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Supporting Information

# Hydrophilic graphene oxide / bismuth selenide nanocomposites for CT imaging, photoacoustic imaging, and photothermal therapy

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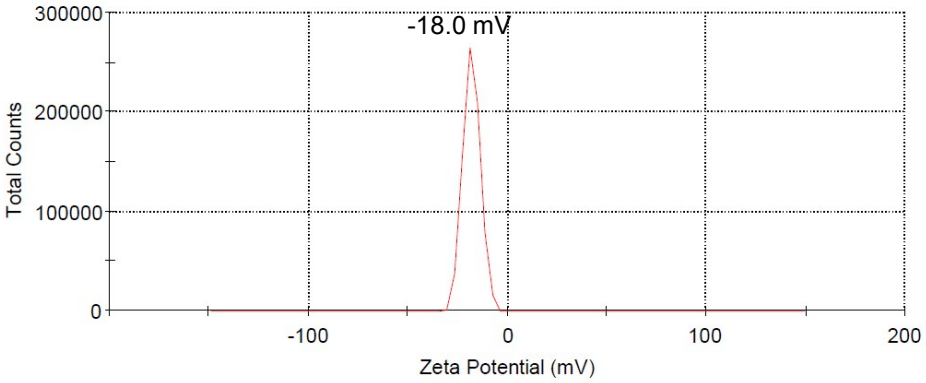


Fig. S1. Zeta potential data of GO. The Zeta potential was measured using a Malvern Zetasizer Nano ZS model ZEN3690.

