

## MoS<sub>2</sub> Nanosheets for the Detoxification of Hg<sup>2+</sup> in Living Cells

Shanshan Xing, Chunqiu Xia, Xinyi Liu, Liangqia Guo,\* Fengfu Fu

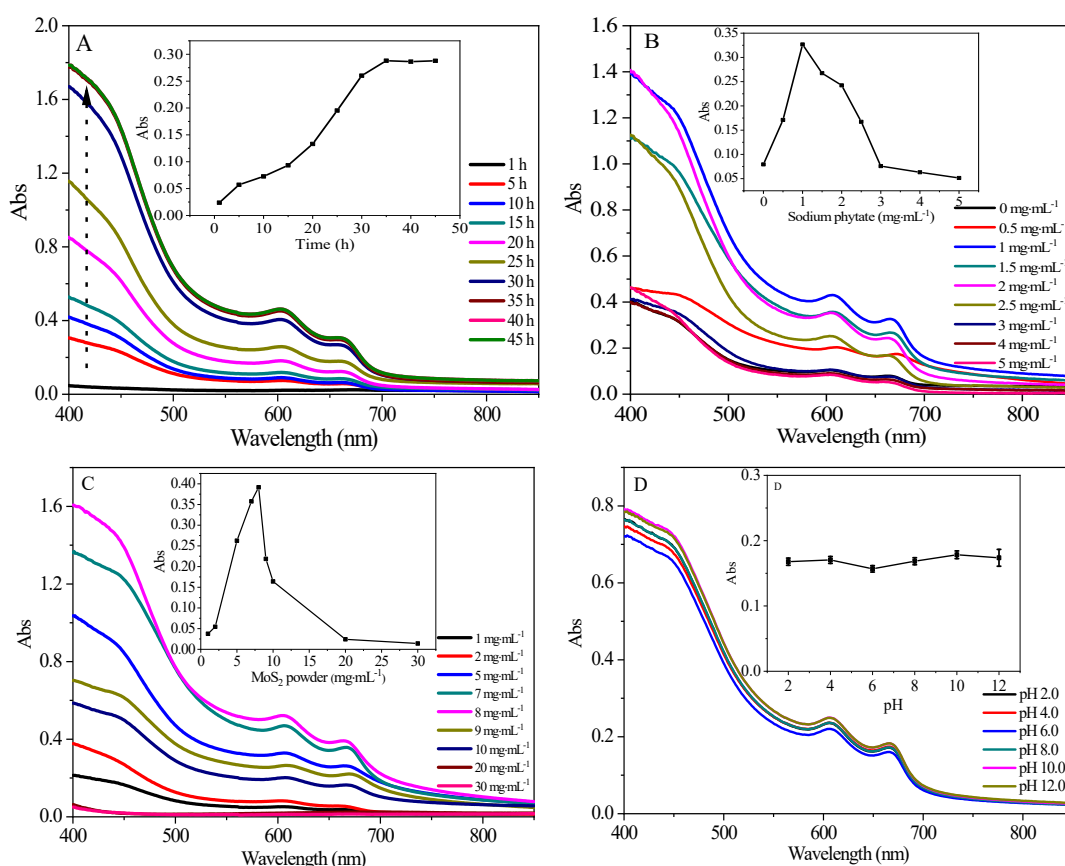
Ministry of Education Key Laboratory for Analytical Science of Food Safety and Biology,  
Fujian Provincial Key Laboratory of Analysis and Detection Technology for Food Safety,  
College of Chemistry, Fuzhou University, Fuzhou 350116, China

\*Corresponding authors, e-mail: [lqguo@fzu.edu.cn](mailto:lqguo@fzu.edu.cn)

