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Surface chemistry regulates optical properties and cellular interactions of ultrasmall MoS_2 quantum dots for biomedical applications

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Experimental

The Cell Lysates

The preparation of cell lysates was based on previous reports.[1] HeLa cells were lysed with a cold 3-[(3-cholamidopropyl) dimethylammonio]-1-propanesulfonate (CHAPS) lysis buffer (10 mM Tris-HCl, pH 7.4, 1 mM $MgCl_2$, 1 mM EGTA, 0.1 mM PMSF, 0.5% CHAPS, and 10% glycerol) supplemented with 20 μM cetrimonium bromide at a density of 1×10^6 cells/mL. The cell suspension was incubated for 30 min on ice, followed by centrifugation at 4 °C for 20 min to remove cell debris. The supernatant was flash frozen and stored at −20 °C before use.

Supporting Figures

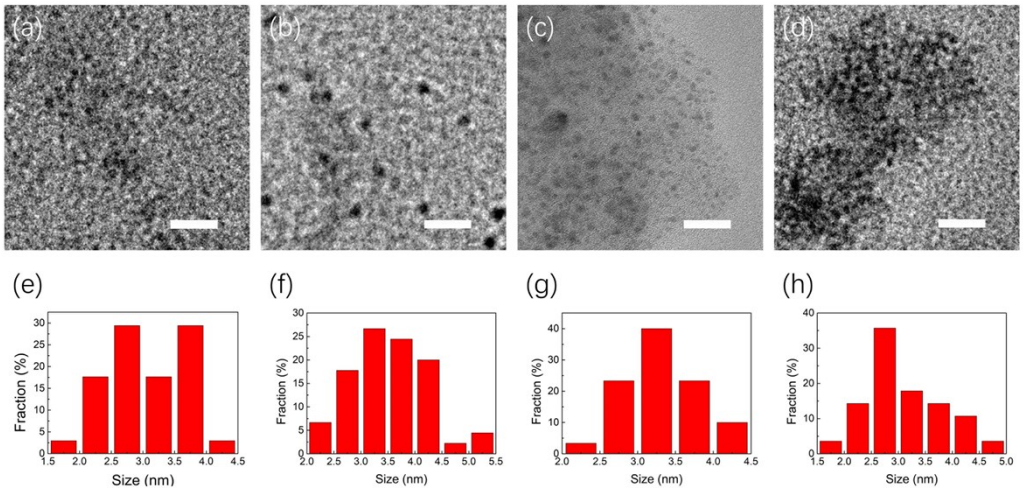

Fig. S1 TEM (a-d) and corresponding size distribution diagrams (e-h) of GSH-MoS_2 QDs (a, e); Cys-MoS_2 QDs (b, f); MSA-MoS_2 QDs (c, g) and TA-MoS_2 QDs (d, h), respectively. Scale bars: 20 nm.

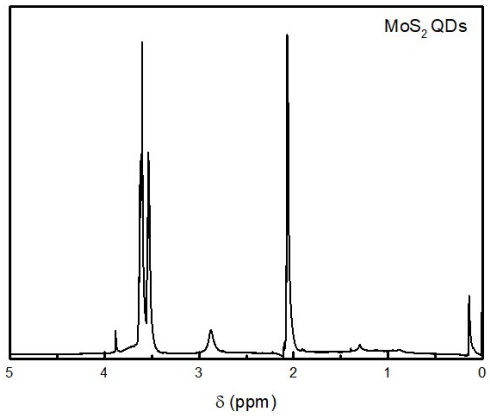

Fig. S2 The ^{1}H-NMR spectrum of pristine MoS_2 QDs.

