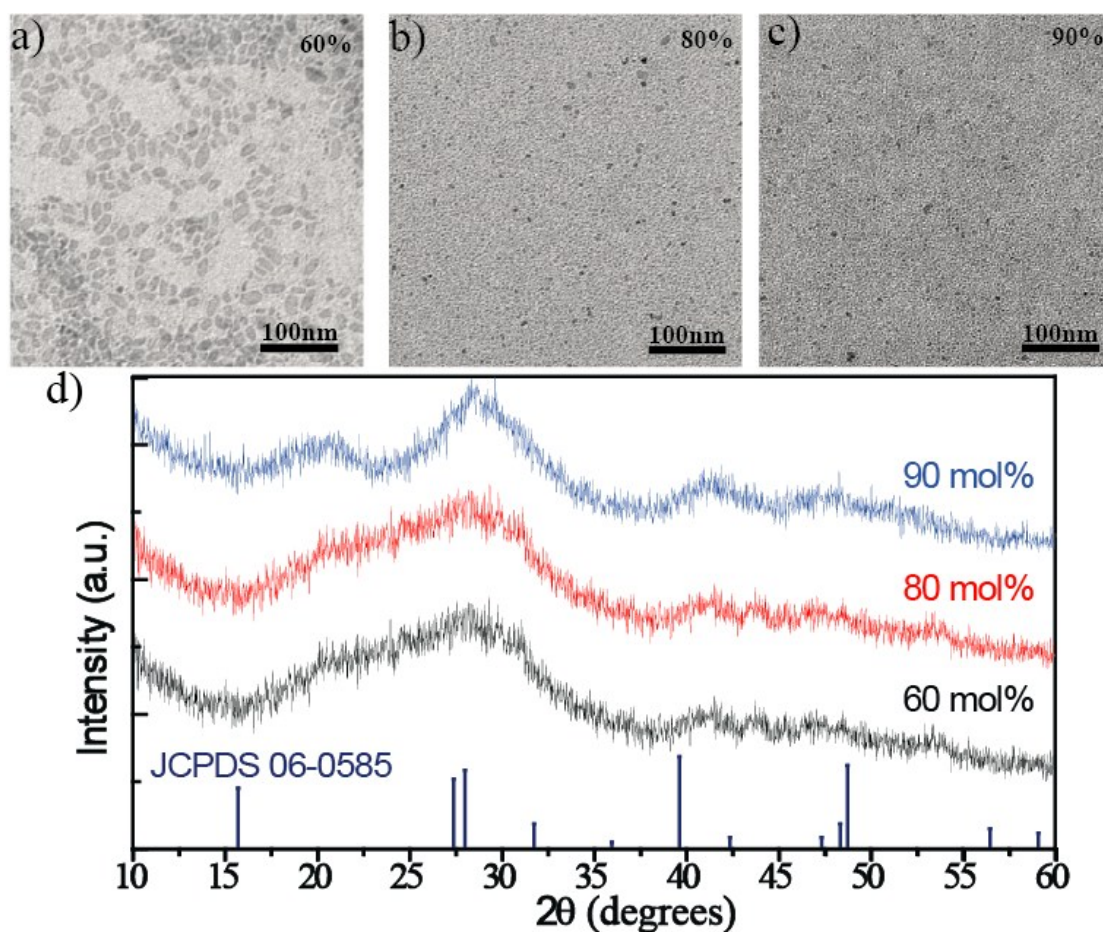


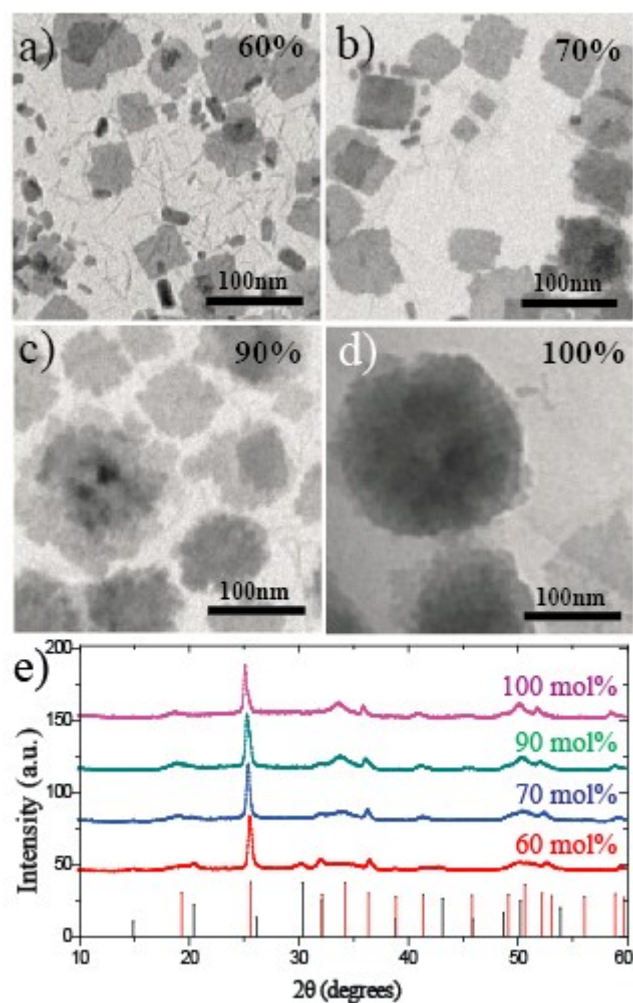
## Supporting Information

### Intentional Anion Incorporation to Rational Modulate Size, Shape and Optical Property of