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Electronic Supplementary Information

## InP/ZnSe/ZnS Quantum Dots with Strong Dual Emissions: Visible Excitonic Emission & Near-Infrared Surface Defect Emission and Their Application in In Vitro and In Vivo Bioimaging<sup>†</sup>

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**Figure S1.** (a) UV–vis absorption and (b) PL spectra of InP core QDs taken at various reaction time at 180 °C.



**Figure S2.** (a) Absorption and (b) PL spectra of InP core QDs, InP/ZnSe QDs and InP/ZnSe/ZnS QDs. The heating time of InP core QDs is 15 min.



**Figure S3.** (a) Absorption and (b) PL spectra of InP core QDs, InP/ZnSe QDs and InP/ZnSe/ZnS QDs. The heating time of InP core QDs is 20 min.



**Figure S4.** (a) Absorption and (b) PL spectra of InP core QDs, InP/ZnSe QDs and InP/ZnSe/ZnS QDs. The heating time of InP core QDs is 40 min.



**Figure S5.** (a) Absorption and (b) PL spectra of InP core QDs and InP/ZnSe QDs with different heating time for ZnSe shell growth.



**Figure S6.** (a) Absorption and (b) PL spectra of InP core QDs, InP/ZnS QDs and InP/ZnS/ZnS QDs. The heating times for the first ZnS shell and the second ZnS shell were 30 min.



**Figure S7.** Absorption and PL spectra of InP/ZnSe/ZnS QDs with strong excitonic emission and negligible surface defect emission synthesized by using InP QDs with short heating time as the cores, in which the band-to-band emission could be tuned from green to red by changing In precursor (namely, InCl<sub>3</sub> for red emission, InBr<sub>3</sub> for orange emission and InI<sub>3</sub> for green emission), similar to previous reports.<sup>1,2</sup>



Figure S8. HR-TEM image of InP core QDs (60 min of heating).



Figure S9. Multi-peak fitting of the PL spectrum of the dual emissive InP/ZnSe/ZnS QDs.



**Figure S10**. Schematic illustration of the four strategies used for water transfer: replacing the original oil-soluble ligands using (a) NAC or (b) SPH, (c) encapsulating the oil-soluble QDs using chitosan-based micelles, (d) wrapping the oil-soluble QDs using PAA-based amphiphilic polymer.



**Figure S11.** Multi-peak fittings of the PL spectra of initial oil-soluble InP/ZnSe/ZnS QDs and resultant water-soluble InP/ZnSe/ZnS QDs wrapped by PAA-based amphiphilic polymers.



**Figure S12.** Cytotoxicities of PAA-based polymer wrapped InP/ZnSe/ZnS QDs, NAC-capped InP/ZnSe/ZnS QDs and NAC-capped CdTe QDs on normal human liver cells (L02 cells) were evaluated using MTT assay. The concentrations were the final QD concentrations in cell culture medium.

## References

 (1) Tessier, M. D.; Dupont, D.; De Nolf, K.; De Roo, J.; Hens, Z. Economic and Size-Tunable Synthesis of InP/ZnE (E = S, Se) Colloidal Quantum Dots. *Chem. Mater.* 2015, *27*, 4893–4898.
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