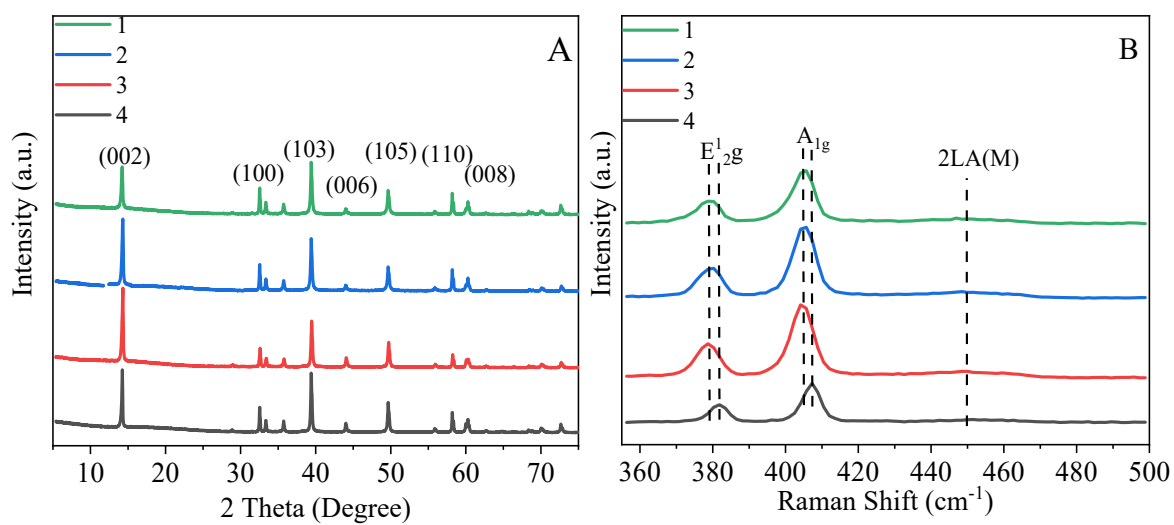
### Experimental

#### Supporting Figures

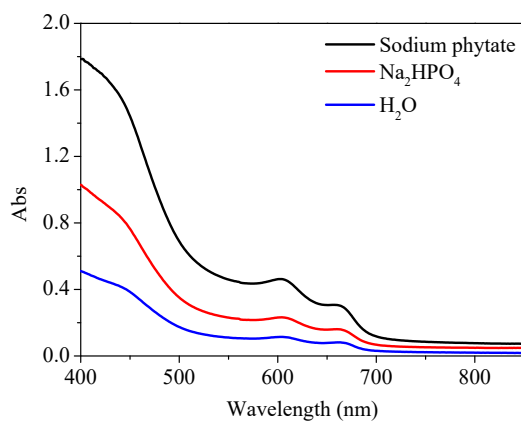
UV-Vis absorption spectra were recorded on a Lambda 750 UV-Vis spectrophotometer. Dynamic light scattering data (DLS) were measured by a Malvern Zetasizer Nano-2s laser particle size and Zeta potential analyzer. X-ray diffraction (XRD) pattern was performed on a Rigaku Ultima-IV X-ray diffractometer in the range of 5–75° by using a Cu K $\alpha$  radiation source ( $\lambda = 1.5418$ ). Raman spectrum was measured by a Renishaw inVia Raman microscope. Transmission electron microscopic (TEM) images were collected by a Thermo Scientific Talos F200S G2 scanning/transmission electron microscope at an accelerated voltage of 200 kV. Atomic force microscopic (AFM) images were taken by a Bruker Nanoscope IIIID scanning probe microscope. X-ray photoelectron spectroscopy (XPS) was measured by an ESCALAB 250 X-ray photoelectron spectrometer. Agilent 7500 inductively coupled plasma mass spectrometer (ICP-MS) was used to determine the concentration of Hg<sup>2+</sup>. The absorbance for cytotoxicity assay was measured by a TECAN Spark multimode microplate reader.



