

1. *Elemental analysis.* To determine whether the nanocomposite is successfully prepared, it has been investigated using X-ray photoelectron spectroscopy (XPS) and Energy Dispersive Spectrometer (EDS). Figure S1(a) showed that element peaks corresponding to S, Cd, Ti and O, indicating that CdS-TiO<sub>2</sub> has been successfully prepared. The element content of CdS is about 75.62%, which was due to the thin shell thickness of TiO<sub>2</sub>. Figure S1(b) indicated that binding energy at 405.14 eV and 564.81 eV were the energy spectrum characteristic peaks of Cd<sub>3d5</sub> and Te<sub>3d5</sub>, respectively. Binding energy at 458.53 eV and 531.84 eV were the energy spectrum characteristic peaks of Ti<sub>2p3</sub> and O<sub>1s</sub> Ti-O, respectively. Therefore, it proved that there are CdTe and TiO<sub>2</sub> in CdTe-TiO<sub>2</sub>. Figure S1(c) showed element peaks corresponding to Se, Cd, Ti and O, indicating that CdSe-TiO<sub>2</sub> had been successfully prepared. The results showed that the samples contained a large amount of element C, which might be due to the surface modification of folic acid. It indicated that FA-CdSe-TiO<sub>2</sub> had been successfully prepared.

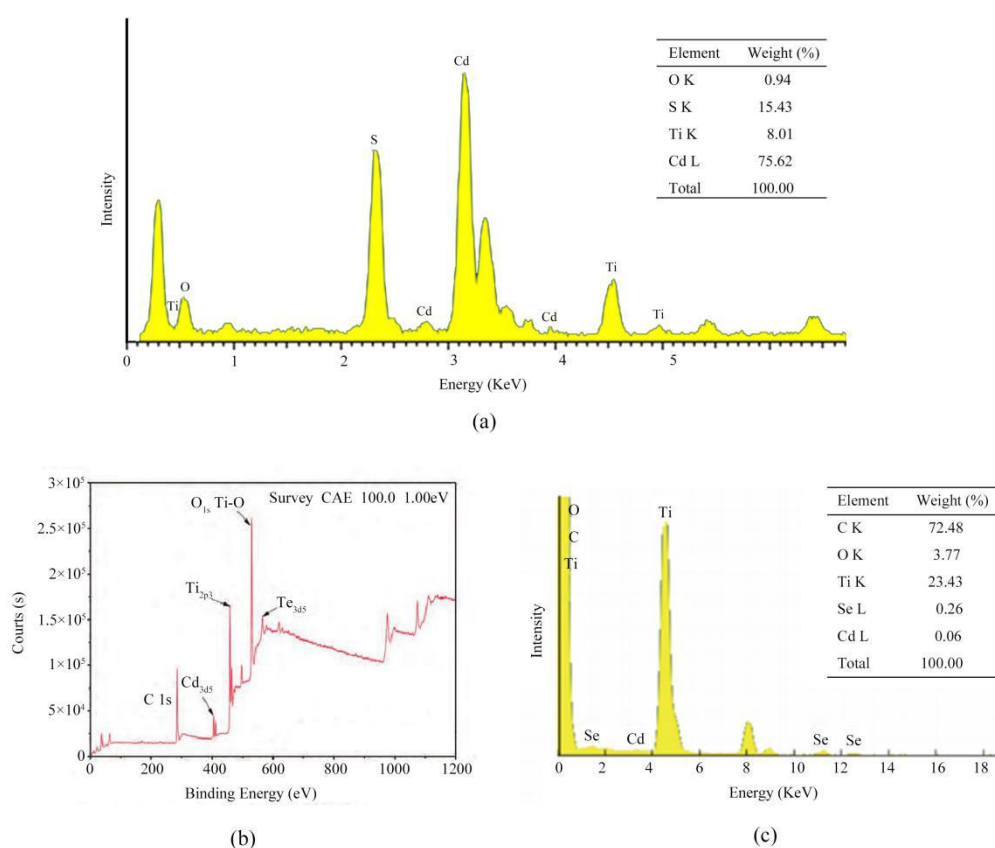


Figure S1: (a) Energy Dispersive Spectrometer (EDS) of CdS-TiO<sub>2</sub>-0.2 (CdS-based nanocomposite A). (b) X-ray photoelectron spectroscopy (XPS) of CdTe-TiO<sub>2</sub> (CdTe-based nanocomposite B). (c) EDS of FA-CdSe-TiO<sub>2</sub> (CdSe-based nanocomposite C).

