Support Information

Gd\(^{3+}\)-doped MoSe\(_2\) nanosheets as a theranostic agent for bimodal imaging and high efficiency cancer photothermal therapy

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**Figure S1.** (A) Photographs of the suspensions of (a) raw MoSe\(_2\) and (b) MoSe\(_2\) treated with grinding and sonication.

(B) The separation process by addition of hexane and then chloroform, maybe followed by centrifugation.

- (a) MoSe\(_2\) dispersed in NMP after addition of hexane (NMP:hexane=1:1, v:v).
- (b) The dispersion in after addition of chloroform (NMP:chloroform=1:1, v:v), maybe accompanied by a small amount of precipitation.
- (c) Samples after centrifuging at 5,000 rpm for 10 min.
Figure S2. TEM image of PEGylated MoSe$_2$(Gd$^{3+}$-3) nanosheets.

Figure S3. Photos of MoSe$_2$(Gd$^{3+}$)-PEG nanosheets in water and physiological solutions, including phosphate buffered saline (PBS), cell culture medium, and fetal bovine serum (FBS), after 0 (upper) or 15 days (bottom).
**Figure S4.** Stability of doped Gd$^{3+}$ in of MoSe$_2$(Gd$^{3+}$-3)-PEG nanosheets in PBS(A) or in cell culture medium(B) for different stored time. Those samples were determined by the ICP-AES to measure Gd$^{3+}$ percentages. No abrupt change of Gd$^{3+}$-content in those samples was observed, suggesting no obvious leakage of doped Gd$^{3+}$ from of MoSe$_2$(Gd$^{3+}$-3)-PEG nanosheets. p values:

* $p < 0.05$, ** $p < 0.01$.

**Figure S5.** (A) UV-vis-NIR absorption spectrum of MoSe$_2$(Gd$^{3+}$)-PEG. (B) Photothermal heating curves of MoSe$_2$(Gd$^{3+}$)-PEG at the same concentrations under different NIR laser irradiation.
Figure S6. UV-vis-NIR spectra of the MoSe$_2$(Gd$^{3+}$)-PEG nanosheets under 808 nm laser before and after irradiation at 2 W/cm$^2$ for 60 min.

Figure S7. (A&B) Cell relative viabilities of 4T1 cells and SGC-7901 cells after being incubated with different concentrations of MoSe$_2$(Gd$^{3+}$-3) or MoSe$_2$(Gd$^{3+}$-3)-PEG for 24 h and then being exposed to the 808 nm NIR laser for 5 min.
Figure S8. (A) PA images of tumors on mice before and after i. t. or i. v. injection with MoSe$_2$(Gd$^{3+}$-3)-PEG. (B) Photoacoustic signals inside the tumors before and after i. t. injections or i. v. injections of MoSe$_2$(Gd$^{3+}$-3)-PEG. The injection dosages of i.t. injection and i.v. injection were 10 or 100 μL at the concentration of 0.2 mg/mL, respectively.

Figure S9. Corresponding photographs of mice before treatment and after 14 days various treatments. Group (i): saline as the control; Group (ii): Only NIR laser irradiation; Group (iii): i.v. injection with MoSe$_2$(Gd$^{3+}$-3)-PEG; Group (iv): i.v. injection with MoSe$_2$(Gd$^{3+}$-3)-PEG+NIR.