Supporting Information

Sensitive and Direct Electrochemical Detection of Bisphenol S Based on 1T&2H-MoS_2/CNTs-NH_2 Nanocomposites

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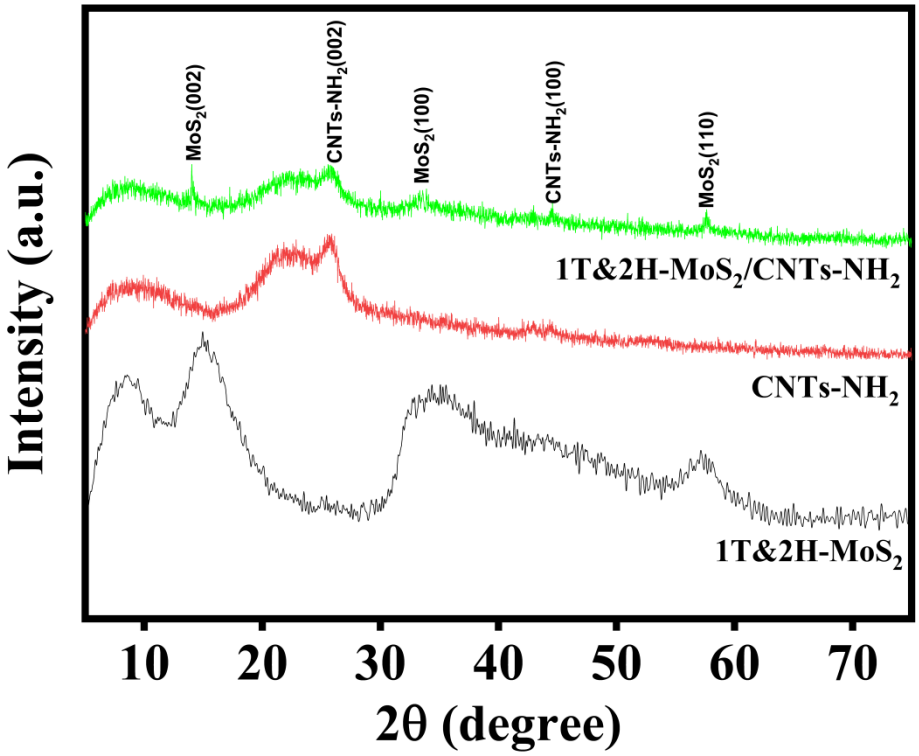

Fig. S1 XRD spectra of CNTs-NH_2, 1T&2H-MoS_2 and 1T&2H-MoS_2/CNTs-NH_2 nanocomposite.

1T&2H-MoS_2 nanosheets exhibit three diffraction peaks at 2θ=14.30°, 33.34°and 58.94°, which can be indexed with the (002), (100) and (110) diffraction planes of 1T&2H-MoS_2 crystals containing hexagonal structure[1]. The two typical diffraction peaks indexed at 2θ = 25.6°, 44.4° for CNTs-NH_2 are associated with the (002), (100) crystal planes of CNTs-NH_2, respectively [2]. In the XRD spectra of 1T&2H-MoS_2/CNTs-NH_2, diffraction peaks of both 1T&2H-MoS_2 and CNTs-NH_2 appear, indicating that the formation of 1T&2H-MoS_2/CNTs-NH_2 nanocomposite.

