Supplementary Information

Bio-based metal−organic aerogel (MOA) adsorbent for capturing tetracycline from aqueous solution

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1. **Fig. S1.** Effect of solvent type on TC adsorption capacity of Fe-MOA.
2. **Fig. S2.** Effect of the mole ratio of ferric salt and FDCA on TC adsorption capacity of Fe-MOA.
3. **Fig. S3.** Effect of the concentration of FDCA on TC adsorption capacity of Fe-MOA.
4. **Fig. S4.** Effect of synthesis temperature on TC adsorption capacity of Fe-MOA.
5. The cartesian coordinate of TC molecule obtained by DFT calculation.

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Three common solvents including DMF, EtOH, and H_2O were tested as the single or binary solvents for preparing the Fe-MOA. When using single solvent, only the DMF solvent was valid for obtaining the gel-like Fe-MOA product. This can be attributed to the better solubility of FDCA in the DMF than that in the E_tOH and H_2O. Thus, the solvent systems, i.e., “DMF+ H_2O” and “DMF+ EtOH” were considered. It was found that the two mixing solvent systems could be used to synthesize the Fe-MOA. Subsequently, those Fe-MOAs obtained by different solvent systems were used to test the solvent effect on the TC adsorption capacity. As shown in Fig. S1, the Fe-MOA obtained by DMF+ EtOH solvent gave the higher adsorption capacity of TC than that by single DMF solvent and DMF+ H_2O solvent. Thus, the binary DMF+ EtOH solvent was selected for preparing Fe-MOA in following experiment.

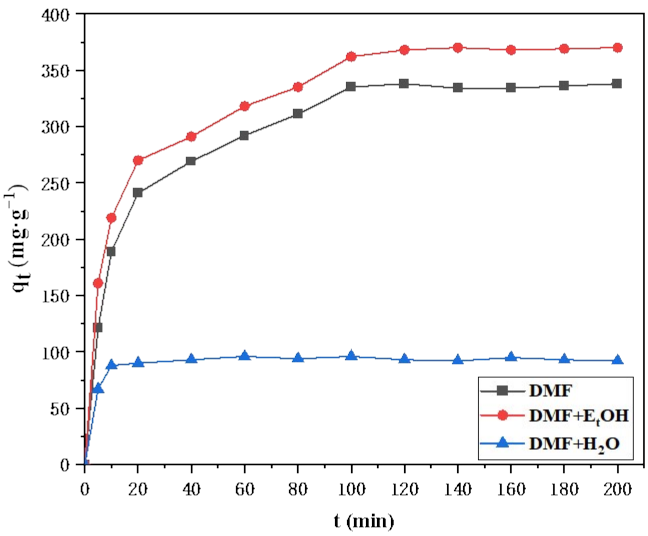

Fig. S1. Effect of solvent type on TC adsorption capacity of Fe-MOA (conditions: the mole ratio of ferric salt and FDCA is 2:1; the concentration of FDCA is 0.06 mol·L^{-1}; synthesis temperature is 110 ℃).

The mole ratio of ferric salt and FDCA plays a significant role in determining the coordination mode between Fe^{3+} and FDCA during the coordination self-assembly process, thus affecting the structure of Fe-MOA. The effect of the reactant mole ratio on the TC adsorption capacity was explored. It can be seen in Fig. S2 that with increasing the mole ratio of ferric salt and FDCA, the TC adsorption capacity presented a first increase and then decrease trend. And when the mole ratio of ferric salt and FDCA was 1:1, the obtaining Fe-MOA gave the highest adsorption. Thus, the ferric salt/FDCA mole ratio of 1:1 was selected as in following preparing experiment.

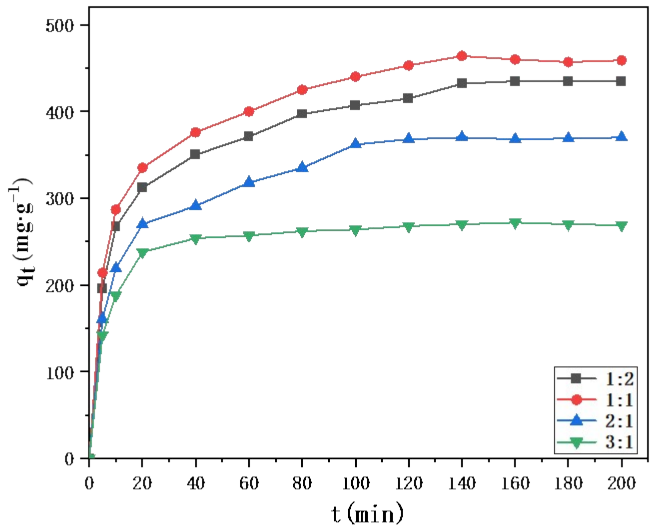

Fig. S2. Effect of the mole ratio of ferric salt and FDCA on TC adsorption capacity of Fe-MOA (conditions: solvent is DMF+EtOH; the concentration of FDCA is 0.06 mol·L^{-1}; synthesis temperature is 110 ℃)

The reactant concentration effect was also assessed. As displayed in Fig. S3, the reactant concentration played an insignificant role in the TC adsorption capacity.