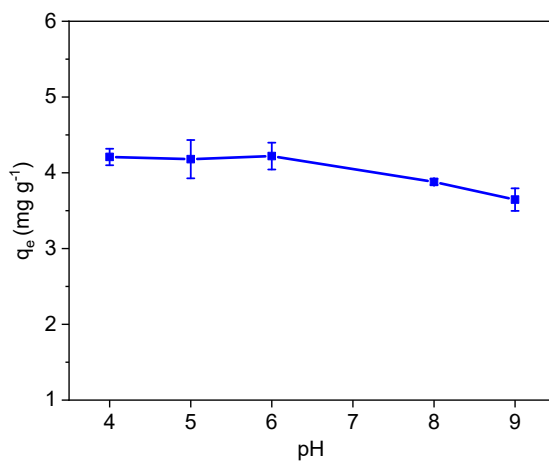
**Figure S1.** Absorption spectra of MoS<sub>2</sub> nanosheets exfoliated with different ultrasonic times (A), different concentrations of sodium phytate (B), different concentrations of MoS<sub>2</sub> powders (C); Absorption spectra of MoS<sub>2</sub> nanosheets (0.2 mg·mL<sup>-1</sup>) dispersed in different pH phosphate buffer (10 mmol·L<sup>-1</sup>) for three days (D). Insert of A, B and C is effect of ultrasonic time, concentration of sodium phytate, mass concentration of MoS<sub>2</sub> powder on the absorbance of MoS<sub>2</sub> nanosheets solution at 665 nm, respectively. Insert of D is the absorbance of MoS<sub>2</sub> nanosheets (0.2 mg·mL<sup>-1</sup>) at 665 nm in different pH buffer. The pH was adjusted by 1.0 mol·L<sup>-1</sup> HCl or NaOH solution.



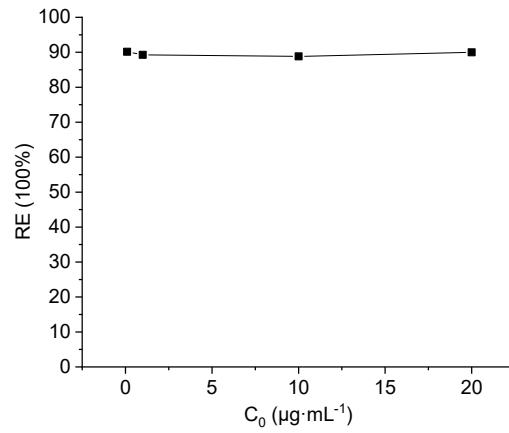
**Figure S2.** XRD patterns (A), and Raman spectra (B) of MoS<sub>2</sub> nanosheets exfoliated by sodium phytate (1), MoS<sub>2</sub> nanosheets exfoliated by Na<sub>2</sub>HPO<sub>4</sub> (2), MoS<sub>2</sub> nanosheets exfoliated by H<sub>2</sub>O (3), and bulk MoS<sub>2</sub> powder (4).



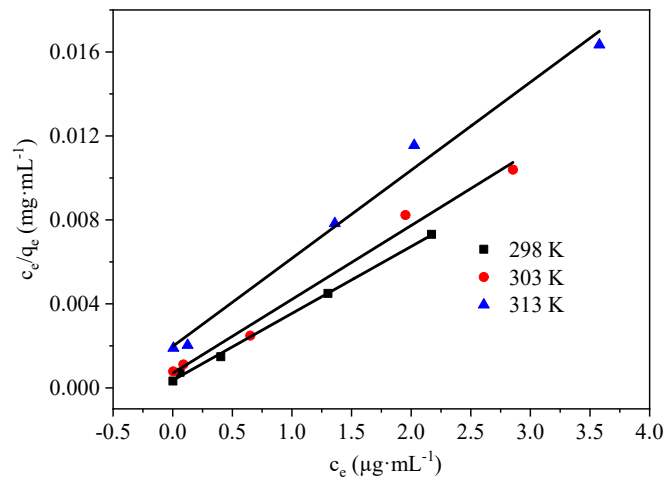
**Figure S3.** Absorption spectra of MoS<sub>2</sub> nanosheets obtained by ultrasonic exfoliation for 35 h in sodium phytate (1 mg·mL<sup>-1</sup>), Na<sub>2</sub>HPO<sub>4</sub> (3 mg·mL<sup>-1</sup>) and water. The mass concentration of MoS<sub>2</sub> powder was 5 mg·mL<sup>-1</sup>.



