

## Three-photon imaging using defect-induced photoluminescence in biocompatible ZnO nanoparticles

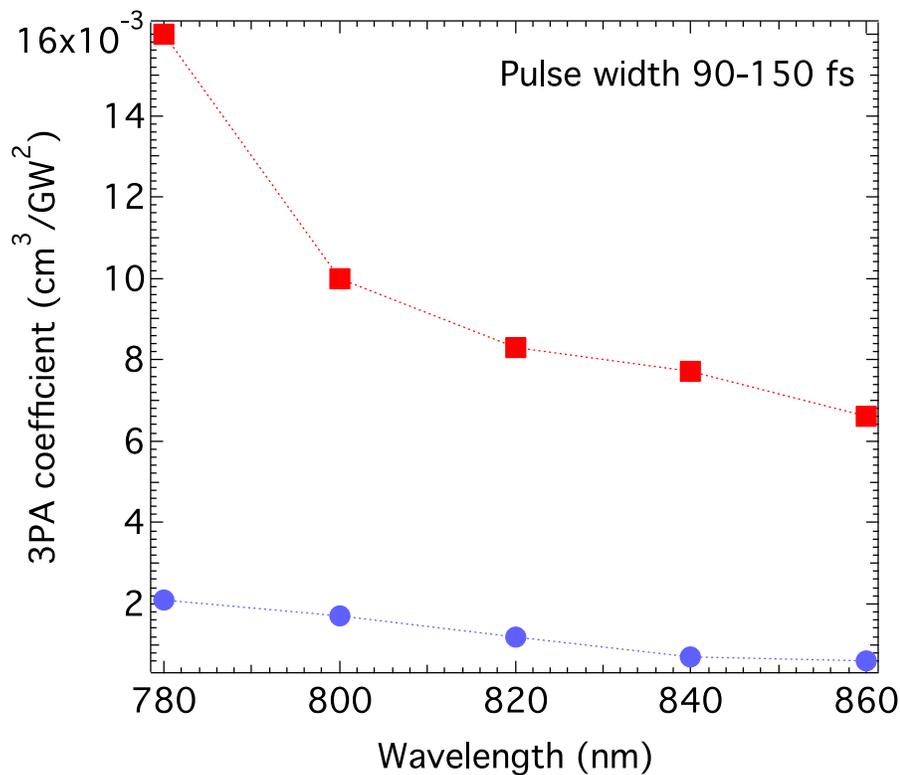
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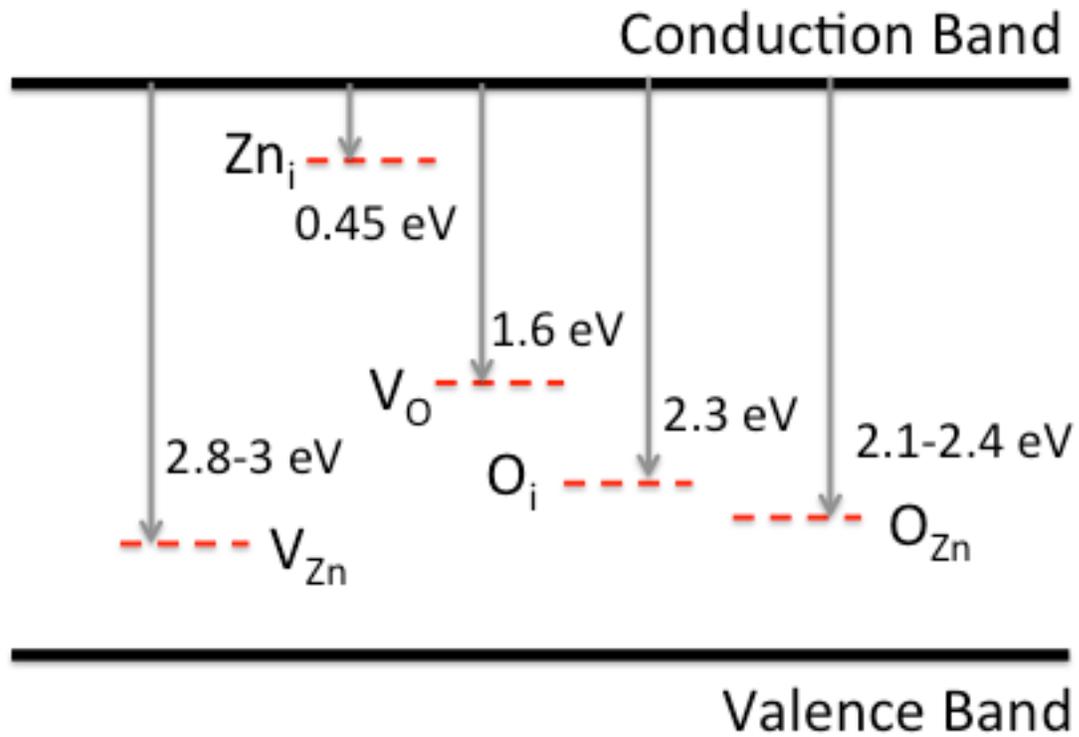
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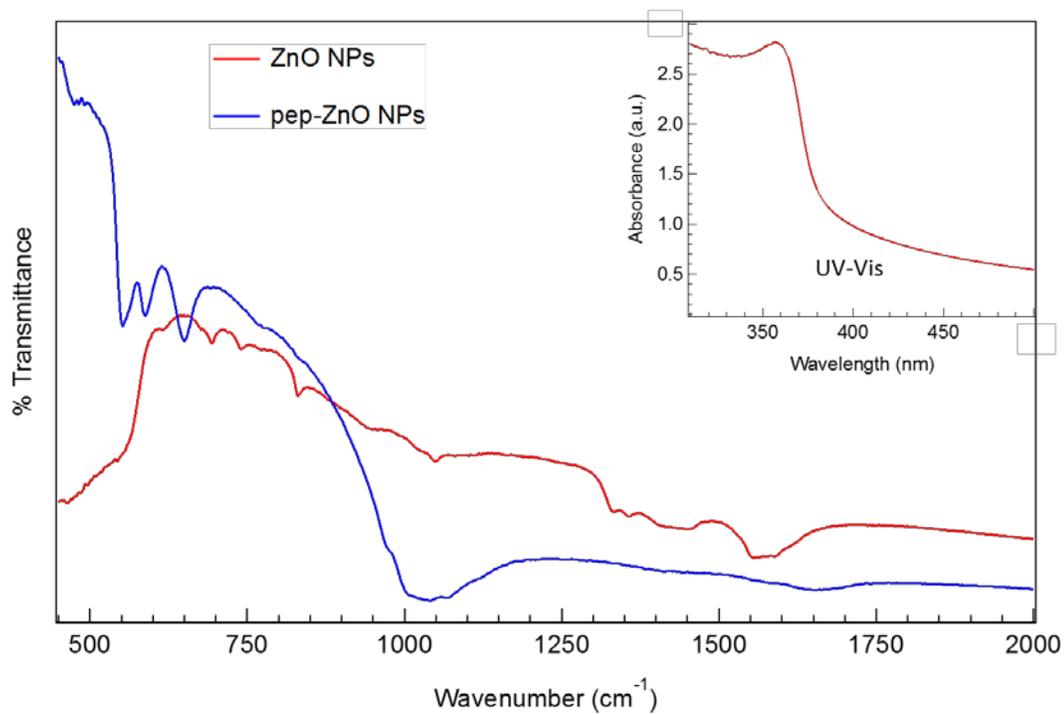
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**Fig. S1** Three-photon absorption coefficients for ZnO (red squares) and ZnS (blue dots) NPs measured using ultra-fast fs Z-scan measurements (J. He et al., OPTICS EXPRESS vol. 13, 23, 9235).