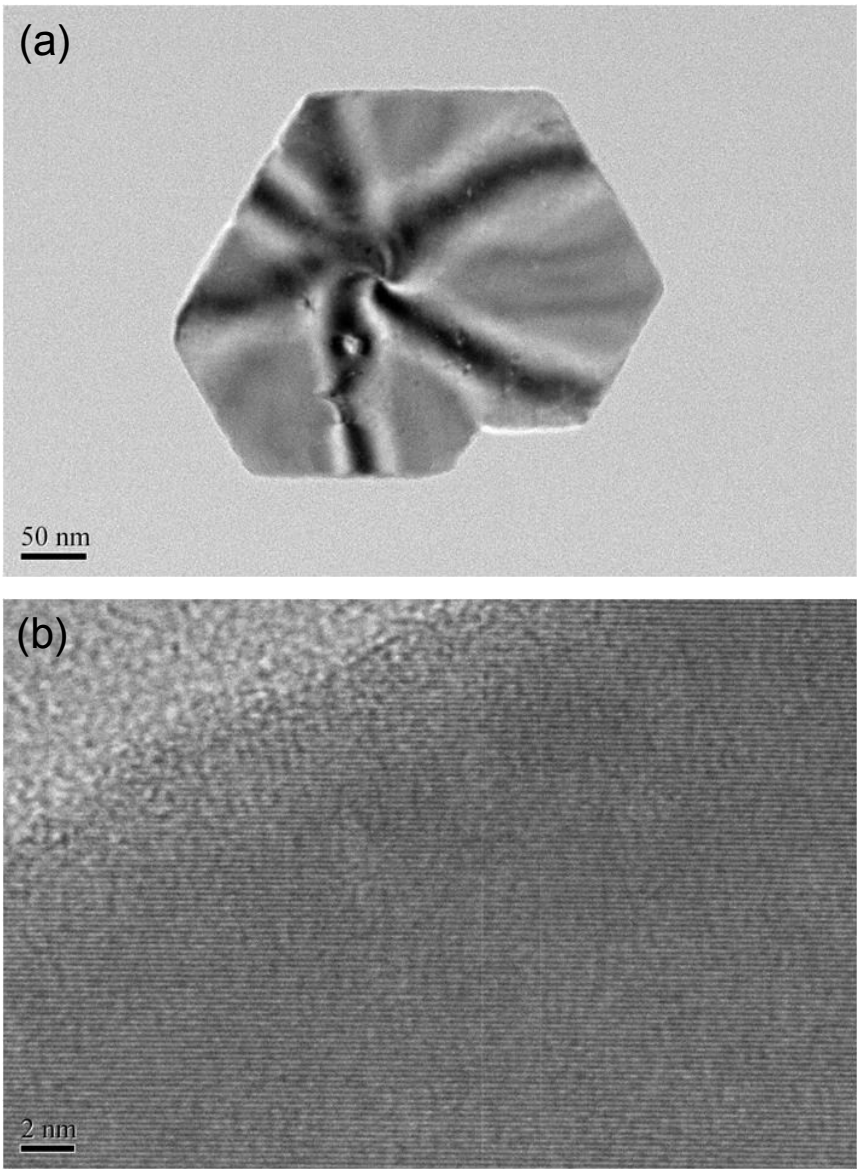


Fig. S2. The TEM (a) and HR-TEM (b) micrographs of a $Bi_2Se_3$/PVP nanosheet. $Bi_2Se_3$/PVP was synthesized under the same reaction conditions for GO/$Bi_2Se_3$/PVP. In the absence of GO, $Bi_2Se_3$/PVP tends to form the sheet structure under similar conditions. The HR-TEM image in (b) show clear and uniform lattice fringes of a $Bi_2Se_3$ sheet. The lattice spacing is 0.21 nm, attributed to the d value of (1 1 0) plane of $Bi_2Se_3$.

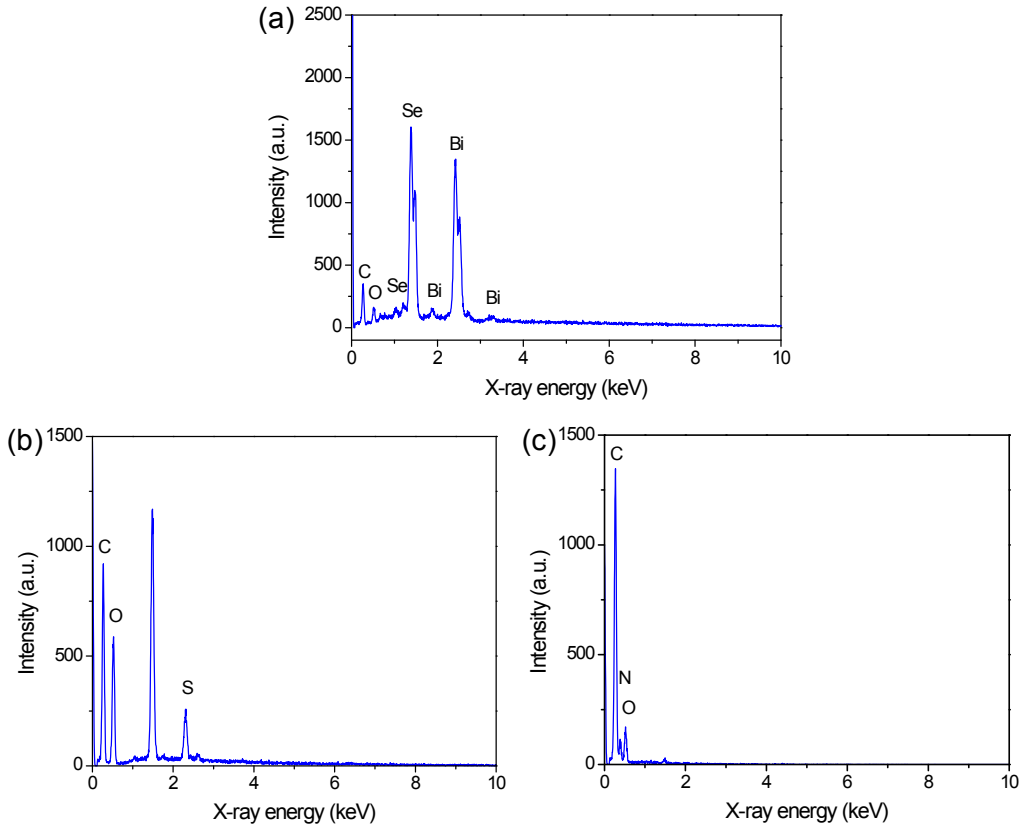


Fig. S3. EDS spectra of GO/$Bi_2Se_3$/PVP (a), GO (b) and PVP (c). The EDS data were acquired on a field-emission JEOL JSM-6460 electron microscope. The samples were placed on aluminum foils. There is a small amount of elemental sulfur residue (0.82 at.%) on GO.

