Suppoting Information

Phase-controlled synthesis of plasmonic molybdenum oxide nanoparticles for surface enhanced Raman scattering and photothermal therapy

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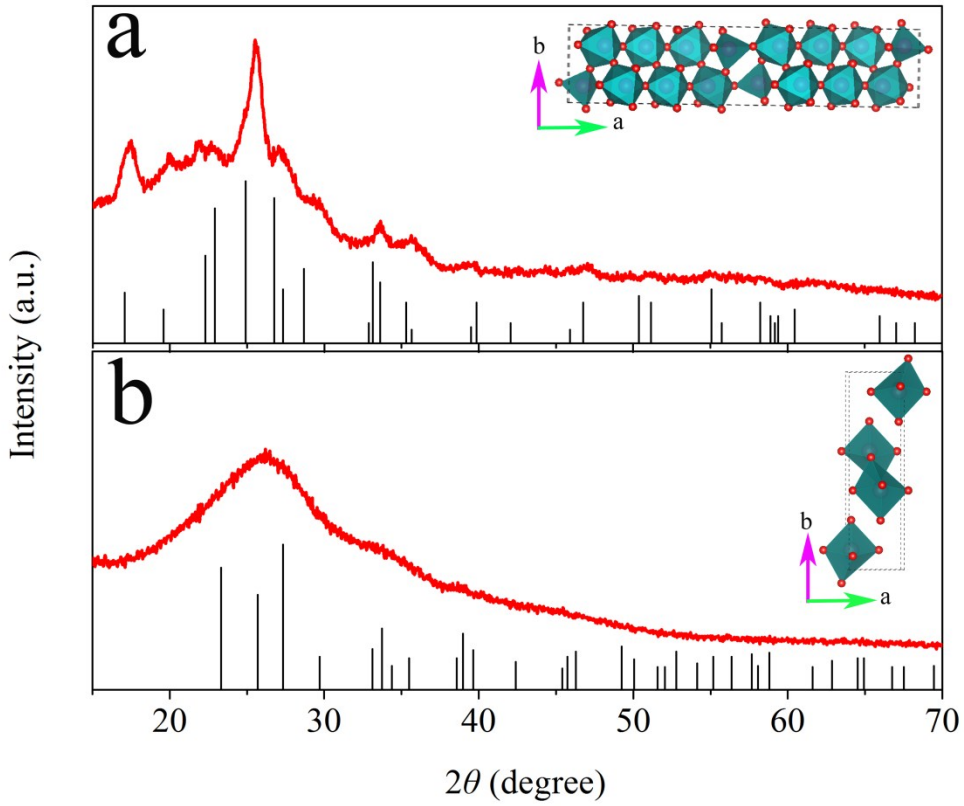

Fig. S1 (a-b) XRD patterns of MoO_{3-x} and MoO_3 NPs. Insets of (a) and (b) represent the crystal structure of MoO_{3-x} and MoO_3 respectively.

