

Electronic Supplementary Information

Size-dependent optical extinction of MoS₂ nanosheets and aptamer-induced dispersion behavior for label-free detection of *Escherichia coli* O157: H7

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Experimental section

Materials: Molybdenum disulfide powder (98%, 2 μ m in size) were purchased from Tianjin Chemical Reagent Factory Kaida chemical plant. Sodium cholate (SC, 98%) and phosphate buffer solution (PBS, 0.01 M, pH = 7.4) were obtained from Shanghai Macklin Biochemical Chemistry Co., Ltd. (Shanghai, China). Anhydrous ethanol and NaCl were purchased from Kelong Chemical Reagent Co., Ltd. (Chengdu, China). The 5'-thiol-modified DNA aptamer of *E.coli* O157: H7 (5'HS-ATC CGT CAC ACC TGC TCT GTC TGC GAG CGG GGC GCG GGC CCG GCG GGG GAT GCG TGG TGT TGG CTC CCG TAT -3')¹ was obtained from Shanghai Sangon Biotech Co., Ltd. All chemicals and reagents were of analytical grade and used as received without further purification, and ultrapure water was used throughout the work. Ultrapure water (18.25 M Ω /cm) was used throughout the experiment.

Apparatus: The SK2510HP ultrasonic bath (250 W, Shanghai Kudos Ultrasonic Instruments Co., Ltd., China) was used for the preparation of MoS₂-NSs. UV- Visible absorption spectrum was recorded by the TU-1950 UV- Visible spectrophotometer (Pgeneral, China). The Visible extinction spectrum was recorded by the custom-made extinction spectroscopy shown in Figure S2. In the extinction spectrum system, the light source was the tungsten halogen lamp (HL-2000-HP, Ocean Optics), and the receiver was the spectrometer (HR4000, Ocean Optics). The morphologies of MoS₂-NSs were observed using a JSM-7800F field-emission SEM (JEOL, Japan) and a dimension icon AFM (Bruker, Germany). Hydrodynamic size distribution and zeta potential were measured on a Malvern Zetasizer Nano ZS analyzer. Centrifugation was conducted using a TG16-WS high-speed centrifuge (Xiangyi, China).

Culture of *E. coli* O157: H7 : *E. coli* O157: H7, *E. coli* ATCC35218, *S. aureus*, and *P. aeruginosa* were obtained from the University-Town Hospital of Chongqing Medical University. Bacteria were inoculated into nutritious broth (NB) and stirred overnight at 37°C. The culture was centrifuged at 4000 rpm for 5 min and then resuspended with PBS buffer. Bacterial suspension was inactivated by boiling at 90 °C for 10 min and stored at 4 °C for later use. The scattered light turbidimeter was used to determine the concentration of bacterial.

Preparation of MoS₂-NSs: The MoS₂-NSs were obtained via two different methods as previously reported,²⁻⁴ and partially optimized. The first method was surfactant-assisted liquid-phase exfoliation MoS₂-NSs. MoS₂ powder (0.5 g, 31.25 mM) and SC (0.15 g, 3.48 mM) were added to water and sonicated at 25-37 °C for 20 h. And then, the dispersion was resting overnight and centrifuged at 3 000 rpm for 30 min to remove bulk MoS₂, collected the yellow-green supernatant. To remove the SC, the dispersion was centrifuged at 10 000 rpm (30 min) for collecting sediment of MoS₂-NSs. Similarly, the sediment was dispersed in pure water and sonicated for 2 min, then repeated the above operation to complete the washing process. Furthermore, to obtain a high dispersibility MoS₂-NSs, the stock solution of MoS₂-NSs should be centrifuged at 3 000 rpm for 10 min to remove re-bulk MoS₂. The MoS₂-NSs prepared by this method were recorded as SC-MoS₂-NSs. Another method was the mixed-solvent strategy Liquid-phase exfoliation MoS₂-NSs. MoS₂ powder (0.5 g, 31.25 mM) was added to 45% ethanol/water (v/v) and sonicated at 25-37 °C for 8 h. Subsequently, the dispersion was resting overnight and centrifuged at 3000 rpm for 30 min to remove bulk MoS₂, collected the yellow-green supernatant. Furthermore, to obtain a high reproducibility, the dispersion was resting overnight and took the top three fourth of the dispersion to use. The MoS₂-NSs prepared by this method were recorded as 45%-MoS₂-NSs. The stock solution of MoS₂-NSs was stored in a refrigerator at 4 °C.

Extinction spectrum measurement: Since the aggregated MoS₂-NSs may exist as suspension and even precipitate, it is very important to guarantee the reproducibility of the experiment. In the experiment, the mixed solution was left setting for 1h at room temperature, and taking the two-thirds (1.4 mL in 2 mL) of the supernatant was diluted with water to 2 mL and measured the extinction spectrum. Taking the supernatant can effectively reduce suspension and precipitate. Furthermore, diluting with water is conducive to its dispersion.