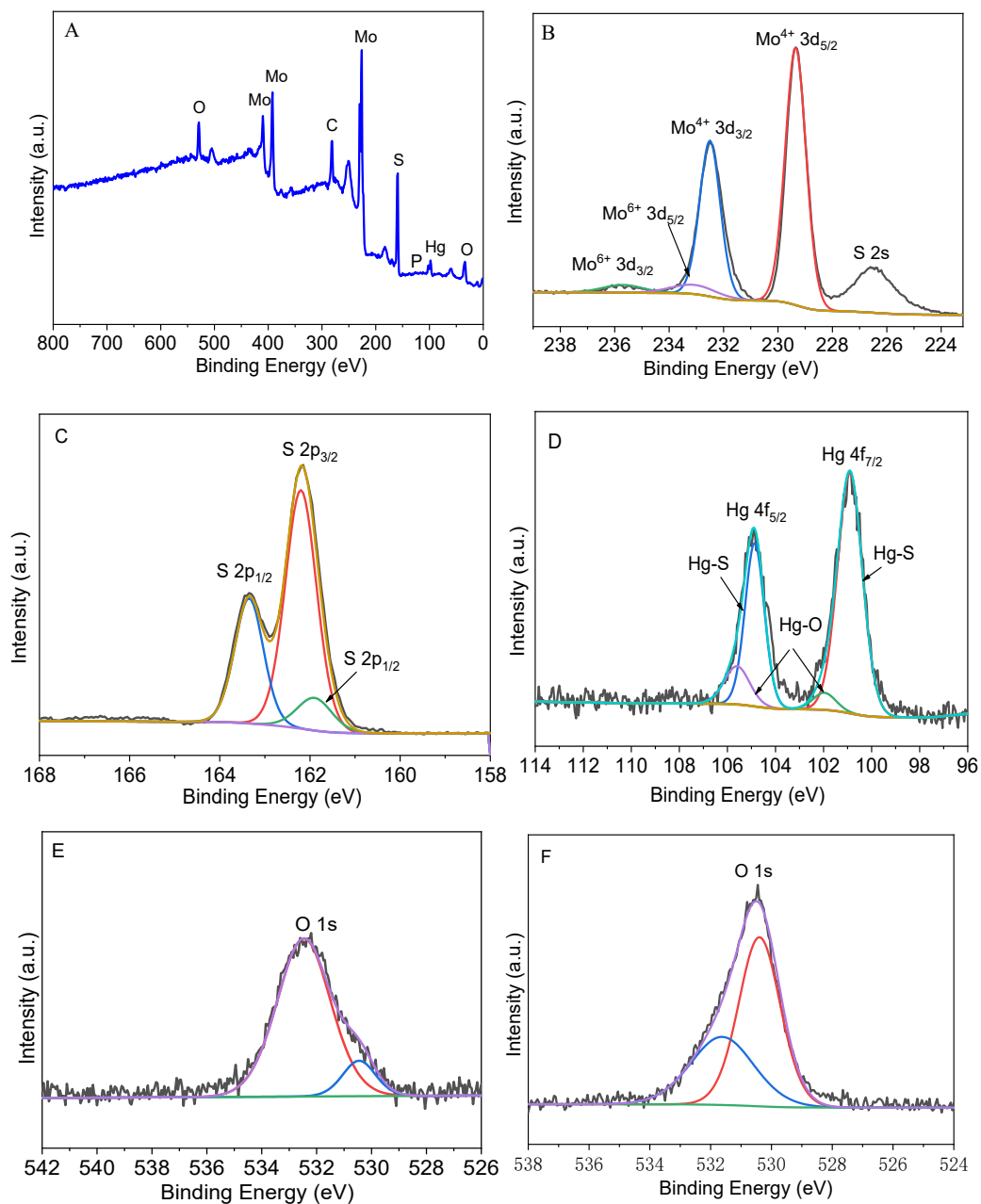
**Figure S4.** Effect of pH on the adsorption amount for Hg<sup>2+</sup> by MoS<sub>2</sub> nanosheets exfoliated by sodium phytate. The mass of MoS<sub>2</sub> nanosheets was 6.4 mg. The initial concentration of Hg<sup>2+</sup> was 1 μg·mL<sup>-1</sup>. The adsorption equilibrium time was 1 h.



