1 Importance of nano-sized molybdenum composite simply synthesized by a microwave oven in

2 sorption enhancement of Au(III) from the aqueous phase

- 3 Chuanhao Yan^a, Xuefeng Yu^a, Jinlong Zhang^a, Jinglei He^a, Wenyi Jia^a, Jianlong Wang^b, Fuqiang Liu^c,
- 4 Junfeng Liu^a, Xilong Wang^{a, *}
- 5 a Laboratory for Earth Surface Processes, College of Urban and Environmental Sciences, Peking
- 6 University, Beijing 100871, China
- 7 ^b College of Food Science and Engineering, Northwest A & F University, Yangling 712100, China
- 8 ° State Key Laboratory of Pollution Control and Resource Reuse, School of the Environment, Nanjing
- 9 University, Nanjing 210023, China
- 10
- 11 Corresponding author. Email address: xilong@pku.edu.cn (X. Wang)
- 12

13 Supplementary information

14

15 Details for calculating the composition of each component in MoCOM

- 16 Base on the XPS spectra of MoCOM (Fig. 3 a-e), We first identified the main components of MoCOM
- 17 was MoS₂, MoO₃, and activated carbon (AC). Considering the relative atomic mass (A_r) of Mo, S, and

....

18 O, we can list the mathematical equations below:

$$W(Mo) = W(MoS_2) \times \frac{A_r(Mo)}{A_r(Mo) + 2 \times A_r(S)} + W(MoO_3) \times \frac{A_r(Mo)}{A_r(Mo) + 3 \times A_r(O)}$$
(S1)

$$W(S) = W(MoS_2) \times \frac{2 \times A_r(S)}{A_r(Mo) + 2 \times A_r(S)} \#(S2)$$

$$W(0+H) = W(MoO_3) \times \frac{A_r(Mo)}{A_r(Mo) + 3 \times A_r(O)} + W(0+H \text{ in } AC) \#(S3)$$
21

22
$$W(AC) = W(MoO_3) + W(O + H in AC) + W(C) + W(N)#(S4)$$

where W (w/w, %) represents the mass fraction of a specific component or element as indicated in the parenthese in MoCOM. There are four unknown terms (W(MoS₂), W(MoO₃), W(AC), and W(O + H in AC)) and four equations. By solving the above equations, we can calculate the composition of MoS₂, 26 MoO₃, and activated carbon in MoCOM, as shown in Fig. 3 f.



32 Table S1. Langmuir, Freundlich, and Temkin model fitting results for sorption isotherms of Au(III) by

Sorption isotherm models	Parameters –	Nanofiber mats	
		CS-Th	CS-MoCOM-Th
Langmuir model	$K_{\rm L} ({\rm mL/mg})$	17.5	21.5
	$Q_{ m m}~(m mg/g)$	2960	4090
	R^2	0.979	0.987
Freundlich model	n	2.63	2.55
	$K_{\rm F}(({\rm mg/g})/({\rm mg/L})^{1/n})$	3320	4760
	R^2	0.895	0.923
Temkin model	$K_{\rm T} (10^5 {\rm mL/mg})$	0.776	1.11
	B_{T}	218	295
	R^2	0.919	0.920

33 CS-Th and CS-MoCOM-Th.

Sorption kinetics models	Parameters -	Nanofiber mats	
		CS-Th	CS-MoCOM-Th
Pseudo-first-order model	$k_1 (10^{-3} \text{ mg/(min \cdot g)})$	3.54	5.58
	$Q_{\rm e}~({ m mg/g})$	1330	1340
	R^2	0.935	0.682
Pseudo-second-order model	$k_2 (10^{-6} \text{g/(min \cdot mg)})$	6.16	7.57
	$Q_{\rm e} ({\rm mg/g})$	2150	2920
	R^2	0.996	0.998
Elovich model	α (mg/min·g)	149	501
	β (10 ⁻³ g/mg)	3.10	2.51
	R^2	0.950	0.956

39 Table S2. Pseudo-first-order, pseudo-second-order, and Elovich model fitting results for sorption
40 kinetics of Au(III) by CS-Th and CS-MoCOM-Th.

41

38





44

Fig. S2. SEM image (a) and EDS mapping (b and c) for CS-MoCOM-Th.



45 46

Fig. S3. The speciation distribution of Au(III) at different pH values.

47