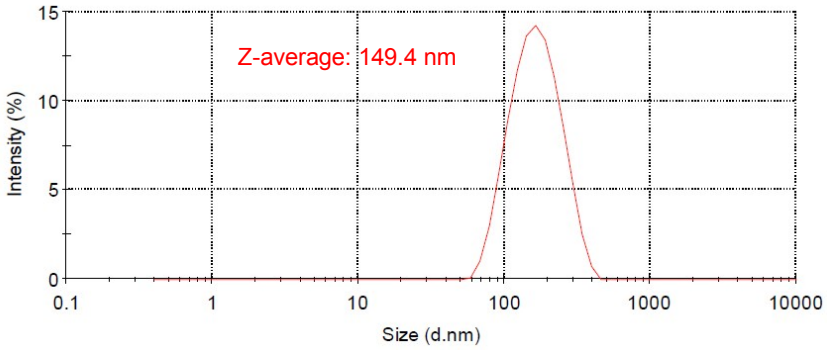


Fig. S4. Hydrodynamic size of GO/$Bi_2Se_3$/PVP nonocomposites dispersed in water.

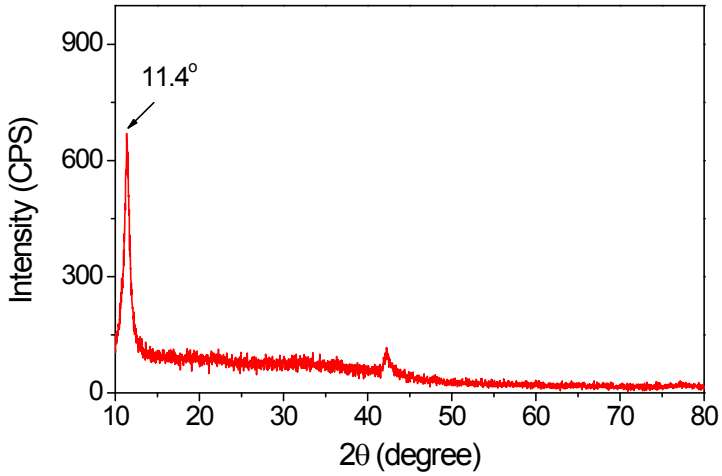


Fig. S5. XRD pattern of as-prepared GO.

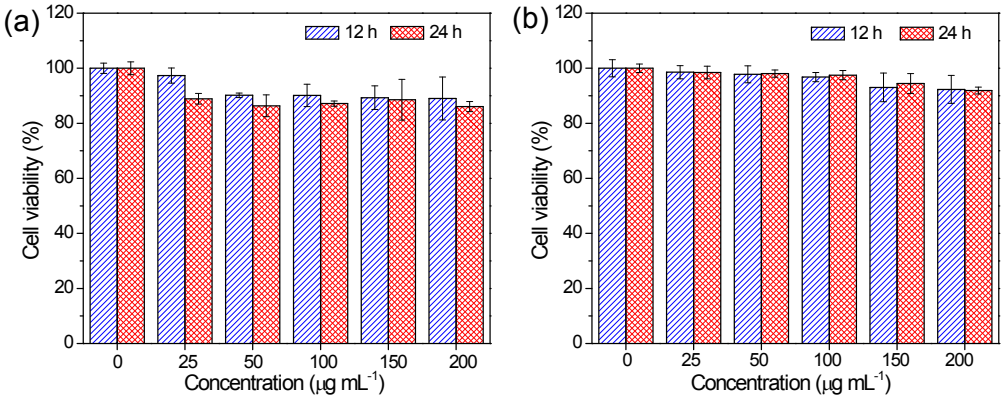


Fig. S6. *In vitro* viabilities of HeLa cells incubated with different concentrations of GO (a) and $Bi_2Se_3$/PVP (b) for 12 and 24 h.