Lanthanide Oxide Nanocrystals

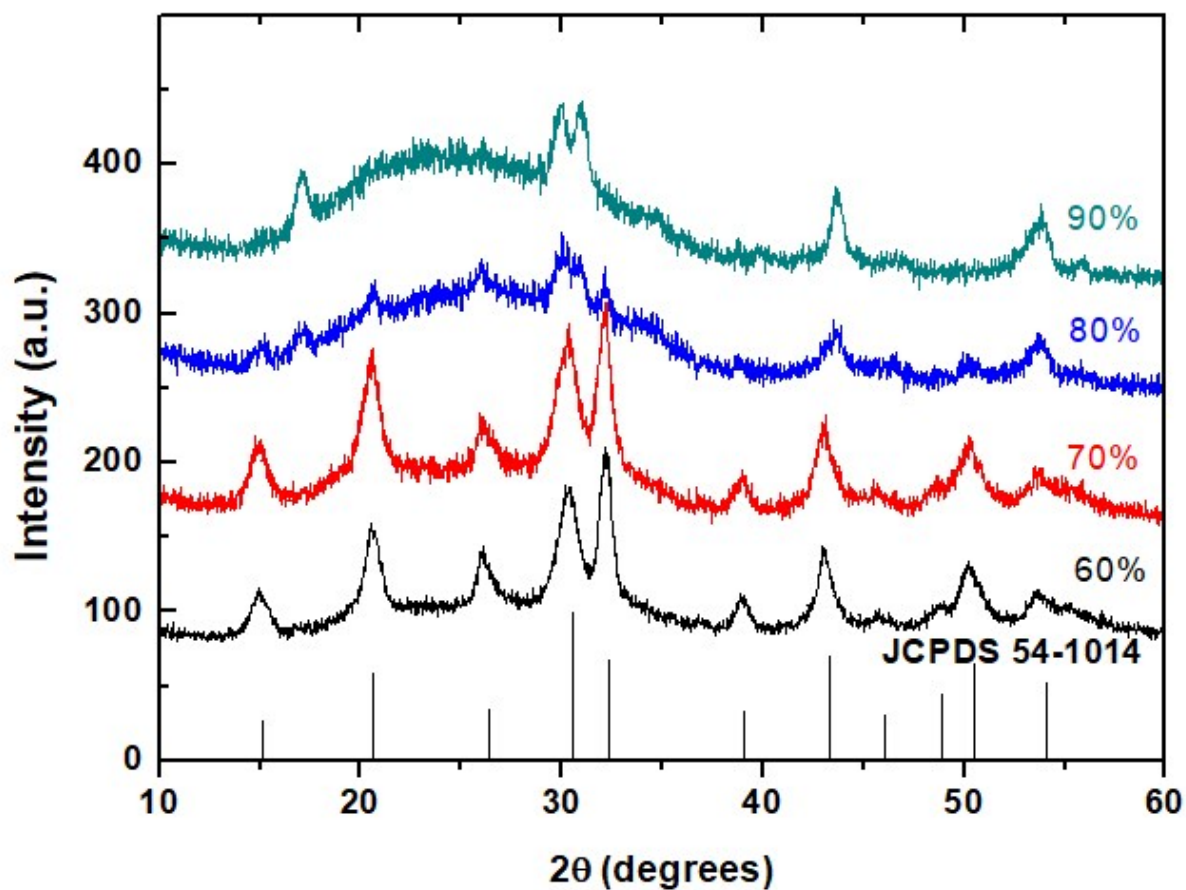
Zhenlan Fang, Fangyu Zhao, Yuwei Zhang, Weilinsen Ding, Lantian Zhang, Meili Liu, Wenlong Xu, Kedar Bahadur Thapa, Wei Huang, Qiang Ju\*



