Supporting Information

Surface-Enhanced Raman Scattering (SERS) as Probe for Detection of Charge Transfer Between TiO_2 and CdS Nanoparticles

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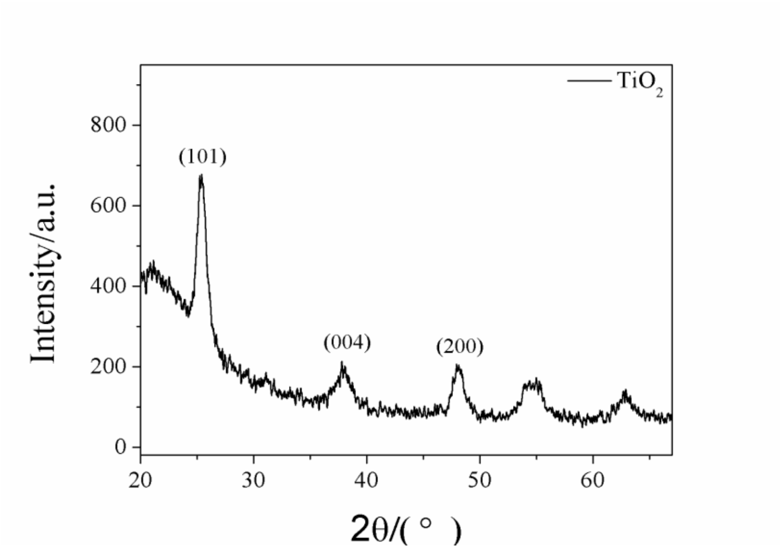

Figure S1. XRD pattern of TiO_2 nanoparticles.

XRD is usually used for identification of the crystal phase structure and estimation of crystallite size for nanoparticles (NPs). The XRD peaks at $2\theta = 25.4^\circ$ (101) and 48° (200) are generally identified as the characteristic diffraction peaks of the anatase crystal phase of TiO_2,[1] which usually holds high surface performance.[2] Figure S1. shows the XRD pattern of TiO_2 NPs. As-prepared TiO_2 NPs exhibits a pure anatase phase with relatively good crystallinity. All XRD peaks are comparatively wide, which is a typical characteristic of nanometer materials. The crystallite size D of the sample is about 8.6 nm, which was estimated from the half band width (β) of the corresponding X-ray spectral peak by the Scherrer formula[1]: $D = k\lambda/(\beta\cos\theta)$.

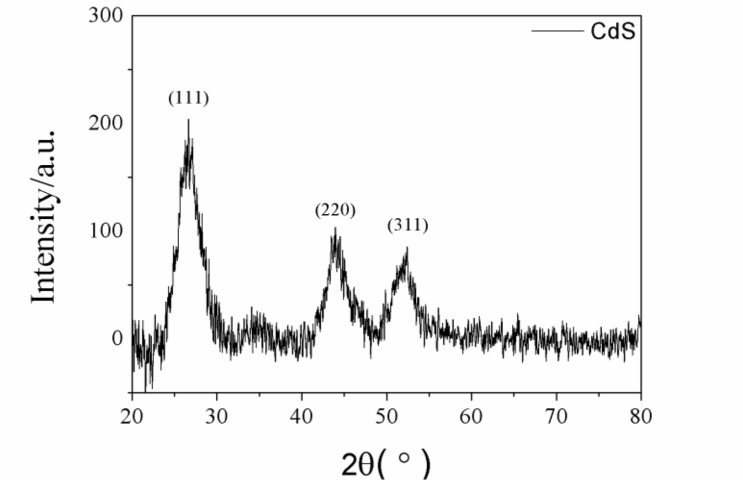

Figure S2. XRD pattern of CdS nanoparticles.

The XRD peaks at 2θ = 26.5˚ (111), 43.9˚ (220) and 51.9˚ (311) are generally identified as the characteristic diffraction peaks of the cubic system of CdS.[3] Figure S2. shows the XRD pattern of CdS NPs. All XRD peaks are comparatively wide, which is a typical characteristic of nanometer materials. The crystallite size D of the sample is about 5.4 nm, which was estimated from the half band width (β) of the corresponding X-ray spectral peak by the Scherrer formula[1]: $D = k\lambda/(\beta\cos\theta)$.