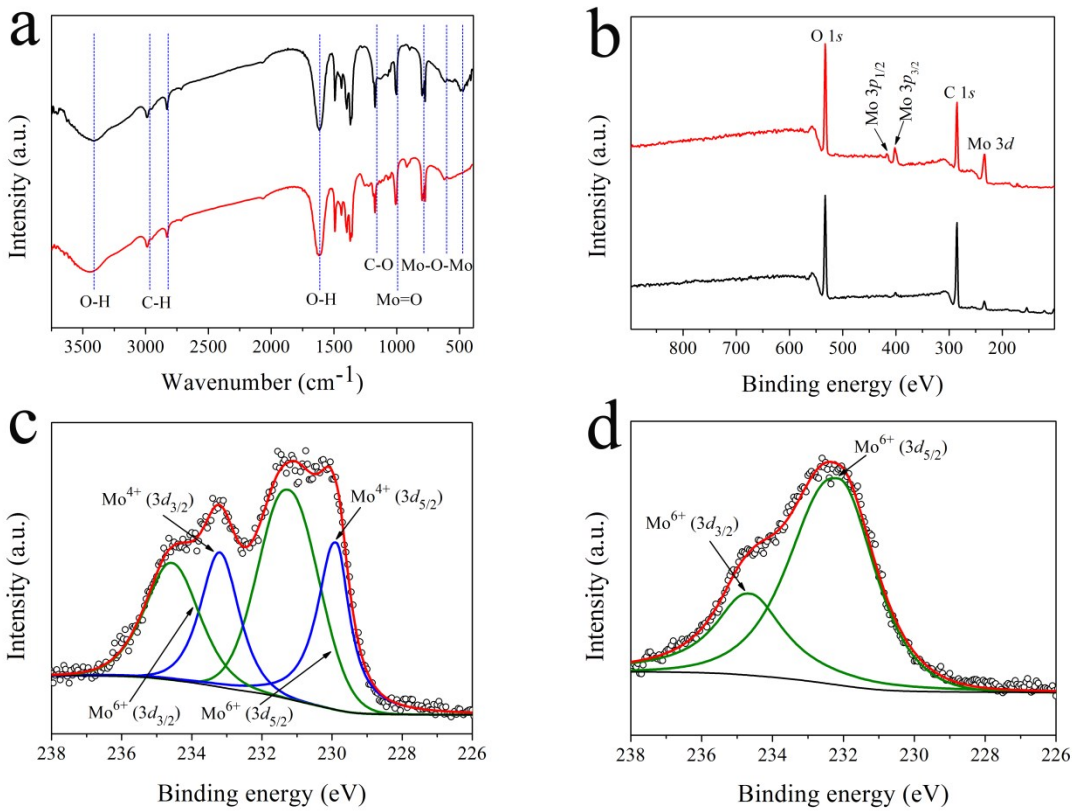

Fig. S2 (a) FTIR spectra of MoO_{3-x} (black) and MoO_3 (red) NPs. (b) XPS survey spectrum of MoO_{3-x} (red) and MoO_3 (black) NPs. (c-d) Mo 3*d* spectrums of MoO_{3-x} and MoO_3 NPs.

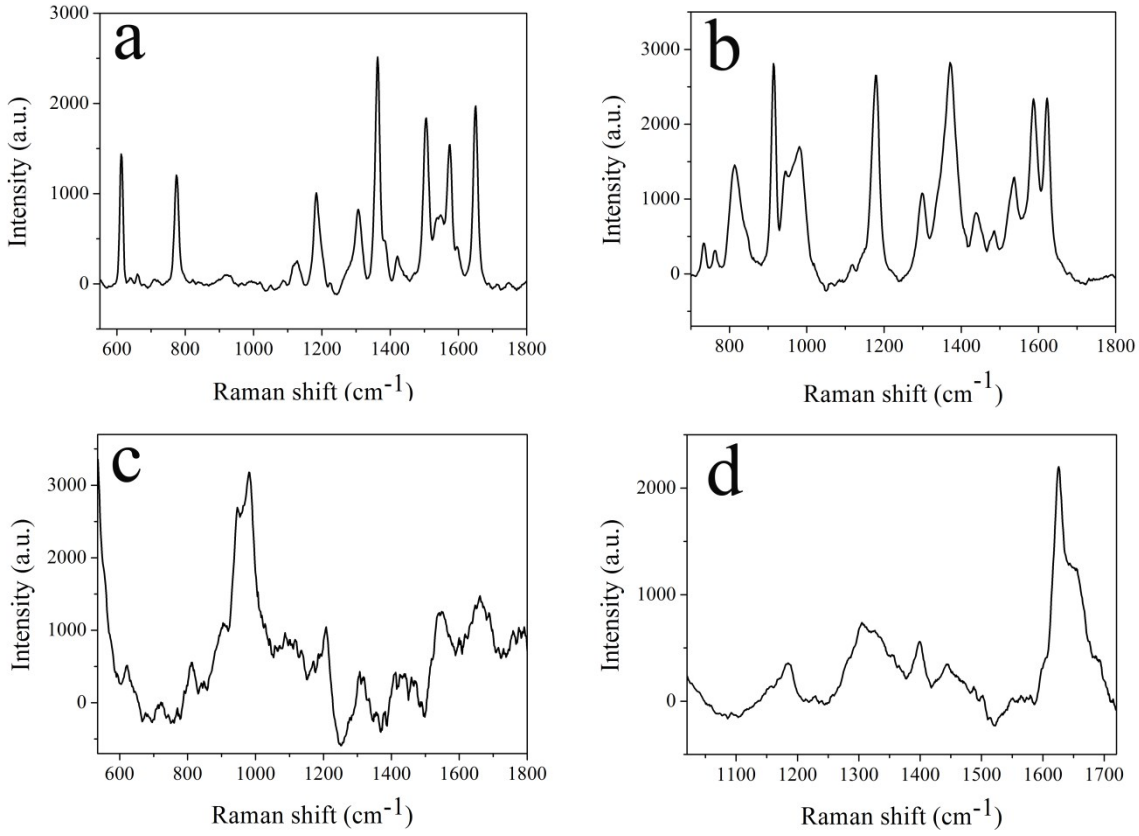

Fig. S3 (a-d) Raman spectra of the reference material of R6G, CV, IR780 and MB, respectively.