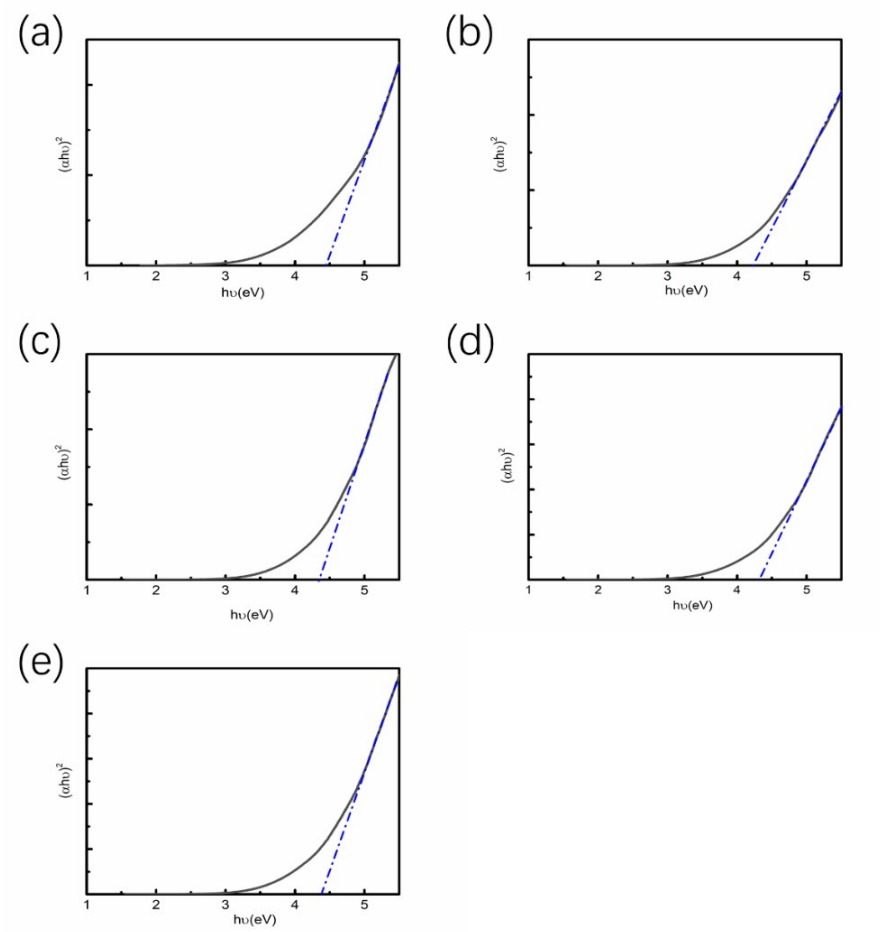

Fig. S3 The Tauc-Plots of MoS_2 QDs and modified MoS_2 QDs. (a) Pristine MoS_2 QDs with band gap of 4.45 eV; (b) GSH-MoS_2 QDs with band gap of 4.23 eV; (c) Cys-MoS_2 QDs with band gap of 4.35 eV; (d) MSA-MoS_2 QDs with band gap of 4.32 eV; (e) TA-MoS_2 QDs with band gap of 4.38 eV. The band gap is estimated from the plot of $(\alpha h\nu)^2$ versus $h\nu$ by extrapolating the straight line to the X axis intercept (where α is the absorbance and $E=h\nu$ is the photonenergy).[2-4]

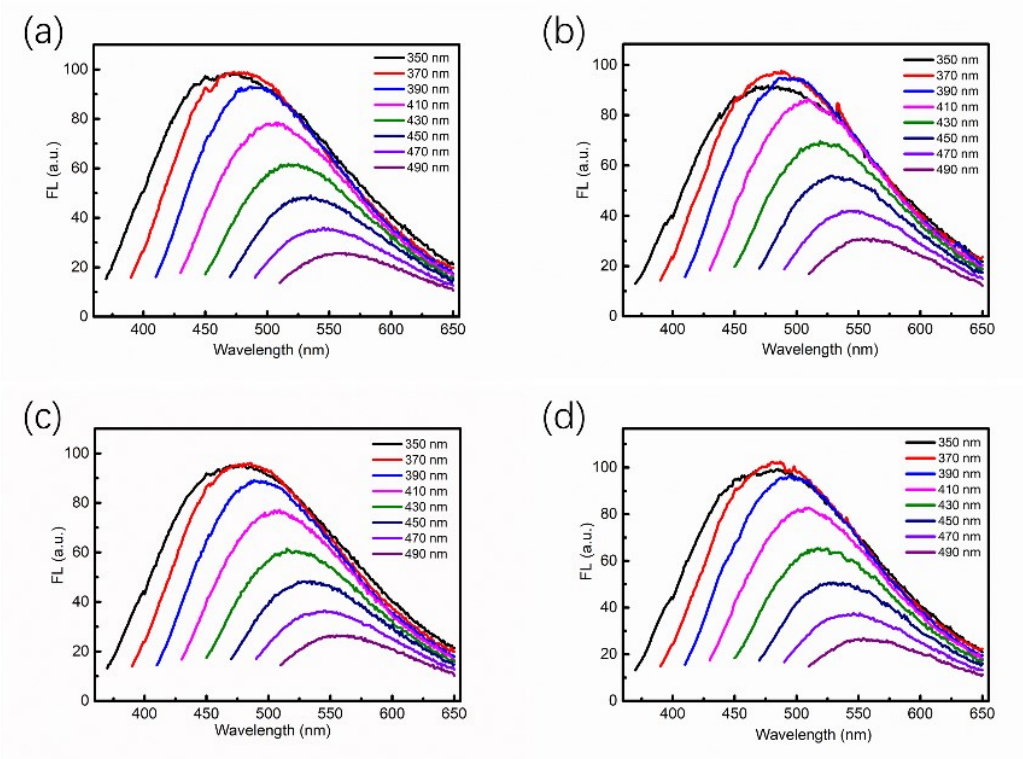

Fig. S4 The fluorescence emission spectra of (a) GSH-MoS_2 QDs; (b) Cys-MoS_2 QDs; (c) MSA-MoS_2 QDs and (d) TA-MoS_2 QDs upon excitation at different wavelengths from 350 nm to 490 nm.