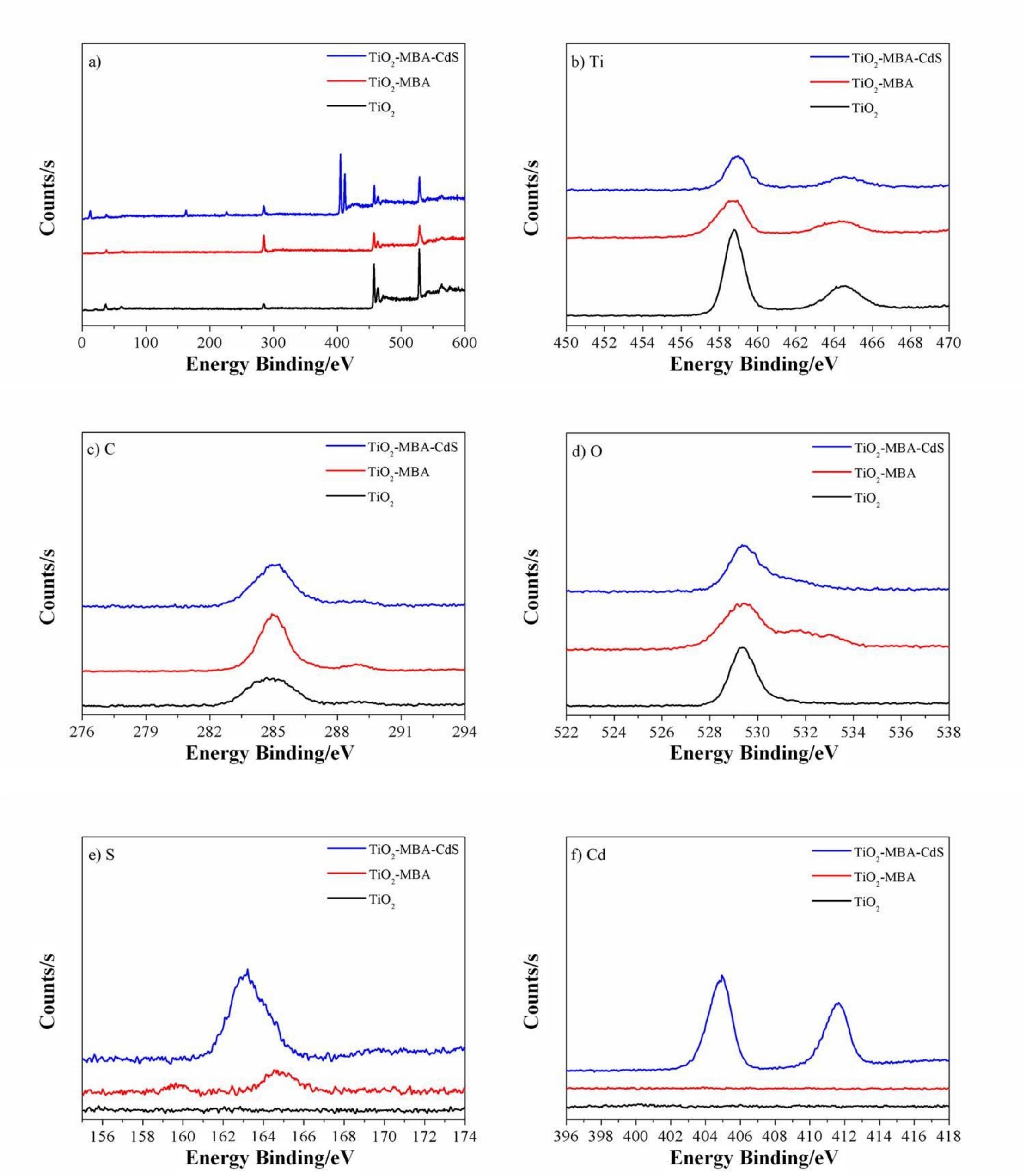

Figure S3. The XPS of the TiO_2-CdS systems, a)full spectrum, b) Ti, c) C, d) O, e) S, f) Cd.

To further identify the elemental composition and chemical state of TiO_2/MBA/CdS charge-transfer system, XPS measurements were carried out. Figure S3. shows that Ti, C, O, S, Cd elements exist on the surface of the charge-transfer systems. The peaks at 458.8eV and 464.4eV are assigned to Ti2p3/2 and 2p1/2(Figure 3b), the doublet separation between the 2p1/2 and 2p3/2 peaks of ~5.6 eV is characteristic of Ti^{4+}. And the peak at 284.7eV is assigned to C (Figure S3c). The peak at 529.3 eV (Figure S3d) is assigned to O1s, which shows the oxygen is bound to tetravalent Ti ions and it means that the surface is partly covered with -COOH groups from the small peak at 531.6 eV. Compared with system TiO_2 in Figure S3e, the systems TiO_2/MBA and TiO_2/MBA/CdS have sulfur element which be attributed to -SH of MBA molecule and CdS NPs are introduced subsequently. The Cd3d photoelectron (Fig S3f) shows a Cd3d5/2 peak at 405.1 eV and a 3d3/2 peak at 411.6 eV in TiO_2/MBA/CdS system.