2. *The advantage of using CdX-TiO<sub>2</sub> for PDT in comparison with previous works.* Hua et al. developed strongly coupled CdX (X=S, Se and Te) quantum dots/TiO<sub>2</sub>

nanocomposites, which had good performance in photocatalytic degradation of benzene [1]. Nideep et al. investigated the good photovoltaic performance of CdX (X=S, Te, Se) QD solar cells [2]. Bansal et al. compared with the visible light absorption spectra of CdX (X=S, Te, Se) nanospheres, CdTe was the most efficient at absorbing solar energy [3]. Due to the lack of research on photodynamic therapy (PDT) about CdX-TiO<sub>2</sub> (X=S, Te, Se) NPs, therefore, it is necessary to research the CdX-TiO<sub>2</sub> (X=S, Te, Se) NPs mediated PDT.

Research work 1: J. H. Hua, M. Wang, Y. Jiao, H. Li and Y. L. Yang, "Strongly coupled CdX (X=S, Se and Te) quantum dots/TiO<sub>2</sub> nanocomposites for photocatalytic degradation of benzene under visible light irradiation," *Optik*, vol. 171, pp. 95-106, 2018.

In this work, Hua et al. proved that CdX (X=S, Te, Se) had a narrow band gap, which could extend the spectral response range of TiO<sub>2</sub> to the visible region. Thus, the photocatalytic degradation efficiency of benzene was improved. CdS-TiO<sub>2</sub> had the narrowest band gap and highest separation efficiency of photo-generated carriers, so the efficiency of photocatalytic degradation of benzene was the highest.

Research work 2: T. K. Nideep, M. Ramya and M. Kailasnath, "An investigation on the photovoltaic performance of quantum dot solar cells sensitized by CdTe, CdSe and CdS having comparable size," *Superlattices and Microstructures*, vol. 141, pp. 11, 2020.

In this work, Nideep et al. investigated that variations in efficiency of the three solar cells sensitized by the CdX (X=S, Te, Se) QDs were explained based on the differences in the effective mass of the charge carriers. The maximum efficiency was obtained for quantum dot sensitized solar cells (QDSSCs) with CdSe QD.

Research work 3: A. Bansal, J. S. Sekhon and S. S. Verma, "Effect Of Surrounding Medium On Light Absorption Characteristics Of CdSe, CdS & CdTe Nanospheres And Their Comparison," in *International Conference on Recent Trends in Applied Physics and Material Science (RAM)*, Ed., pp. 267-268, Amer Inst Physics, Govt Coll Engrg & Technol Bikaner, Bikaner, INDIA, 2013.

In this work, Bansal et al. studied that effect of surrounding medium refractive index on CdX (X=S, Te, Se) by Mie Plot. Absorption efficiency of CdTe was the highest for solar cell applications.

Table S1 Comparisons between recent reports of CdX (X=S, Te, Se) and our work

Works	Band gap energy (eV)			Particle size of CdX	Highest photocatalytic (sensitization) efficiency
	CdS QDs	CdTe QDs	CdSe QDs		
Hua et al.[1]	2.20 (CdS-TiO <sub>2</sub> )	2.81 (CdTe-TiO <sub>2</sub> )	2.48 (CdSe-TiO <sub>2</sub> )	2-5 nm	CdS-TiO <sub>2</sub>
Nideep et al.[2]	2.62	2.18	2.42	4-5 nm	CdSe QDs
Bansal et al.[3]	2.42	1.44	1.74	No mention	CdTe
Our work	2.40	2.36	1.95	2-5 nm	CdSe-TiO <sub>2</sub>

In our works, FA-CdSe-TiO<sub>2</sub> has the highest PDT efficiency and low dark toxicity. Due to CdSe QDs having a narrow band gap, it combined with TiO<sub>2</sub> can extend the visible response range of TiO<sub>2</sub>. The separation efficiency of photo-generated carriers was improved. When FA modified on the surface of CdSe-TiO<sub>2</sub>, FA could specifically recognize FR to improve the efficiency of HL60 cell uptake of nanocomposites.

## References

- [1] J. H. Hua, M. Wang, Y. Jiao, H. Li and Y. L. Yang, "Strongly coupled CdX (X=S, Se and Te) quantum dots/TiO<sub>2</sub> nanocomposites for photocatalytic degradation of benzene under visible light irradiation," *Optik*, vol. 171, pp. 95-106, 2018.
- [2] T. K. Nideep, M. Ramya and M. Kailasnath, "An investigation on the photovoltaic performance of quantum dot solar cells sensitized by CdTe, CdSe and CdS having comparable size," *Superlattices and Microstructures*, vol. 141, pp. 11, 2020.
- [3] A. Bansal, J. S. Sekhon and S. S. Verma, "Effect Of Surrounding Medium On Light Absorption Characteristics Of CdSe, CdS & CdTe Nanospheres And Their Comparison," in *International Conference on Recent Trends in Applied Physics and Material Science (RAM)*, Ed., pp. 267-268, Amer Inst Physics, Govt Coll Engn & Technol Bikaner, Bikaner, INDIA, 2013.