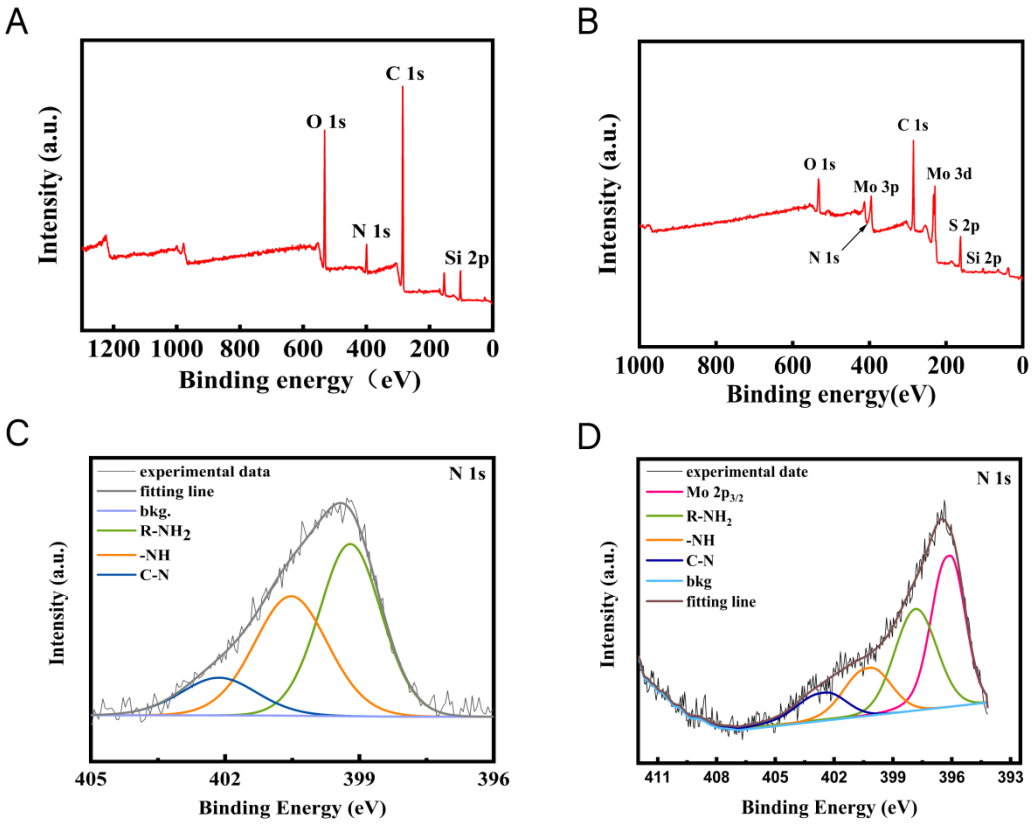

Fig. S2 XPS spectra of CNTs-NH_2 (A) and 1T&2H-MoS_2/CNTs-NH_2 nanocomposite (B). XPS spectra for N 1S of CNT-NH_2(C) and 1T&2H-MoS_2/CNTs-NH_2 nanocomposite (D).

The XPS survey spectrum of CNTs-NH_2 shows the presence of Si(102.40 eV), N(399.46 eV), C(285.03 eV) and O(532.09 eV) elements, meaning that the amino groups were successfully introduced to the carbon nanotubes[3]. The XPS survey spectrum of the 1T&2H-MoS_2/CNTs-NH_2 composite shows the presence of Si(102.41 eV), S(161.47), Mo(228.46 eV), C(284.26 eV), N(399.50) and O(531.43 eV) elements. The N 1s spectrum of CNT-NH2 can be decomposed into three peaks at 399.20, 400.53, 402.14 eV corresponding to R-NH_2, -NH and C-N, respectively[3]. Besides, the N 1s spectrum of 1T&2H-MoS_2/CNTs-NH_2 nanocomposite can be divided into four peaks, the peak observed at 397.84 eV is ascribed to R-NH_2, peaks at 400.17 eV and 402.46 eV to -NH and C-N, respectively, and the peak at 396.09 eV belongs to Mo-N[4, 5]. The appearance of all peaks for 1T&2H-MoS_2/CNTs-NH_2 nanocomposite indicates that 1T&2H-MOS_2 and CNTs-NH_2 were successfully assembled.