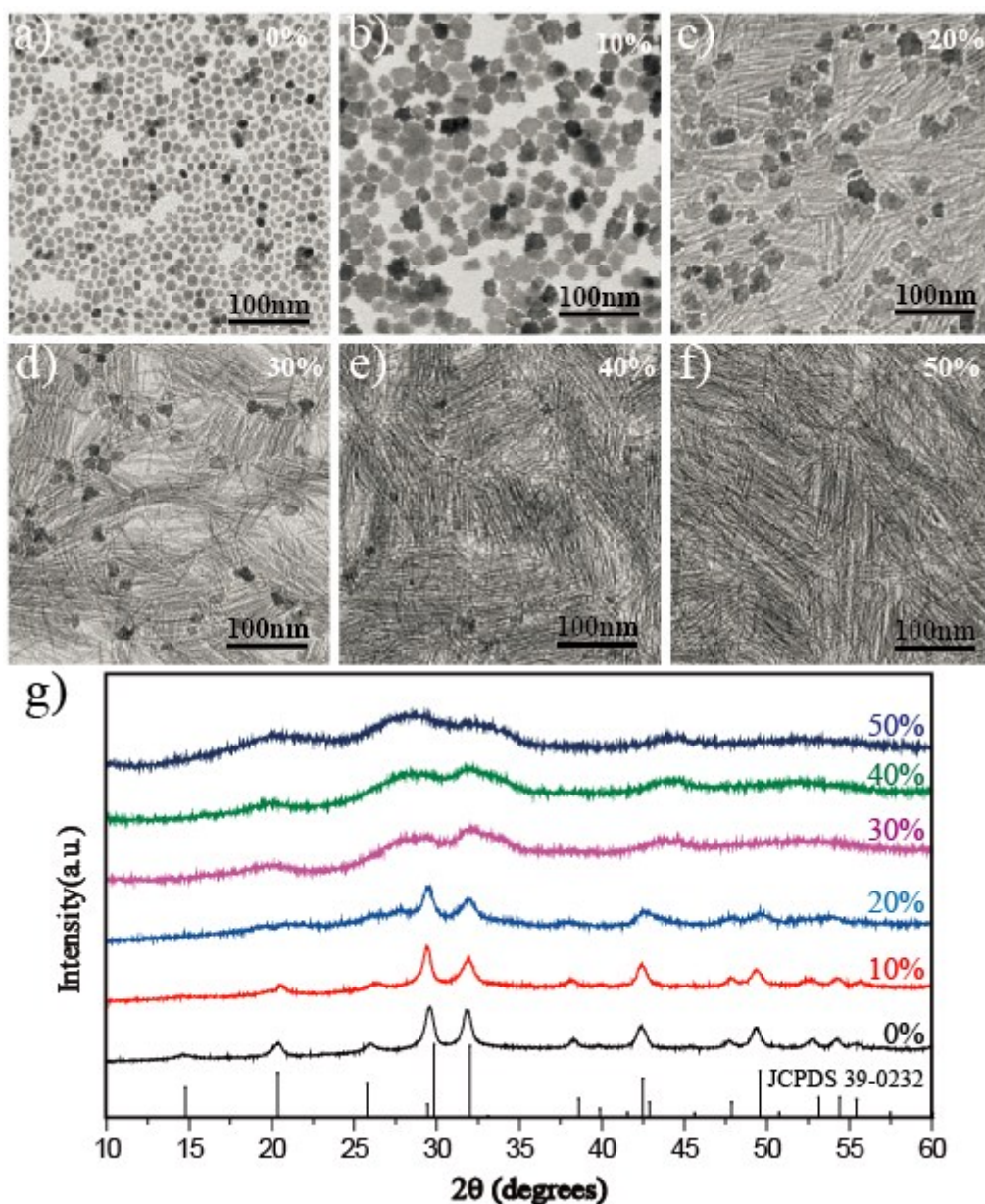
**Figure S1.** TEM images of LaVO<sub>4</sub> nanocrystals incorporated with a) 60 mol% PO<sub>4</sub><sup>3-</sup>, B) 80 mol% PO<sub>4</sub><sup>3-</sup>, and c) 90 mol% PO<sub>4</sub><sup>3-</sup>, respectively; d) XRD patterns of corresponding nanocrystals as well as La(OH)<sub>3</sub> (JCPDS standard card no. 06-0585). There were no LaVO<sub>4</sub> or LaPO<sub>4</sub> detected on the XRD patterns, and the peak position partially overlap with that of La(OH)<sub>3</sub>, implying the presence of La(OH)<sub>3</sub> under this fabrication condition.