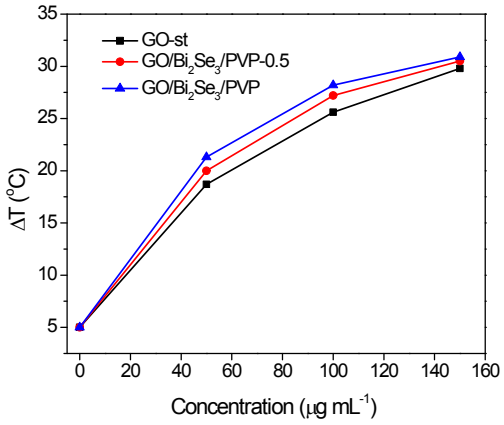


Fig. S7. Temperature increase in GO-st, GO/$Bi_2Se_3$/PVP-0.5, and GO/$Bi_2Se_3$/PVP solutions of different concentrations under 808-nm NIR irradiation (0.4 W $cm^{-2}$) for 5 min. GO-st: GO was treated by solvothermal method in DEG at 200 °C for 3 h. GO/$Bi_2Se_3$/PVP-0.5: The feeding amount of $Bi(NO_3)_3 \cdot 5H_2O$, selenium powder, and $Na_2SO_3$ was decreased to half of the original amount for synthesis of GO/$Bi_2Se_3$/PVP, and other reaction conditions remained unchanged. GO-st showed significantly improved photothermal performance in comparison with pristine GO due to apparent reduction of GO during the hydrothermal treatment. Compared with GO/$Bi_2Se_3$/PVP, GO/$Bi_2Se_3$/PVP-0.5 shows ΔT decrease only by ~ 1 °C. This means that, in GO/$Bi_2Se_3$/PVP nanocomposites, the photothermal performance of $Bi_2Se_3$ NPs is close to that of partially reduced GO. The $Bi_2Se_3$ NPs in GO/$Bi_2Se_3$/PVP show significantly better photothermal property than $Bi_2Se_3$/PVP. This may be due to the small size of $Bi_2Se_3$ NPs and their uniformly distribution on GO. Therefore, both GO and $Bi_2Se_3$ NPs in GO/$Bi_2Se_3$/PVP show important contribution to the photothermal performance of the nanocomposites.

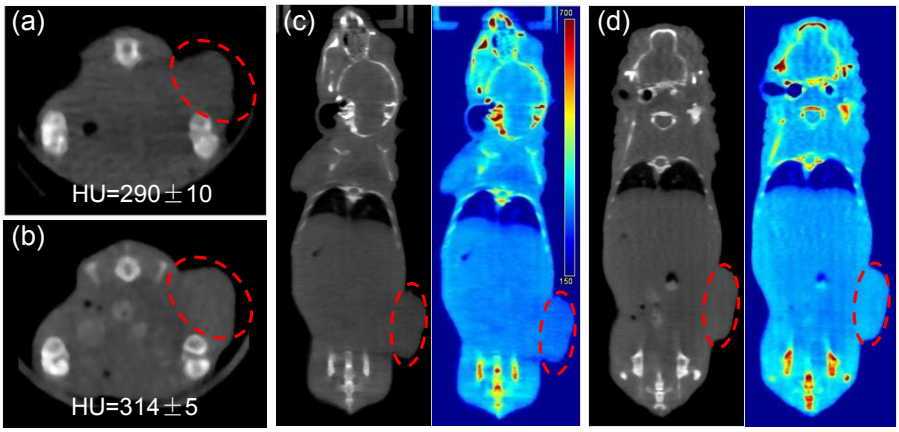


Fig. S8. X-ray transverse CT images of a tumor model before (a, c) and 6 h after (b, d) intravenous injection of GO/$Bi_2Se_3$/PVP (12 mg $mL^{-1}$, 500 μL) via tail vein.