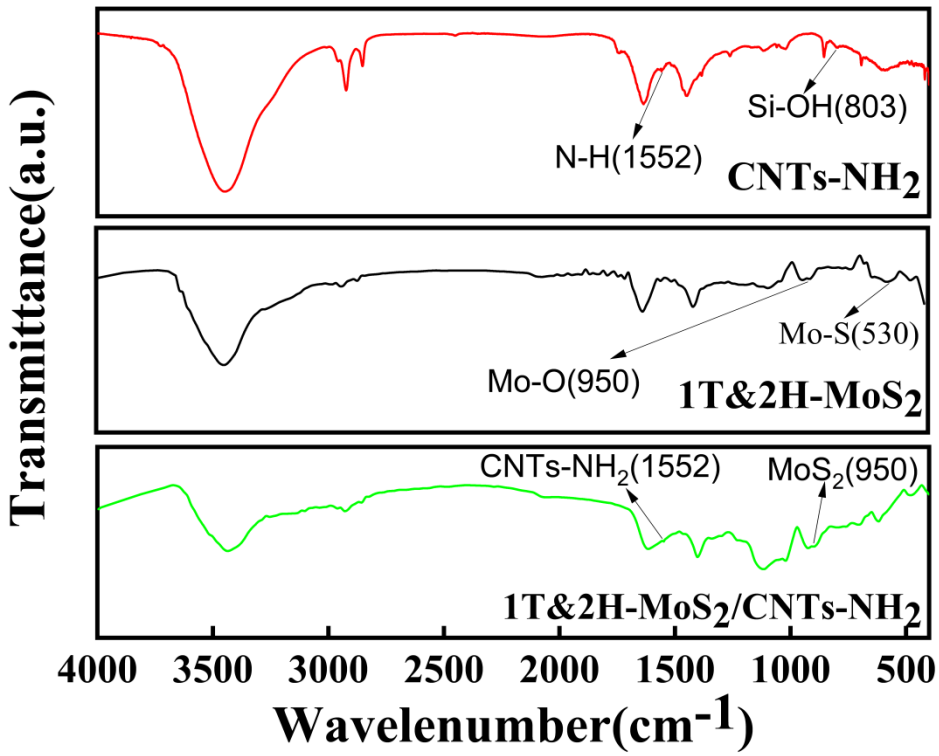

Fig. S3 FT-IR spectra of CNTs-NH_2, 1T&2H-MoS_2 and 1T&2H-MoS_2/CNTs-NH_2 nanocomposite.

In the FT-IR spectrum of CNTs-NH_2, the peak at 1552 cm^{-1} is attributed to the N-H secondary amine group. In addition, the peak observed at 803 cm^{-1} is caused by Si-OH, which confirms the reaction of CNTs-COOH with 3-APTES[6, 7]. The experimental results show that the amine group has been successfully grafted onto the carbon nanotubes. In the FT-IR spectrum of 1T&2H-MoS_2, The peaks at 530 cm^{-1} and 950 cm^{-1} are attributed to Mo-S and Mo-O stretching vibrations, respectively[8]. In FI-TR spectrum of 1T&2H-MoS_2/CNTs-NH_2, the characteristic peaks of both CNTs-NH_2 (1552 cm^{-1}) and 1T&2H-MoS_2 (950 cm^{-1}) appear, indicating the formation of 1T&2H-MoS_2/CNTs-NH_2 hybrids.

