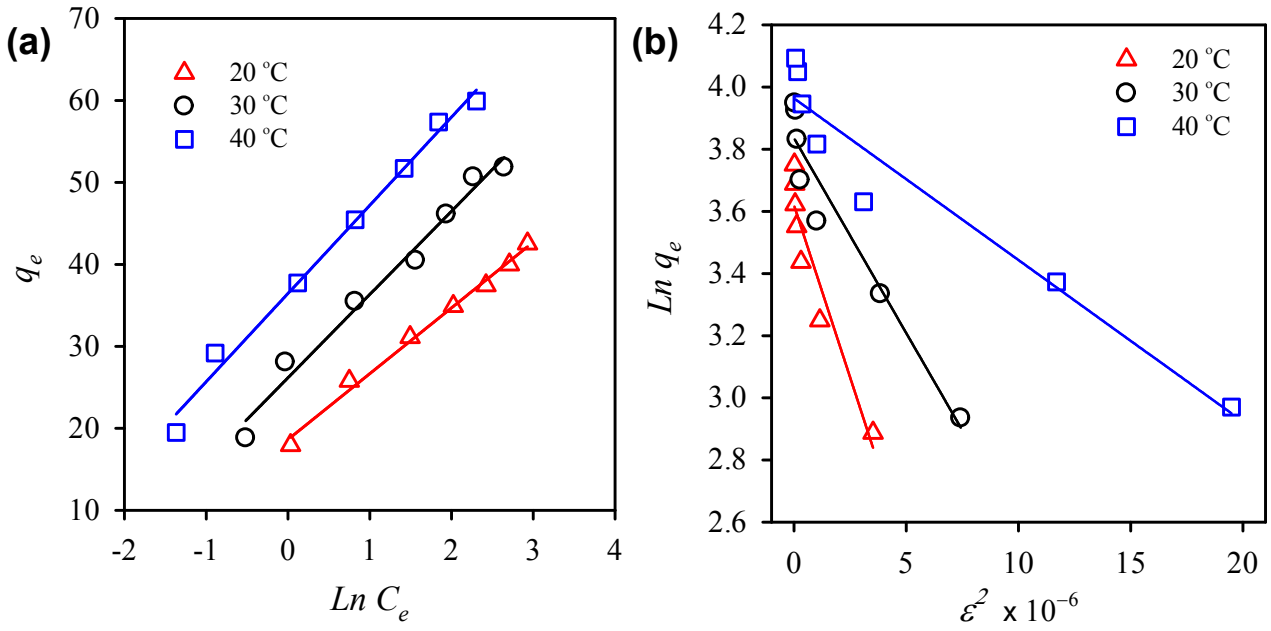

Fig. S5. Modeling of the adsorption isotherm data using the (a) Temkin and (b) Dubinin-Raduskevich isotherms.

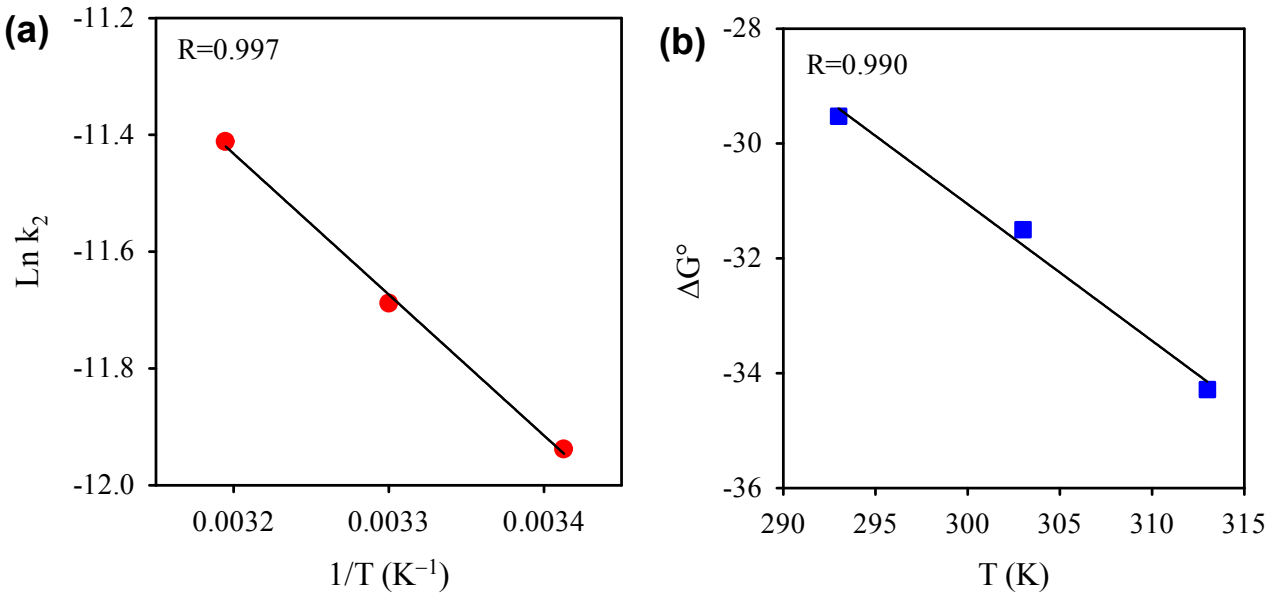

Fig. S6. Thermodynamics of the diclofenac adsorption to CTAB-ZIF-67: (a) a plot for determining the activation energy E_a and the temperature-independent factor *k,* and (b) a plot for determining the free energy (ΔG°), the enthalpy (ΔH°) and entropy (ΔS°) of the adsorption.

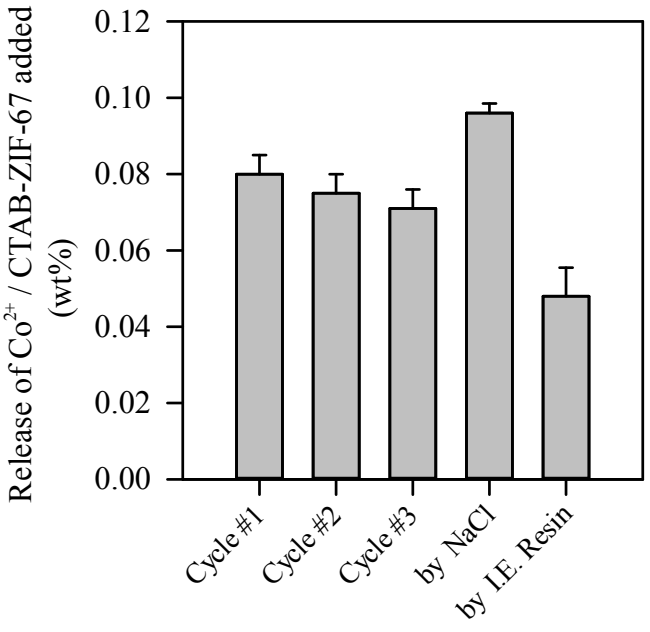

Fig. S7. Release of cobalt from CTAB-ZIF-67 during the adsorption (cycle #1−3) and desorption (in the presence of NaCl and I.E. resin) at ambient temperature.