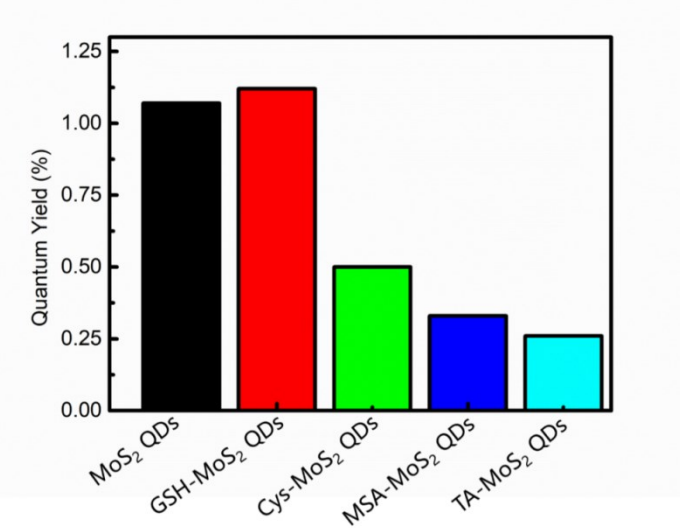

Fig. S5 The quantum yield of pristine MoS_2 QDs and different modified MoS_2 QDs by using quinine sulfate as the reference.

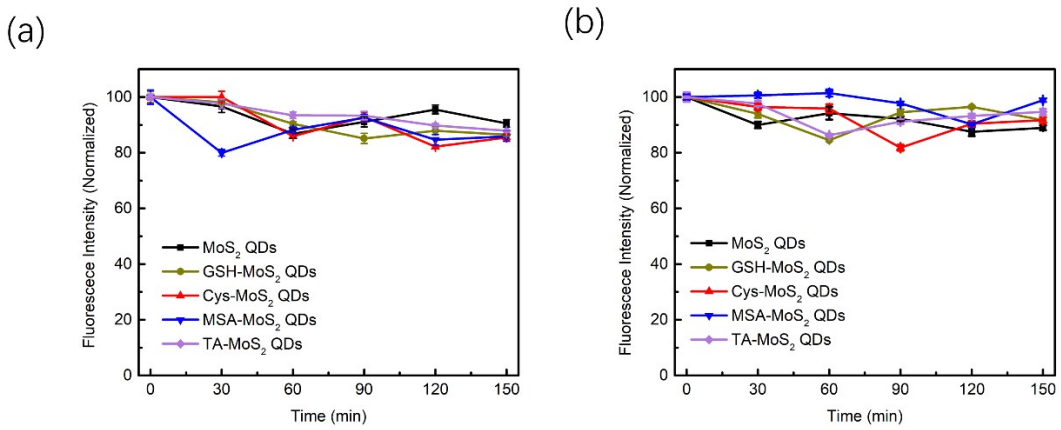

Fig. S6 The colloidal stability of different MoS_2 QDs in (a) PBS and (b) cell lysates. The time-dependent fluorescence intensity of QDs, normalized by the original intensity at time zero, was recorded upon excitation at 405 nm.

Reference

1. J. Deng, K. Wang, M. Wang, P. Yu, and L. Mao, *J. Am. Chem. Soc.*, 2017, **139**, 5877−5882.
2. X. Ren, Q. Wei, P. Ren, Y. Wang and Y. Peng, *Opt. Mater.*, 2018, **86**, 62-65.
3. Y. Feng, S. Lin, S. Huang, S. Shrestha and G. Conibeer, *J. Appl. Phys.*, 2015, **117**, 125701.
4. L. Najafi, B. Taheri, B. Martin-Garcia, S. Bellani, D. Di Girolamo, A. Agresti, R. Oropesa-Nunez, S. Pescetelli, L. Vesce, E. Calabro, M. Prato, A. E. Del Rio Castillo, A. Di Carlo and F. Bonaccorso, *ACS Nano*, 2018, **12**, 10736-10754.