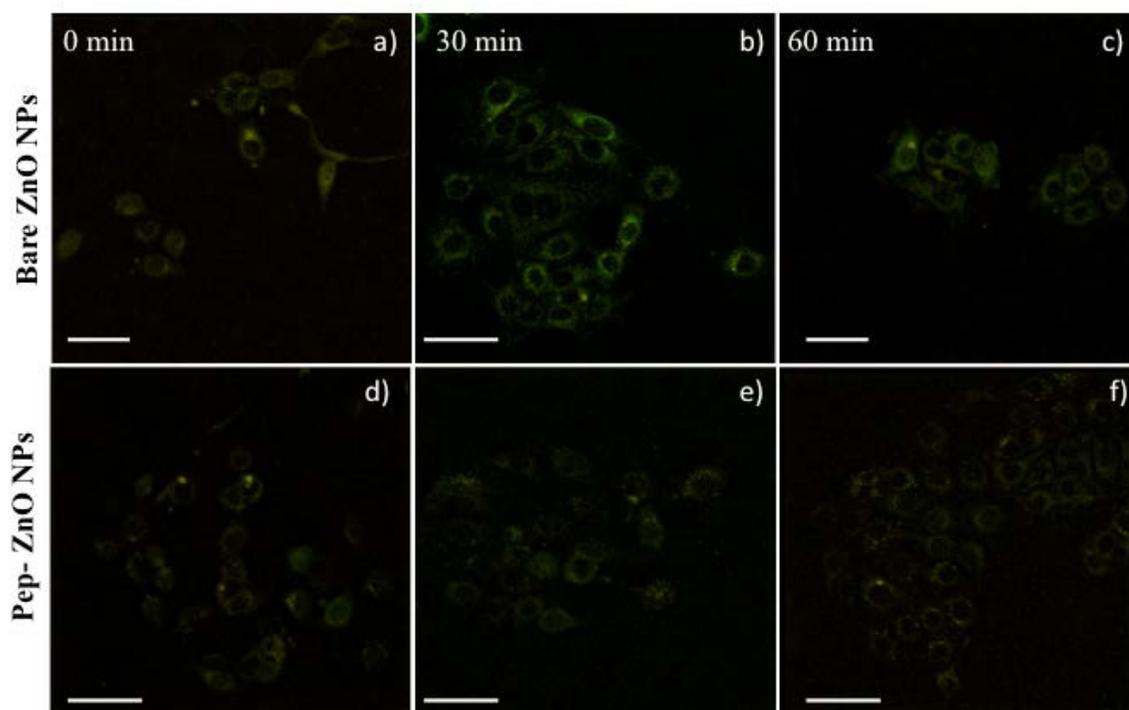


**Fig. S2** Defect-induced electronic states within the band gap of ZnO NPs (B. Lin *et al.* J. Electrochem. Soc. 2001 vol. 148 no. 3 G110-G113)



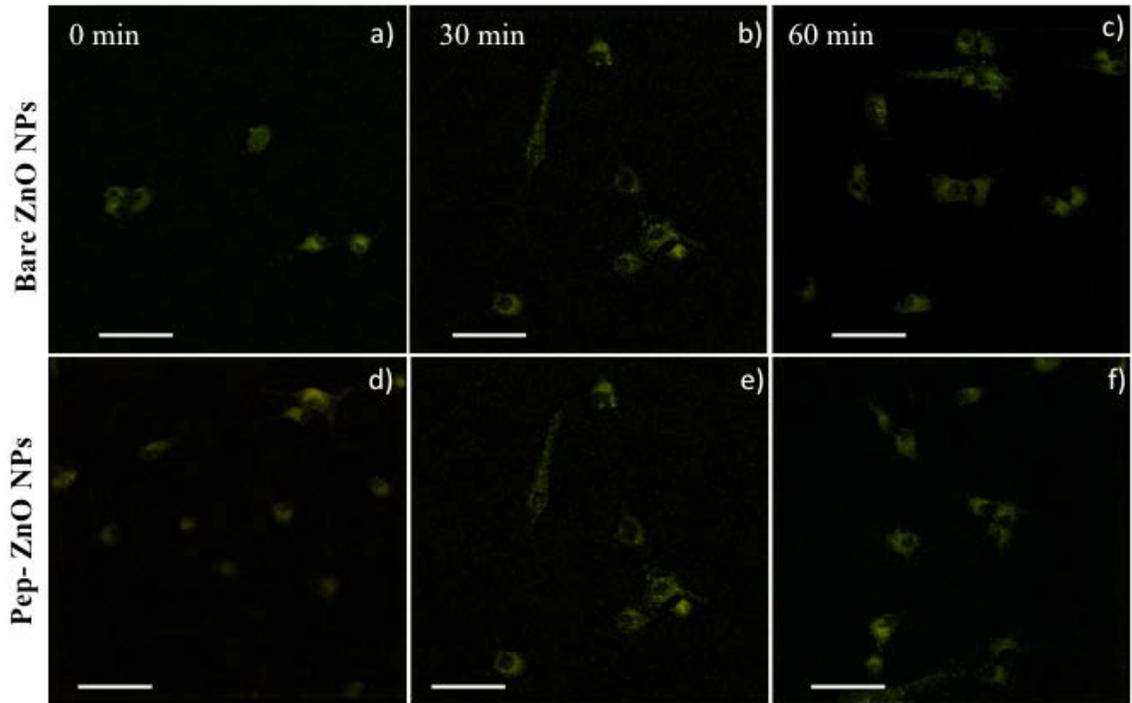
**Fig. S3** FTIR spectra of pep-ZnO NPs show stronger signatures of C-O stretch ( $\sim 1000\text{ cm}^{-1}$ ), carboxyl ( $\sim 1600\text{ cm}^{-1}$ ) unlike pristine ZnO. Inset shows UV-Vis spectrum of bare ZnO NPs showing absorbance peak around 360 nm corresponding to the band edge  $\sim 3.4\text{ eV}$ .