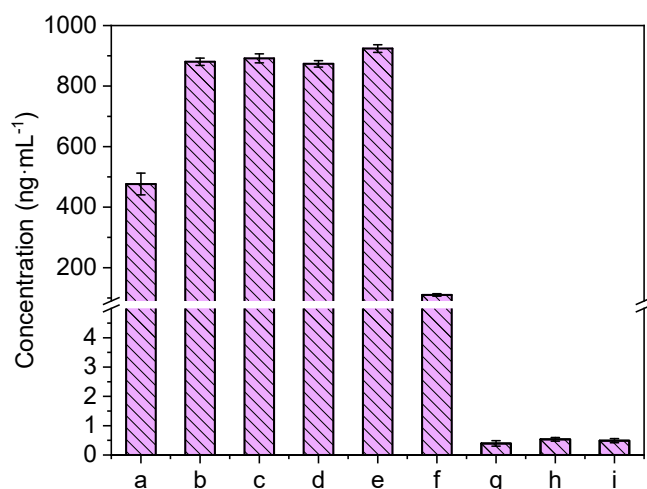
**Figure S5.** Effect of  $C_0$  on the removal efficiency (RE) of  $\text{MoS}_2$  nanosheets exfoliated by sodium phytate at  $25^\circ\text{C}$ .



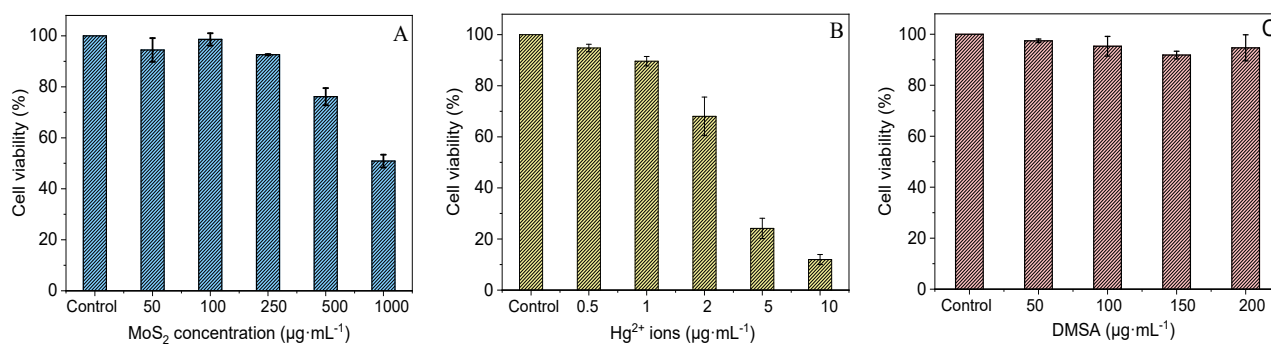
**Figure S6.** Langmuir adsorption isotherms of  $\text{Hg}^{2+}$  by  $\text{MoS}_2$  nanosheets exfoliated by sodium phytate at different temperatures.