Table S1 Comparison of the limit detection and EF with other SERS-active substrate materials.

SERS Substrate	Probe molecule	Excited Wavelength (nm)	Limited Detection (M)	EF	Ref.
Ag NPs	MGITC	632.8	10^{-10}	10^{7}	**1**
Colloidal Ag	R6G	514	10^{-9}	10^{6}	**2**
Au-CdSe nanowires	CV	633	-	10^{4}	**3**
ZnO nanocrystals	4-Mpy	514.5	10^{-3}	10^{3}	**4**
Cu_2O nanopheres	4-MBA	488	10^{-3}	10^{5}	**5**
TiO_2 photonic microarry	MB	532	6×10^{-6}	2×10^{4}	**6**
MoO_2	R6G	532	10^{-7}	3.75×10^{6}	**7**

$W_{18}O_{49}$	R6G	532.8	10^{-7}	3.4×10^{5}	**8**
MoO2 NPs	R6G	514	5×10^{-8}	1.10×10^{7}	This work
MoO2 NPs	CV	514	5×10^{-8}	3.62×10^{5}	This work

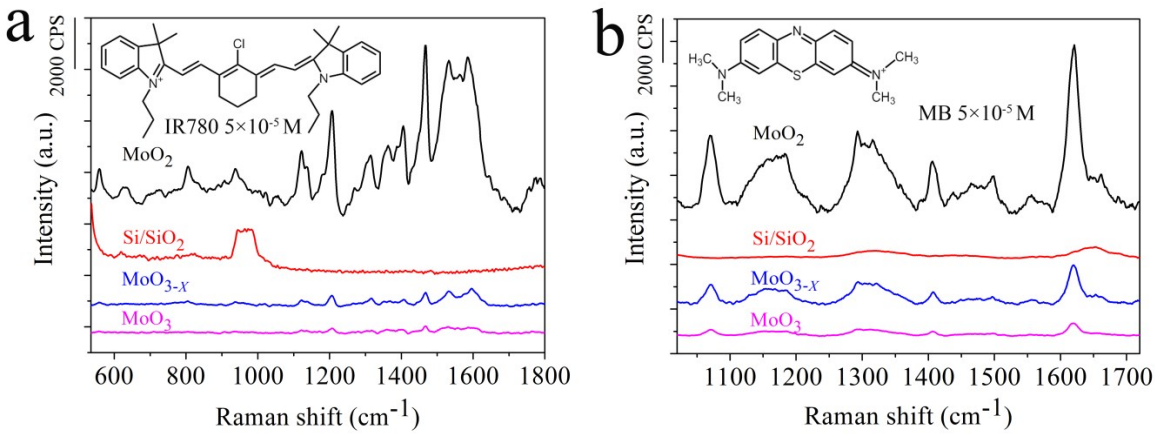

Fig. S4 (a) Raman spectra of IR780 aqueous solution mixed with MoO_2 (black), MoO_{3-x} (green) and MoO_3 (pink) NPs dispersion at the concentration of 5×10^{-5} M and bare silicon slice (red). (b) Raman spectra of MB aqueous solution mixed with MoO_2 (black), MoO_{3-x} (green) and MoO_3 (pink) NPs dispersion at the concentration of 5×10^{-5} M and bare silicon slice (red).