MCF-7; Scale: 50  $\mu$ m

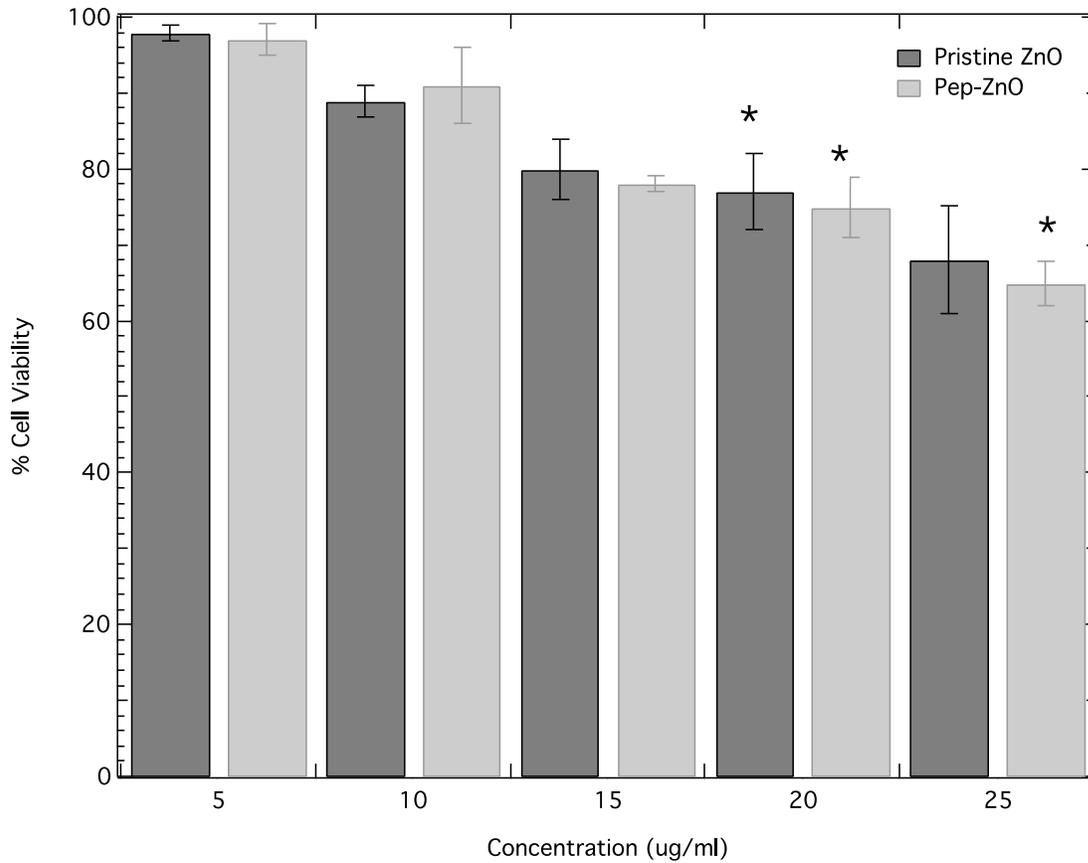


**Fig. S4** Three-photon images for integrin-negative MCF-7 cells at different incubation times with (a-c) bare ZnO NPs and (d-f) pep-ZnO NPs showed no difference in uptake before and after functionalization due to the absence of integrin receptors.

U87MG; Scale: 50  $\mu$ m



**Fig. S5** Three-photon images for U87MG cells at different incubation times with (a-c) bare ZnO NPs and (d-f) pep-ZnO NPs showed increased uptake after functionalization at 60 mins due to selective binding of RGD pep-ZnO NPs with integrin receptors.



**Fig. S6** RAEC Cell viability analyzed after 24 hrs with MTS assay kit showed no significant change in number of viable cells with ZnO NPs and pep-ZnO NPs up to 20 ug/ml concentrations that are relevant to imaging experiments performed in this study.

<b>Multiphoton Imaging of ZnO NPs in cells – Imaging Parameters</b>
Objective Used: Leica HC PL APO CS2 40x/1.10 water
Frame Average: 4
Line Average: 4
<b>Laser Settings</b>
Wavelength: 975 nm (Intensity – 14.3%; Gain – 42.9%; Offset – 33.13%)
Detector 1: HyD6 APD1; HyD standard mode; Gain – 123.7; Pseudocolor = green
Detector 2: HyD7 APD2; HyD standard mode; Gain – 123.7; Pseudocolor = red
Argon Laser Settings: 488 nm (Intensity – 22.517%)
PMT Trans Detector: Gain – 254; Offset – 0
Laser peak power for all images: 905-911 W
Pulse duration: 75-100 fs
Pulse repetition rate: 80 MHz
Average laser power for all images: 5.1-5.5 mW
Average laser power at the sample: 0.5-1 mW

**Table S1** Laser settings and powers used for obtaining three-photon images.