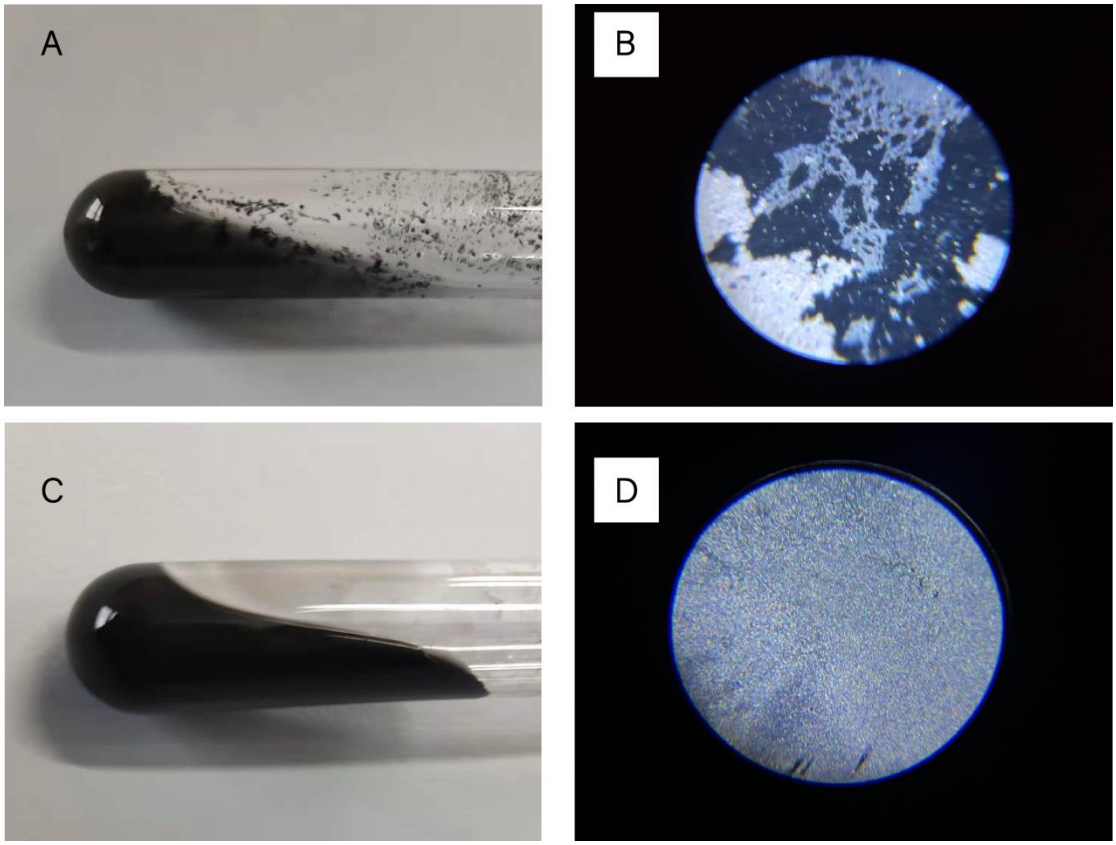

Fig. S4 Photographs of 1 mg/mL CNTs (A) and 1 mg/mL CNTs-NH_2 (C) dispersions in water after sonication 6h, optical microscope images of 1 mg/mL CNTs (B) and 1 mg/mL CNTs-NH_2 (D)modified GCE (coating volume: 8 μL).

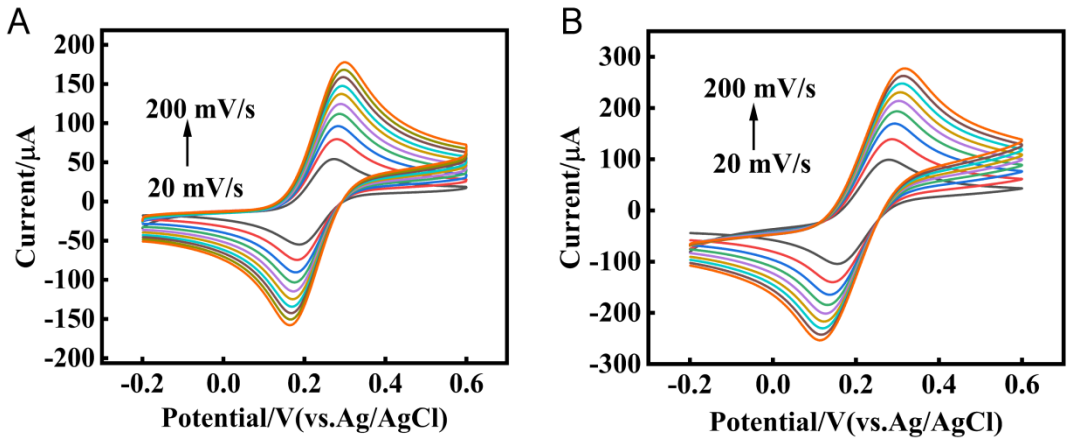

Fig. S5 CV curves of CNTs/GCE (A) and CNTs-NH_2/GCE (B) in 0.1M KCl solution (containing 5.0 mM $Fe(CN)_6^{3-}$/$Fe(CN)_6^{4-}$) at different scan rates (20, 40, 60, 80, 100,120,140, 160,180 and 200 mV/s)