E. coli O157: H7 Detection: The 45%-MoS₂-NSs dispersions (0.2 mL) were first diluted with pure water to 1mL, added with aptamers (40 µL, 1 µM), and then incubated for 1 h. After that, PBS buffer (0.75 mL) with different concentrations of E. coli O157: H7 were added into the solution, and then water was added to 2 mL. The mixed solution was left setting for 1 h at room temperature, and taking the two-thirds (1.4 mL in 2 mL) of the supernatant was diluted with water to 2 mL and measured the extinction spectrum. All the data were collected from at least three independent measurements.

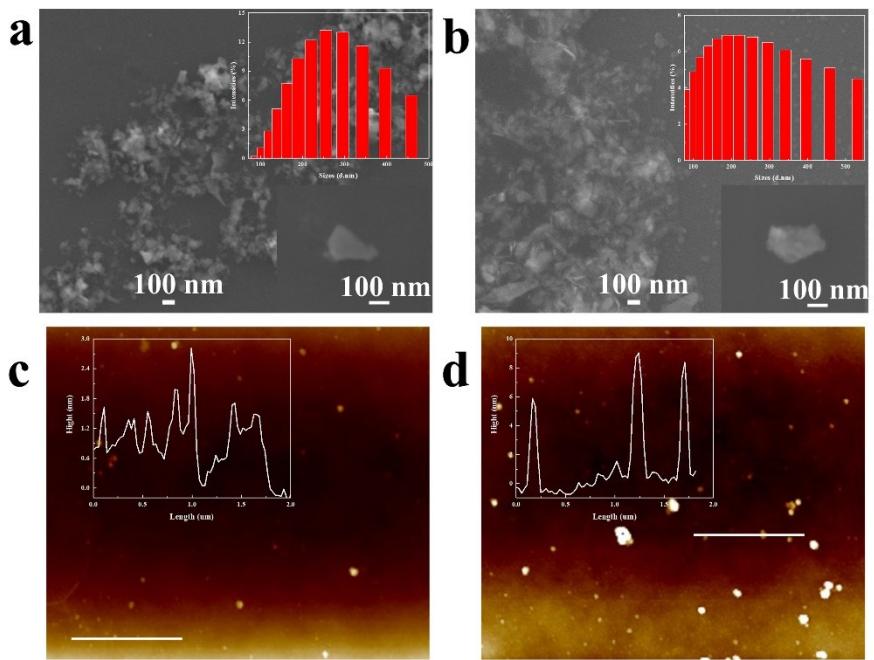


Fig. S1 a) SEM image of 45%-MoS₂-NSs, the upper-right inset is the DLS measured hydrodynamic size distributions of 45%-MoS₂-NSs, and lower-right inset is single 45%-MoS₂-NSs. b) SEM image of SC-MoS₂-NSs, the upper-right inset is the DLS measured hydrodynamic size distributions of SC-MoS₂-NSs, and lower-right inset is single SC-MoS₂-NSs. c) AFM image of 45%-MoS₂-NSs, the inset is the height images of 45%-MoS₂-NSs. d) AFM image of SC-MoS₂-NSs, the inset is the height images of SC-MoS₂-NSs.

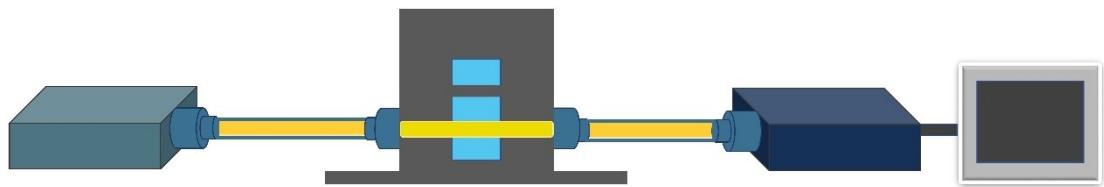


Fig. S2 Schematic diagram of custom-made extinction spectroscopy. From left to right: tungsten halogen lamp, optical fiber, cuvette, optical fiber, spectrometer, and computer.