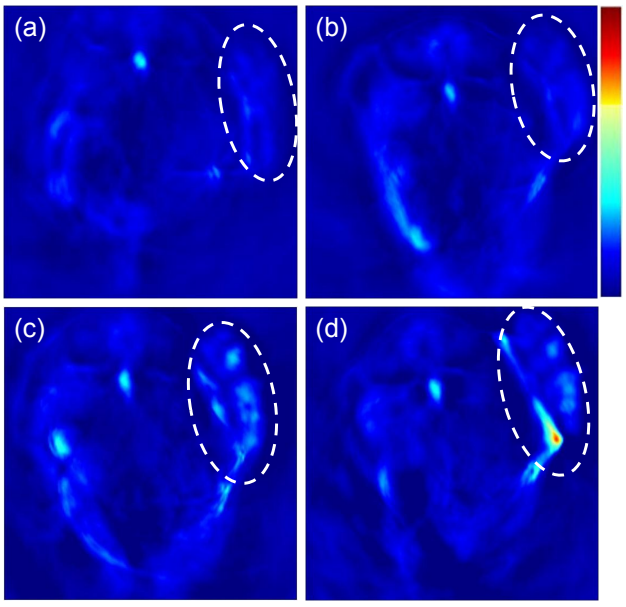


Fig. S9. PA images of the tumors on mice before (a) and 2 h (b), 4 h (c), and 8 h (d) after intravenous injection of GO/$Bi_2Se_3$/PVP.

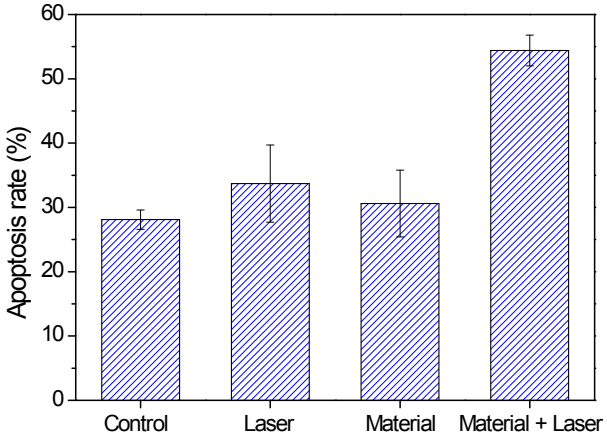


Fig. S10. TUNEL positive percentage of tumor tissue from the 4 groups measured by TUNEL assay.