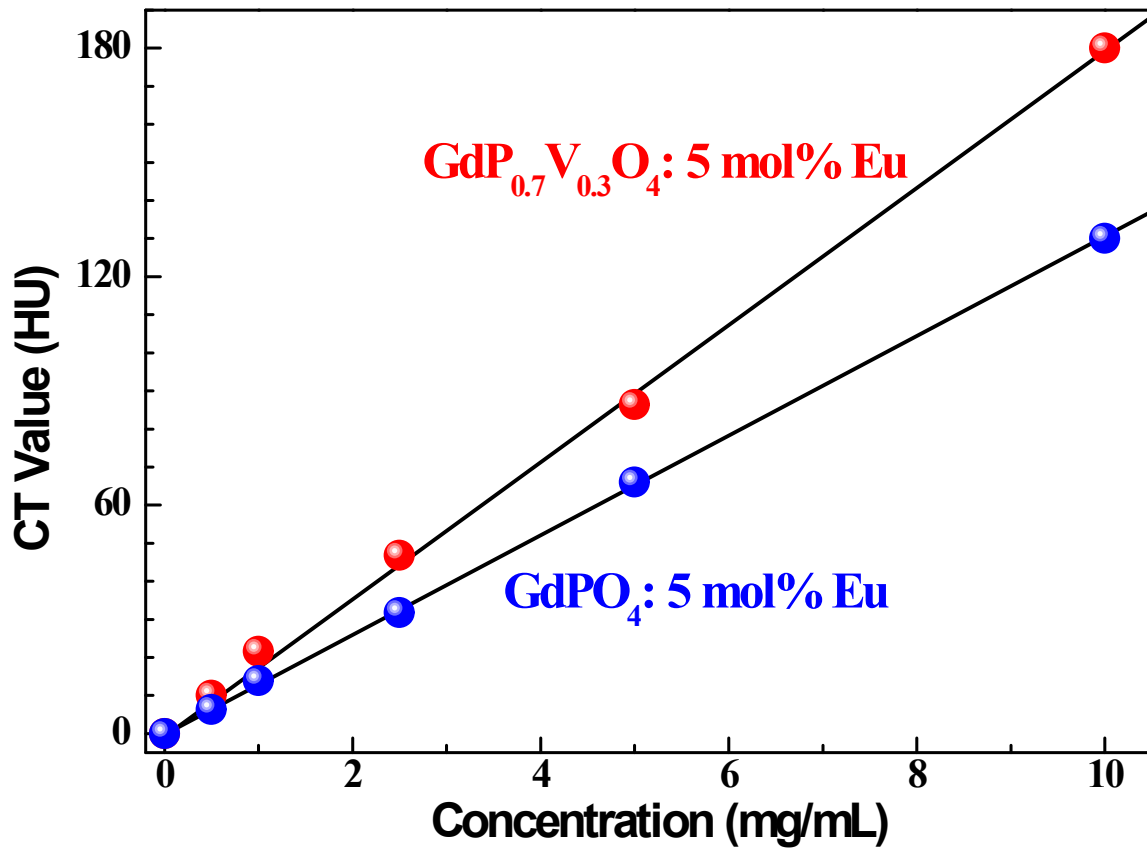
**Figure S2.** TEM images of  $\text{YbPO}_4$  nanocrystals incorporated with a) 60 mol%  $\text{VO}_4^{3-}$ , b) 70 mol%  $\text{VO}_4^{3-}$ , c) 90 mol%  $\text{VO}_4^{3-}$ , and d) 100 mol%  $\text{VO}_4^{3-}$ , respectively; e) XRD patterns of corresponding nanocrystals as well as  $\text{YbPO}_4$  (JCPDS standard card no. 54-1014, black line) and  $\text{YbVO}_4$  (JCPDS standard card no. 72-0271, red line). The size of nanoparticles gradually enlarged as more  $\text{VO}_4^{3-}$  entered, and meanwhile, XRD patterns were dominated by  $\text{YbVO}_4$ .