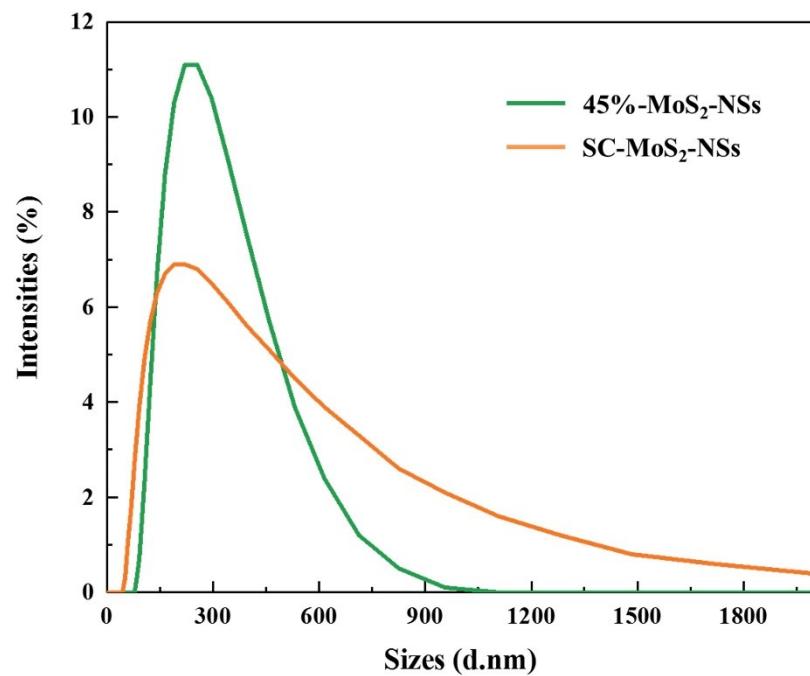


Fig. S3 DLS measured hydrodynamic size distributions of 45%-MoS₂-NSs and SC-MoS₂-NSs.

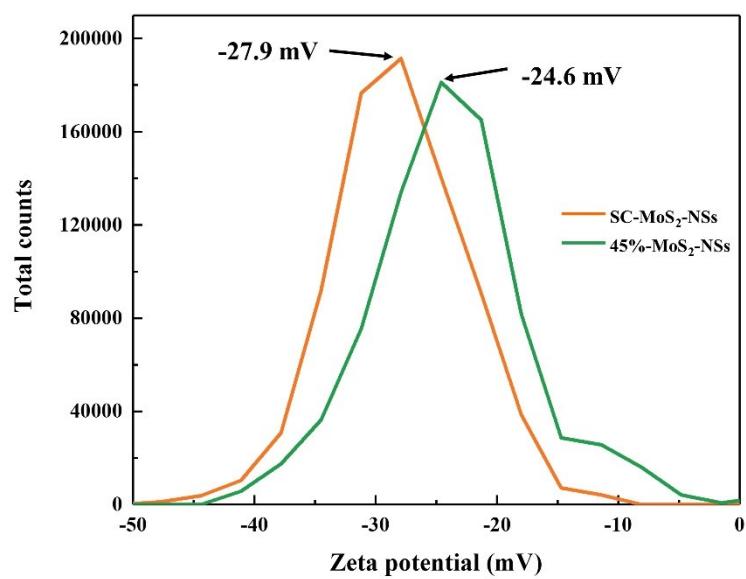


Fig. S4 The zeta potential of 45%-MoS₂-NSs and SC-MoS₂-NSs.

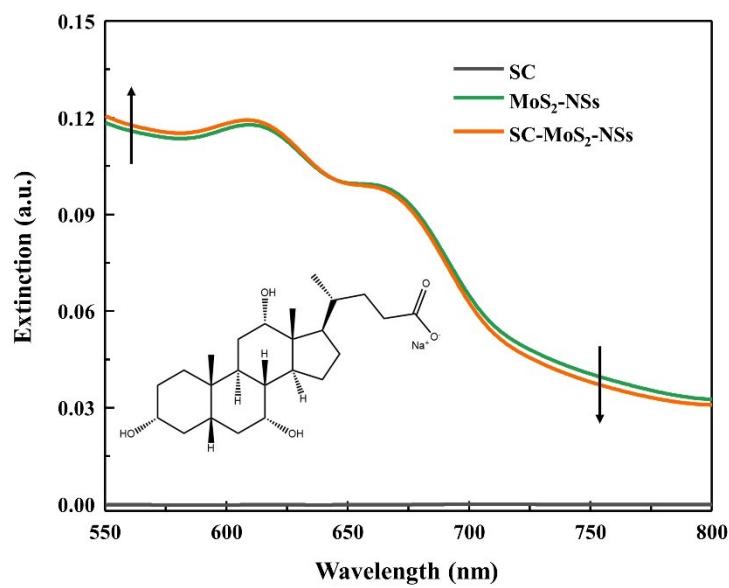


Fig. S5 The effect of SC on the extinction spectrum of MoS₂-NSs, the inset is the molecular structure of SC.