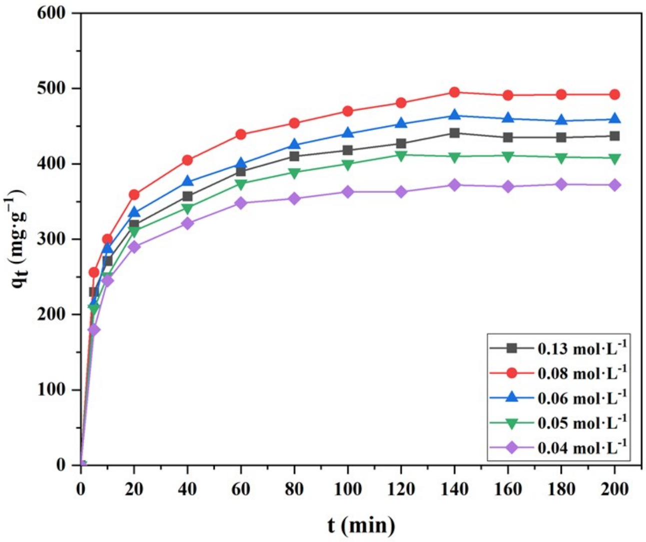

Fig. S3. Effect of the concentration of FDCA on TC adsorption capacity of Fe-MOA (conditions: solvent is DMF+EtOH; the mole ratio of ferric salt and FDCA is 1:1; synthesis temperature is 110 ℃).

Generally, the temperature is one of the most important parameters for the material preparation with hydrothermal/solvothermal method. Herein, different temperatures ranging from 50 to 140 ℃ were considered in the Fe-MOA fabrication. One can see in Fig. S4 that the TC adsorption capacities on the Fe-MOA adsorbents obtained under different temperatures varied greatly. With elevating the temperature, the TC adsorption on Fe-MOAs exhibited a first increase and then decrease trend and the Fe-MOA fabricated at 110 °C gave the most optimistic TC adsorption. The trend agreed well with that of specific surface area and pore structure as presented in Table 1. Accordingly, the all Fe-MOA employed for the following adsorption experiments were synthesized at 110 ℃.

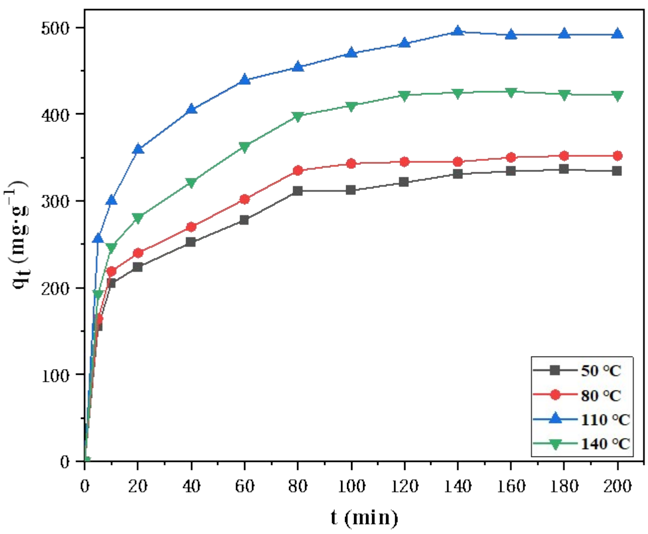

Fig. S4. Effect of synthesis temperature on TC adsorption capacity of Fe-MOA (conditions: solvent is DMF+EtOH; the mole ratio of ferric salt and FDCA is 1:1; the concentration of FDCA is 0.08 mol·L^{-1}).

The cartesian coordinate of TC molecule obtained by DFT calculation.

C	-3.6685	1.4133	0.0002
C	-4.8819	0.7235	0.0004
C	-4.8898	-0.6678	0.0003
C	-3.6844	-1.3714	0.0001
C	-2.4551	-0.6915	0.
C	-2.447	0.7195	0.
C	-1.2335	-1.385	-0.0001
C	0.004	0.7044	-0.0002
C	-1.2176	1.399	0.
C	1.2175	-1.399	-0.0002
C	2.447	-0.7195	-0.0003
C	2.455	0.6915	-0.0003
C	1.2335	1.385	-0.0002
C	3.6685	-1.4133	-0.0003
C	4.8897	0.6678	-0.0005
C	3.6843	1.3714	-0.0004
H	-1.21384	2.03324	-0.86176
H	5.8452	1.2128	-0.0006
H	3.6971	2.4713	-0.0005
O	3.66876	-2.8433	-0.0003
H	4.57375	-3.16359	-0.00205
O	1.20879	-2.82897	-0.00007
C	1.23848	2.29756	1.24029
H	2.11327	2.91354	1.22642
H	0.36598	2.91689	1.23096
H	1.23963	1.6963	2.12538
O	1.23803	2.23255	-1.15196
H	2.14413	2.42051	-1.40739
O	-1.24117	-2.81498	0.00003
H	-0.3378	-3.13983	0.00006
O	-3.70091	-2.8013	-0.00016
O	-6.11591	1.44607	0.00066
C	-6.22746	-1.43086	0.00044
O	-6.6415	-1.66729	-1.34773
H	-1.2137	2.03299	0.86194
N	-7.2478	-0.63097	0.69326
H	-8.0787	-0.59722	0.13786
H	-7.4549	-1.04877	1.57788
N	-3.66877	2.8833	0.00033
C	-4.36249	3.37306	1.20024
C	-4.36115	3.37328	-1.20026

H	-3.76056	4.1147	1.68248
H	-5.30106	3.80309	0.91904
H	-4.53081	2.5579	1.8726
H	-3.75847	3.18065	-2.06314
H	-5.29982	2.86967	-1.30116
H	-4.52914	4.42618	-1.11037
H	-6.78813	0.93152	-0.45207
C	-0.0041	-0.7044	-0.0002
O	-0.00415	-0.71818	1.42973
H	0.19006	-1.60508	1.74166
C	4.8818	-0.7236	-0.0003
H	5.80512	-1.26433	-0.00015
H	0.00395	0.70971	-1.07019