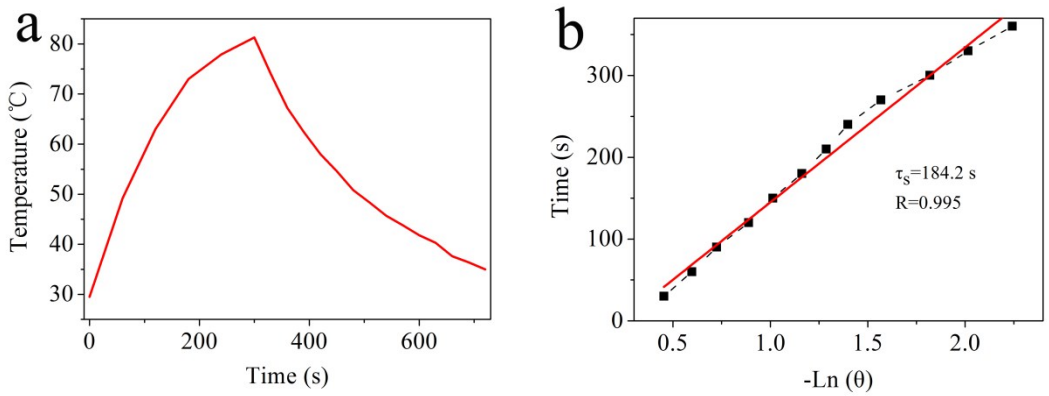

Fig. S5 (a) Photothermal effect of 100 μg/mL MoO_2 NPs irradiated by 808 nm laser for 5 min with a power density of 2 W cm^{-2} and shutting off the laser. (b) Time constant for heat transfer from the system is estimated to be τ_S = 184.2 S via applying the liner data of the cooling period of panel (a) *versus* negative natural logarithm of

driving force temperature.

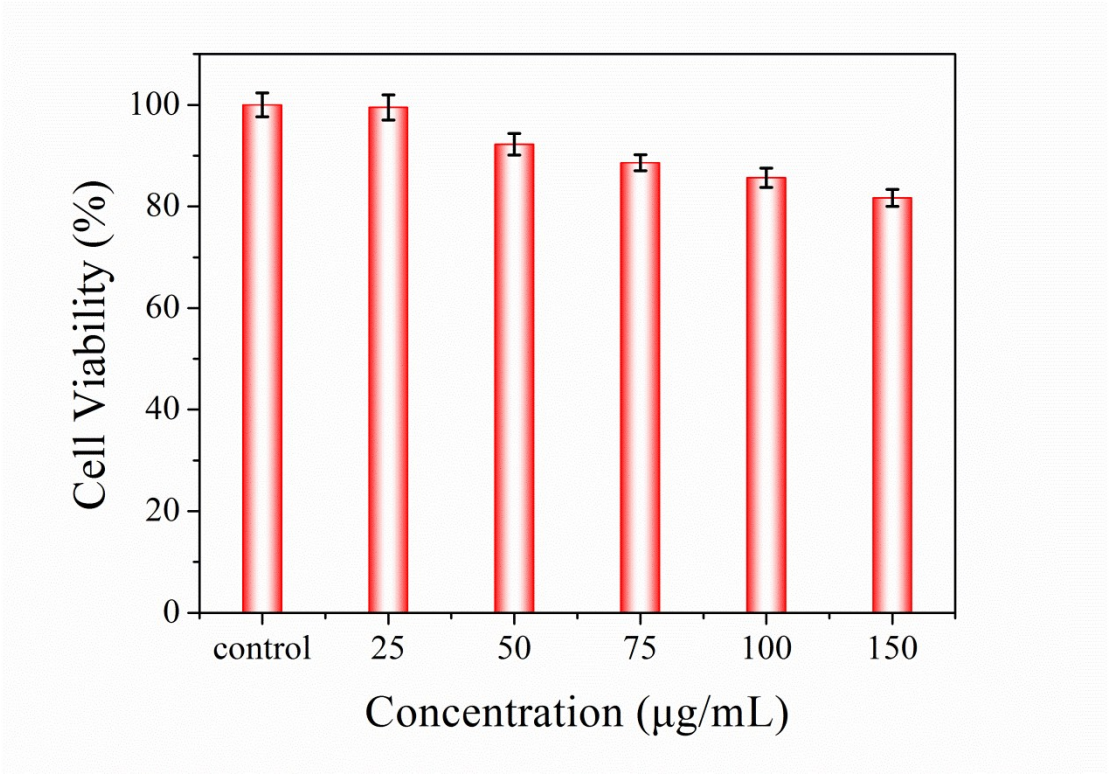

Fig. S6 Dose-dependent viability of HepG2 cells incubated with different concentrations of MoO_2 NPs ranging from 25 to 150 μg/mL for 24 h. Each date point refers to the mean value of three independent experiments.

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