**Figure S7.** The survey (A), Mo 3d (B), S 2p (C), Hg 4f (E) and O 1s (E) core-level XPS spectra of MoS<sub>2</sub> nanosheets after Hg<sup>2+</sup> adsorption, O 1s (F) core-level XPS spectra of MoS<sub>2</sub> nanosheets exfoliated by sodium phytate.



**Figure S8.** Concentration of residual metal ions after adsorption by MoS<sub>2</sub> nanosheets exfoliated by sodium phytate. (Concentrations of (a) Pb<sup>2+</sup>, (b) Cd<sup>2+</sup>, (c) Cr<sup>3+</sup>, (d) Mn<sup>2+</sup>, (e) Zn<sup>2+</sup>, (f) Hg<sup>2+</sup> were 1 μg·mL<sup>-1</sup>, respectively; (g) Hg<sup>2+</sup>: 100 ng·mL<sup>-1</sup>; (h) Mixture 1: Hg<sup>2+</sup>, Pb<sup>2+</sup>, Cd<sup>2+</sup>, Cr<sup>3+</sup>, Mn<sup>2+</sup>, Zn<sup>2+</sup> are all 100 ng·mL<sup>-1</sup>; (i) Mixture 2: Hg<sup>2+</sup>, NO<sub>2</sub><sup>-</sup>, NO<sub>3</sub><sup>-</sup>, SO<sub>4</sub><sup>2-</sup>, CO<sub>3</sub><sup>2-</sup> are all 100 ng·mL<sup>-1</sup>; MoS<sub>2</sub> nanosheets: 6.4 mg, adsorption time: 1 h).



**Figure S9.** Viability of HepG2 cells after incubation in different concentrations of MoS<sub>2</sub> nanosheets exfoliated by sodium phytate (A), Hg<sup>2+</sup> (B) and DMSA (C) for 12 h.

**Table S1.** Comparison of yields of MoS<sub>2</sub> nanosheets prepared by liquid ultrasonic exfoliation

Solvent/auxiliary reagent	Exfoliation time (h)	Yield	References
NMP	48 h	21%	[1]
ethyl alcohol/Water	8 h	0.6%	[2]
chloroform/acetonitrile	1 h	13.3%	[3]
alkali lignin	80 h	17.5%	[4]
TOCNs	4 h	18%	[5]
chitosan	5 h	25.5%	[6]
sodium cholate	16 h	10%	[7]
BSA	35 h	27.2%	[8]
tannin	2 h	60.5%	[9]
BSA-caged Au <sub>25</sub> clusters	48	24%	[10]
ATP	30 h	23.6%	[11]
water	35 h	2.3%	This work
sodium phytate	35 h	18.1%	This work

**Table S2.** Adsorption dynamics model parameters

C <sub>0</sub> (μg·mL <sup>-1</sup> )	Pseudo-second order model		
	q <sub>e,exp</sub> (mg·g <sup>-1</sup> )	q <sub>e,cal</sub> (mg·g <sup>-1</sup> )	R <sup>2</sup>
0.1	0.42	0.43	0.9992
1	4.19	4.22	0.9996
10	43.66	43.71	0.9969
20	85.30	86.73	0.9979



**Table S3.** The maximal adsorption capacity and correlation coefficient of Langmuir isotherms at different temperatures

Temperature	$q_{\max}$ (mg·g <sup>-1</sup> )	R <sup>2</sup>
298 K	313.48	0.9976
303 K	284.09	0.9857
313 K	238.1	0.9842

**Table S4.** Comparison of the maximum adsorption capacity of MoS<sub>2</sub> for Hg<sup>2+</sup>

Adsorbent	$q_{\max}$ (mg·g <sup>-1</sup> )	Reference
MoS <sub>2</sub> nanosheets exfoliated by sodium phytate	312.5 (25 °C)	This work
MoS <sub>2</sub> nanosheets exfoliated directly in water	85.47 (25 °C)	This work
MoS <sub>2</sub> powder	41.49 (25 °C)	This work
widened defect-rich nanoMoS <sub>2</sub> nanosheets	2563	[12]
2D MoS <sub>2</sub>	254 (20 °C)/305 (35 °C)	[13]
Porous Au/Fe <sub>3</sub> O <sub>4</sub> /MoS <sub>2</sub> CAAs aerogel	1527	[14]
oxygen-incorporated MoS <sub>2</sub> nanosheets	1995.72	[15]
cellulose/MoS <sub>2</sub> /Fe <sub>3</sub> O <sub>4</sub> composite	469.48	[16]