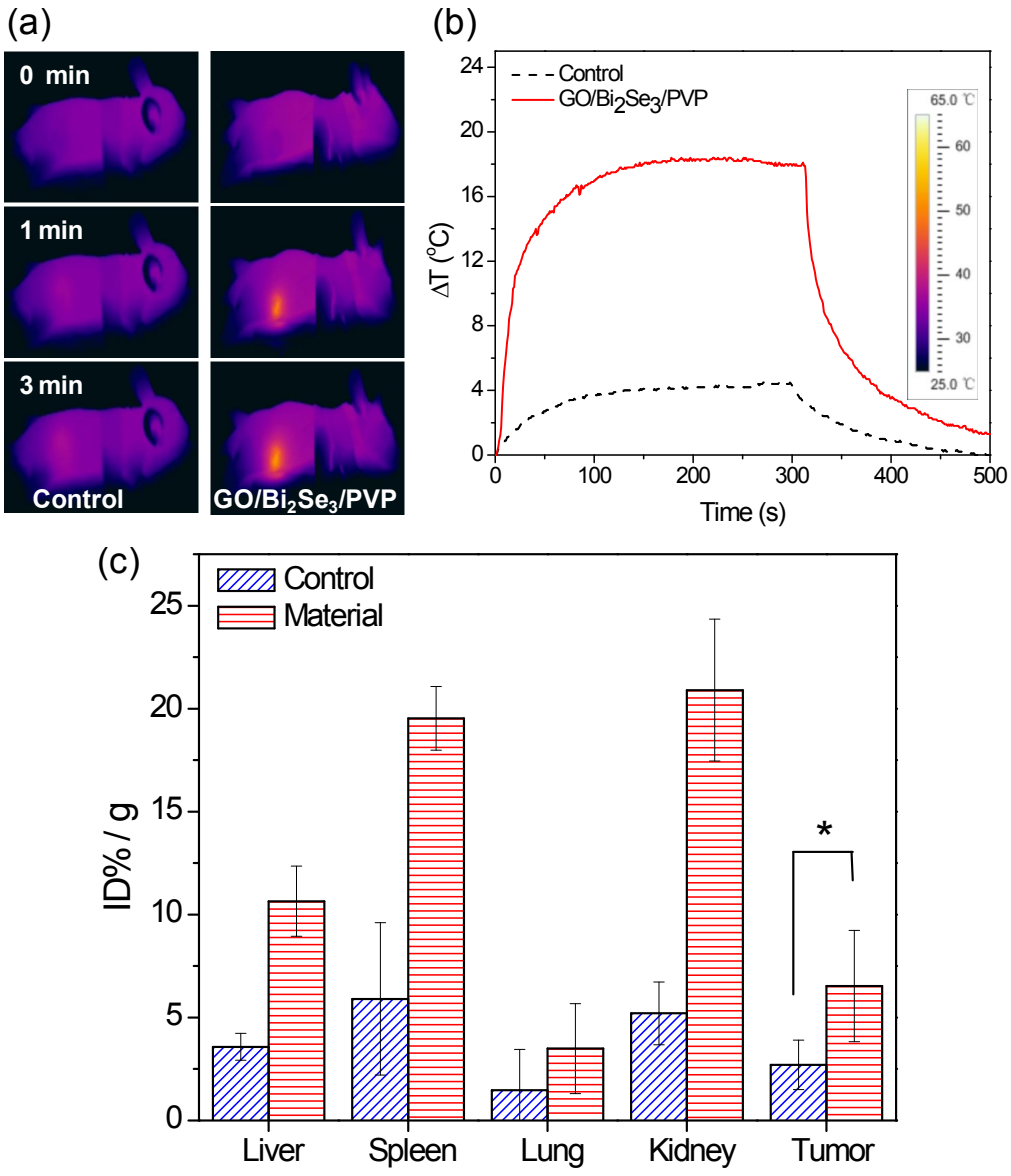


Fig. S11. (a) *In vivo* photothermal images of tumor-bearing mice 24 h after intravenous injection with PBS (as control) or $GO/Bi_2Se_3/PVP$ (2 mg $mL^{-1}$, 200 μL) exposed to laser irradiation (808 nm, 1.0 W $cm^{-2}$) for 5 min. (b) Temperature change curves of the tumor site exposed to laser irradiation. (c) Biodistribution of $GO/Bi_2Se_3/PVP$ in HeLa tumor-bearing mice at 24 h after intravenous injection (n = 4). *$P < 0.05$. Bi content in the organs and tumors was determined by a high-resolution sector field inductively coupled plasma atomic emission spectroscopy instrument

(Varian). The ICP data of heart before and after injection is very close to zero, so the data of heart are not presented in the figure.

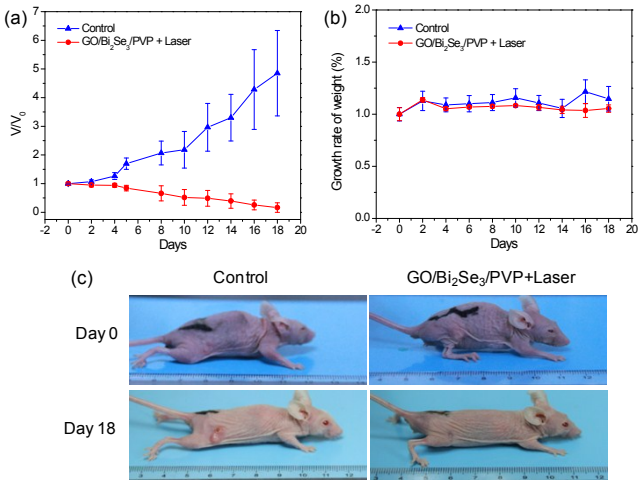


Fig. S12. (a) The changes of relative tumor volume as a function of days for the control group and PTT group (n = 4). (b) Body weight (normalized to day 0) curves of mice after the beginning of treatments. (c) Representative photographs of mice after photothermal treatment. The nude mice bearing HeLa tumors were intravenously injected with GO/$Bi_2Se_3$/PVP (2 mg $mL^{-1}$, 200 μL). At 24 and 48 h after injection, the HeLa tumors were exposed to an 808-nm laser (1.0 W $cm^{-2}$) for 10 min.