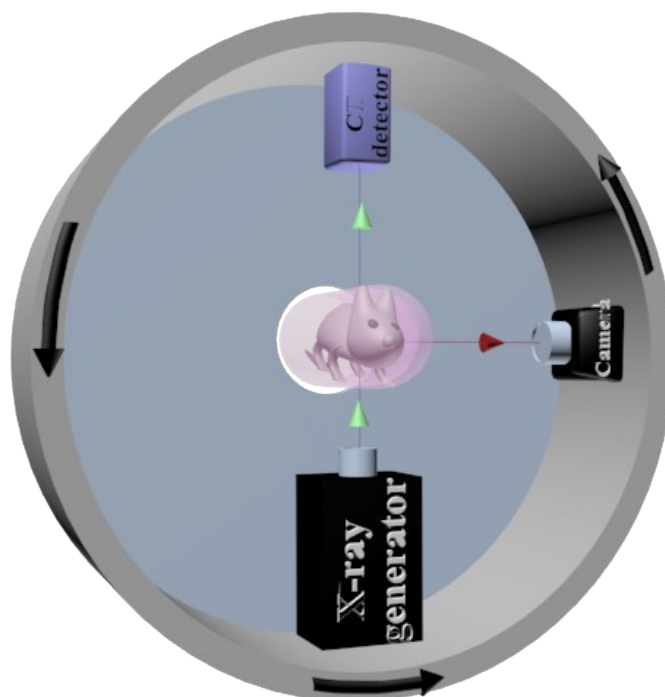
**Figure S3.** XRD patterns of YbPO<sub>4</sub> nanocrystals incorporated with 60 mol%, 70 mol%, 80 mol% and 90 mol% BO<sub>3</sub><sup>3-</sup> as well as the JCPDS standard card of YbPO<sub>4</sub> (no. 54-1014), indicating that there were no crystalline YbBO<sub>3</sub> nanocrystals generated.



**Fig. S4.** TEM images of GdPO<sub>4</sub> incorporated with a) 0%, b) 10%, c) 20% d) 30%, e) 40%, and f) 50 % BO<sub>3</sub><sup>3-</sup>; and g) XRD patterns of corresponding nanocrystals as well as GdPO<sub>4</sub> (JCPDS standard card no. 39-0232). Although there is no GdBO<sub>3</sub> detected out as shown in the XRD, the added BO<sub>3</sub><sup>3-</sup> can effectively modify size and morphology of GdPO<sub>4</sub> nanocrystals.



**Figure S5.** CT value (HU) of aqueous solution of GdP<sub>0.7</sub>V<sub>0.3</sub>O<sub>4</sub>: 5 mol% Eu and GdPO<sub>4</sub>: 5 mol% Eu nanocrystals as a function of concentration. The the CT value at a concentration of 10 mg mL<sup>-1</sup> is measured to be 178.4 and 127.8 HU, respectively. This result demonstrate that the incorporation of VO<sub>4</sub><sup>3-</sup> could significantly improve the CT contrast capability. As Iopromide (a common used CT contrast agent in clinical application) is 135.4 HU, GdP<sub>0.7</sub>V<sub>0.3</sub>O<sub>4</sub>: 5 mol% Eu could serve as efficient CT contrast agents.



**Figure S6.** Schematic illustration of the simultaneous optical and CT deep tissue dual-modal imaging under the single X-ray irradiation assisted by  $\text{Gd}_{0.95}\text{Eu}_{0.05}\text{P}_{0.7}\text{V}_{0.3}\text{O}_4$  nanocrystals.