## References

1. J. Z. Huang, X. L. Deng, H. Wan, F. S. Chen, Y. F. Lin, X. J. Xu, R. Z. Ma and T. Sasaki, *ACS Sustain. Chem. Eng.*, 2018, **6**, 5227-5237.
2. K. G. Zhou, N. N. Mao, H. X. Wang, Y. Peng and H. L. Zhang, *Angew. Chem. Int. Ed.*, 2011, **50**, 10839-10842.
3. S. L. Zhang, H. Jung, J. S. Huh, J. B. Yu and W. C. Yang, *J. Nanosci. Nanotechnol.*, 2014, **14**, 8518-8522.

4. W. S. Liu, C. Y. Zhao, R. Zhou, D. Zhou, Z. L. Liu and X. H. Lu, *Nanoscale*, 2015, **7**, 9919-9926.
5. Y. Y. Li, H. L. Zhu, F. Shen, J. Y. Wan, S. Lacey, Z. Q. Fang, H. Q. Dai and L. B. Hu, *Nano Energy*, 2015, **13**, 346-354.
6. X. M. Feng, X. Wang, W. Y. Xing, K. Q. Zhou, L. Song and Y. Hu, *Compos. Sci. Technol.*, 2014, **93**, 76-82.
7. R. J. Smith, P. J. King, M. Lotya, C. Wirtz, U. Khan, S. De, A. Neill, G. S. Duesberg, J. C. Grunlan, G. Moriarty, J. Chen, J. Z. Wang, A. I. Minett, V. Nicolosi and J. N. Coleman, *Adv. Mater.*, 2011, **23**, 3944-3948.
8. G. J. Guan, S. Y. Zhang, S. Liu, Y. Q. Cai, M. Low, C. P. Teng, I. Y. Phang, Y. Cheng, K. L. Duci, B. M. Srinivasan, Y. Zhang, Y. W. Zhang and M. Y. Han, *J. Am. Chem. Soc.*, 2015, **137**, 6152-6155.
9. C. Zhang, D. F. Hu, J. W. Xu, M. Q. Ma, H. B. Xing, K. Yao, J. Ji and Z. K. Xu, *ACS Nano*, 2018, **12**, 12347-12356.
10. G. J. Guan, S. H. Liu, Y. Cheng, Y. W. Zhang and M. Y. Han, *Nanoscale*, 2018, **10**, 10911-10917.
11. X. L. Liu, H. Chen, J. Lin, Y. Li and L. Q. Guo, *Chem. Commun.*, 2019, **55**, 2972-2975.
12. K. Ai, C. P. Ruan, M. X. Shen and L. H. Lu, *Adv. Fun. Mater.*, 2016, **26**, 5542-5549.
13. F. F. Jia, Q. M. Wang, J. S. Wu, Y. M. Li and S. X. Song, *ACS Sustain. Chem. Eng.*, 2017, **5**, 7410-7419.
14. L. H. Zhi, W. Zuo, F. J. Chen and B. D. Wang, *ACS Sustain. Chem. Eng.*, 2016, **4**, 3398-3408.
15. W. Zhan, F. Jia, Y. Yuan, C. Liu, K. Sun, B. Yang and S. Song, and *J. Hazard. Mater.*, 2020, **384**, 121382.
16. P. Gao, J. Lei, J. Tan, G. Wang, H. Liu and L. Zhou, *Compos. Commun.*, 2021, **25**, 100736.