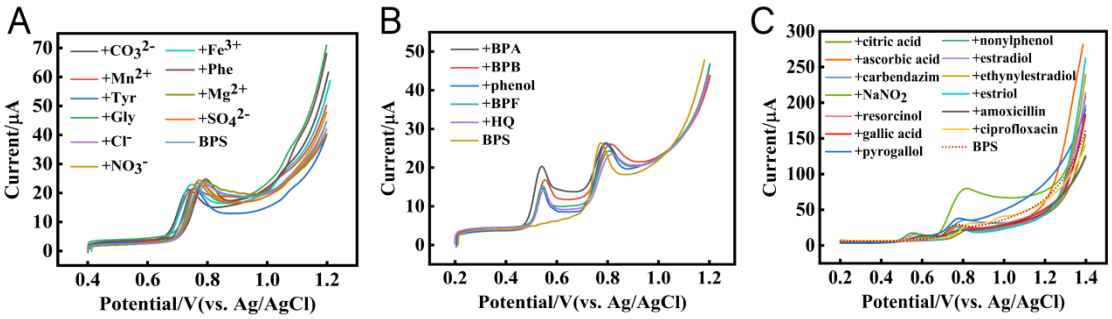

Fig. S6 LSV curves of 1T&2H-MoS_2/CNTs-NH_2/GCE to 10 μmol/L BPS in the absence or presence of (A) 1 mmol/L different common inorganic ions(Mn^{2+}, Mg^{2+}, NO_3^-, Fe^{3+}, SO_4^{2-}, CO_3^{2-}, Cl^- and phenylalanine, glycine and tyrosine) and (B) 10 μmol/L other bisphenolic and phenolic compounds(BPA, BPB, BPF, phenol, hydroquinone). (C) 1 mmol/L citric acid, ascorbic acid, $NaNO_2$, and 10 μmol/L carbendazim, resorcinol, gallic acid, pyrogallol, nonylphenol, estradiol, ethynylestradiol, estriol, amoxicillin and ciprofloxacin. (scan rate: 100 mV/s)