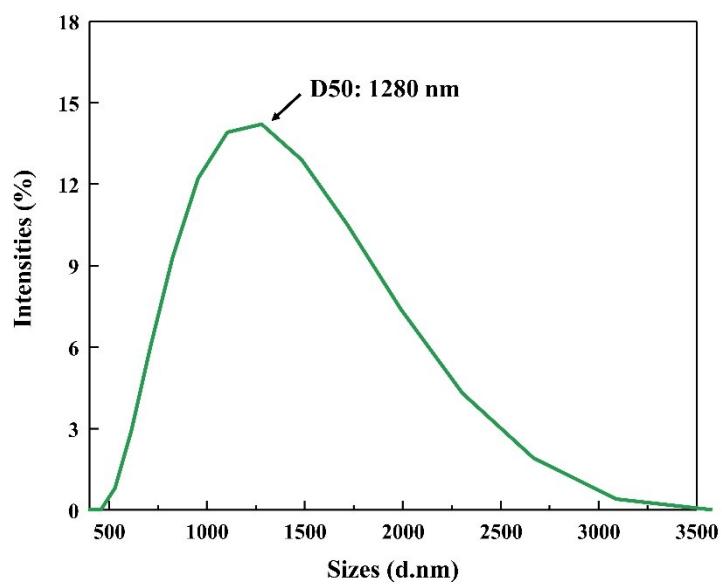


Fig. S6 After the addition of NaCl (20 μ L, 5 M) for 1 h, DLS measured hydrodynamic size distributions of 45%-MoS₂-NSs.

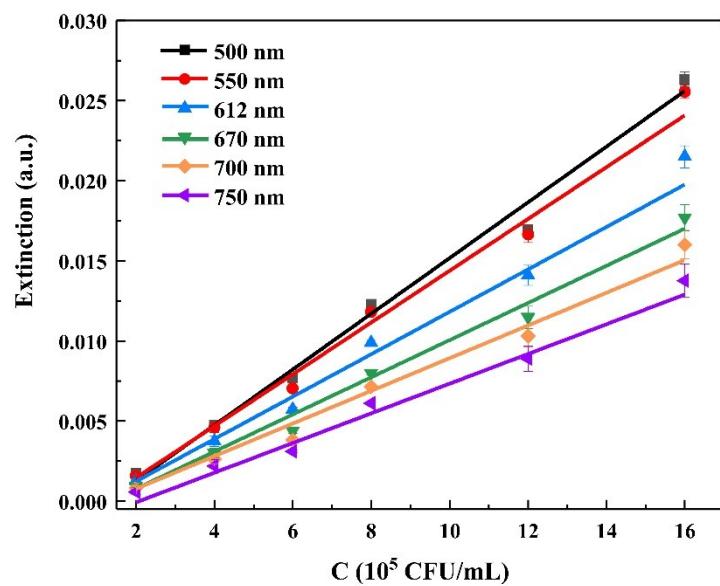


Fig. S7 Calibration curve of extinction spectra detection of *E. coli* O157: H7 at different wavelengths (500, 550, 610, 670, 700, 750 nm).

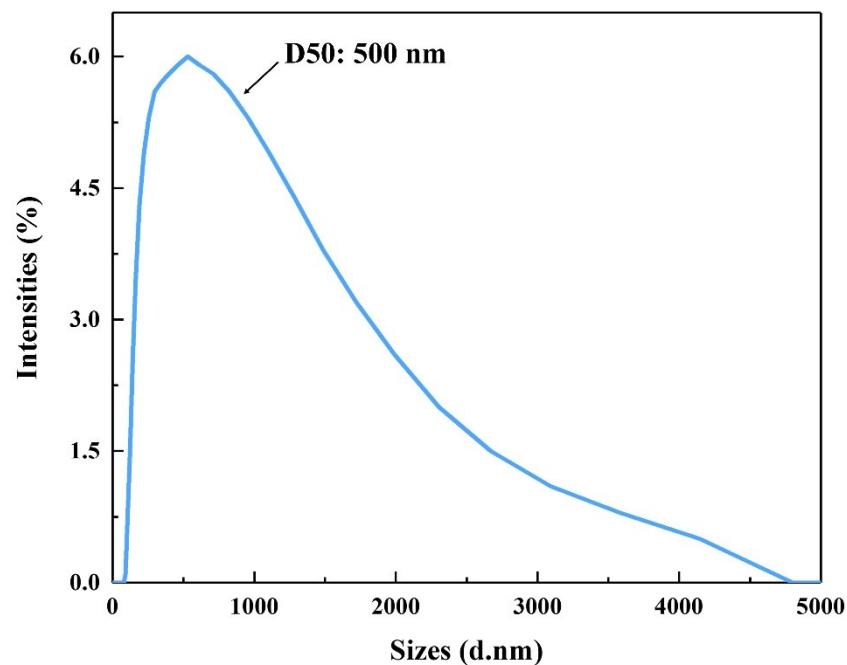


Fig. S8 After the addition of *E. coli* O157: H7 (750 μ L, 10^4 CFU/mL) for 1 h, DLS measured hydrodynamic size distributions of aptamer-based MoS₂-NSs.

References

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