

Supporting information for

Highly concentrated MoS₂ nanosheets in water achieved by thioglycolic acid as stabilizer and used as biomarkers

Rajeshkumar Anbazhagan^{1†}, Hsing-Ju Wang^{2†}, Hsieh-Chih Tsai^{1,*}, Ru-Jong Jeng^{2,*}

1. Graduate Institute of Applied Science and Technology, National Taiwan University of Science and Technology, Taipei, Taiwan

2. Institute Polymer Science and Engineering, National Taiwan University, Taipei, Taiwan.

[†] These authors contributed equally.

[*] To whom correspondence and reprint requests should be addressed.

Materials:

Molybdenum disulphide (MoS_2 10-30 μm) was purchased from Rose Mill Company (West Hartford USA). Thioglycolic acid (CAS number: 68-11-1) was purchased from Merck Millipore Company (Germany). All solution and reagents were used without any further purification.

Characterization

MoS_2 materials were coated on calcium fluoride pellets and investigated by Infrared spectroscopy (JASCO FTIR-4100). UV-visible spectrum was recorded by the JASCO, V-650 spectrometer. Zeta-potentials of MoS_2 solutions were analyzed using Horiba sz-100. The MoS_2 solution was dropped on the holey-carbon grids for TEM observation and on cleaned silica wafer substrates for AFM, Raman and XRD studies. TEM images were obtained by Technai F20 FEI-TEM. AFM images were obtained using Bruker Scanasyt. Raman measurements with the excitation wavelength of 632.8 nm were performed using a Horiba Jobin Yvon Raman HR800. Diffraction patterns were collected from XRD system (Bruker D2 PHASER) with reference $\text{CuK}\alpha 1$ radiation ($\lambda = 1.54056 \text{ \AA}$). Fluorescence spectroscopy was investigated by using HITACHI, F-7000.

Optimize the TGA concentration:

To determine the optimized concentration of TGA for this reaction, first the MoS_2 concentration (in water) was fixed at 5 mg/ml to be mixed with various TGA concentrations such as, 0.1, 0.25, 0.5, 1, 1.5 and 2 M. A well suspended solution in water was obtained for the mixtures with a TGA concentration higher than 1 M. When TGA was mixed with MoS_2 in water, the thiol moiety of TGA would lose the hydrogen and turn into a thiolate group. This thiolate moiety partially gave an electron to a vacant site of MoS_2 to promote the thiol

chemistry reaction. This would reduce the re-stacking nature of MoS₂. Due to the depression of hydrophobic nature and Van der Waals force between the MoS₂ layers in the presence of TGA, successful exfoliation of MoS₂ in water was achieved.

Measurement of concentration of MoS₂ monolayers

To measure the dispersion concentration of MoS₂ monolayers in the supernatant from centrifugation, we calculated the weight of the MoS₂ monolayers. A measured 20 ml of dispersion was filtered under high vacuum on a membrane filter of known weight. The obtained film was dried in a vacuum oven at 75 C° for 24 h. The mass of the MoS₂ nanosheets on film was taken from a microbalance.

$$\begin{aligned} \text{Concentration} &= \frac{\text{Membrane weight with sample} - \text{Empty Membrane weight}}{\text{Total Volume of the Solvent}} \\ &= \frac{0.3171 - 0.1219}{0.02} \\ &= 9.76 \text{ mg/ml} \end{aligned}$$

| Sonication time | Concentration (yield) of MoS ₂ |
|-----------------|---|
| 2 h | 3.49 mg/ml |
| 3 h | 5.64 mg/ml |
| 5 h | 9.76 mg/ml |