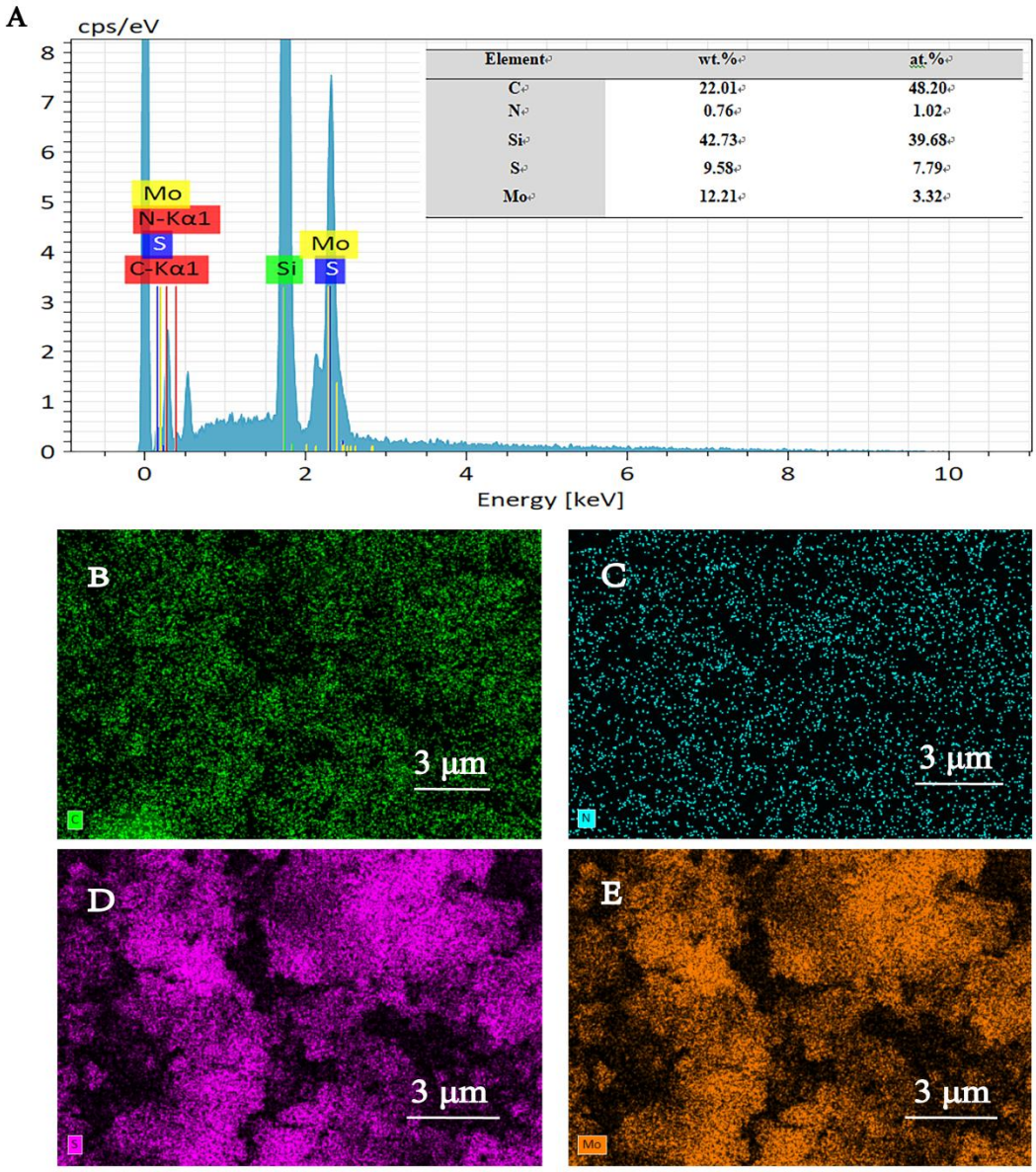

Fig. S7 (A) EDX spectrum of 1T&2H-MoS_2/CNTs-NH_2. EDX elemental mapping images of C(B), N(C), S(D) and Mo(E).

The elemental analysis of 1T&2H-MoS_2/CNTs-NH_2 nanocomposites was performed using EDX spectroscopy, as shown in Fig. S7A. The results confirm the presence of Mo, S, C and N elements, indicating the successful preparation of 1T&2H-MoS2/CNTs-NH_2. The high percentage of Si element was due to the use of Si wafer as the substrate for EDX analysis. In addition, the elemental mapping images in Fig. S7B~E reveals that there is a homogeneous distribution of C, N, S, and Mo elements, showing that CNTs-NH_2 interspersed well in 1T&2H-MoS_2.

References

1. J. Prasad, A. K. Singh, K. K. Haldar, V. Gupta and K. Singh, *Journal of Alloys and Compounds*, 2019, **788**, 861-872.
2. A. Mohammadi, E. Heydari-Bafrooei, M. M. Foroughi and M. Mohammadi, *Microchemical Journal*, 2020, **158**, 105154.
3. G. Yu, W. Wu, Q. Zhao, X. Wei and Q. Lu, *Biosensors and Bioelectronics*, 2015, **68**, 288-294.
4. N. Lingappan and D. J. Kang, *Electrochimica Acta*, 2016, **193**, 128-136.
5. X. Dai, Z. Li, K. Du, H. Sun, Y. Yang, X. Zhang, X. Ma and J. Wang, *Electrochimica Acta*, 2015, **171**, 72-80.
6. J. Kathi, K.-Y. Rhee and J. H. Lee, *Composites Part A: Applied Science and Manufacturing*, 2009, **40**, 800-809.
7. S. Zarghami, T. Mohammadi, M. Sadrzadeh and B. Van der Bruggen, *Science of The Total Environment*, 2020, **711**, 134951.
8. L. N. Long, P. T. Thi, P. Trung Kien, P. T. Trung, M. Ohtani, Y. Kumabe, H. Tanaka, S. Ueda, H. Lee, P. B. Thang and T. V. Khai, *Applied Surface Science*, 2020, **504**, 144193.