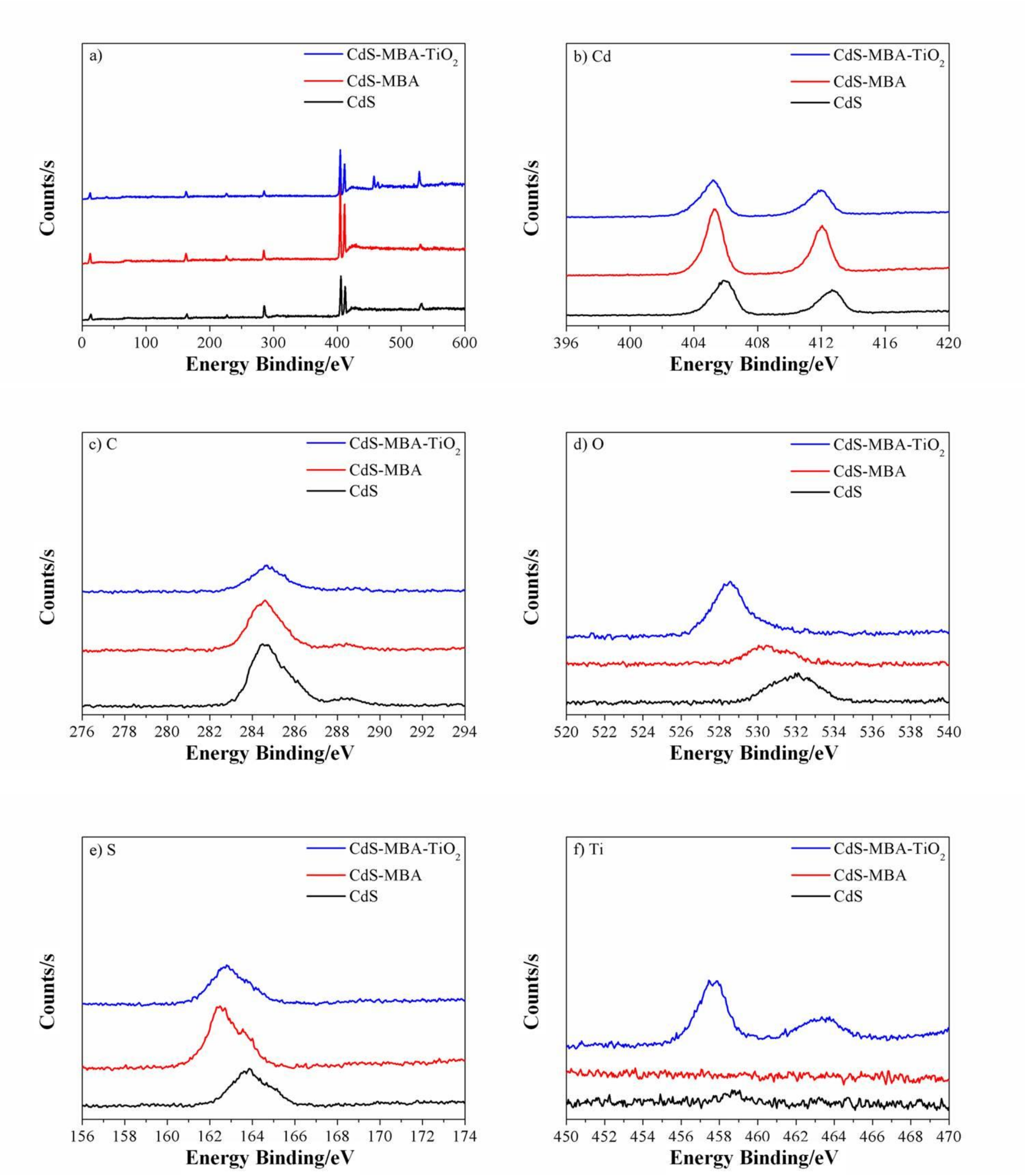

Figure S4. The XPS of the CdS-TiO$_2$ systems, a)full spectrum, b) Cd, c) C, d) O, e) S, f) Ti.

Figure S4. shows that Cd, C, O, S, Ti elements exist on the surface of the charge-transfer systems. The peaks at 405.8eV and 412eV are assigned to Cd3d5/2 and 3d3/2(Figure S4b), the doublet separation between the 3d5/2 and 3d3/2 peaks of ~6.2 eV is characteristic of Cd^{2+}. And the peak at 284.6eV is assigned to C (Figure S4c). The peak of CdS at 532.1eV (Figure S4d) is assigned to O1s, which may be attributed to the residual of nitrate ions in the process of synthesizing CdS. The peak of CdS/MBA at 530.4eV and CdS/MBA/TiO$_2$ at 528.6 are assigned to O1s which be attributed to MBA and TiO$_2$ are introduced subsequently. Compared with system CdS in Figure S4e, the systems CdS/MBA and CdS/MBA/TiO_2 have sulfur element which be attributed to -SH of MBA molecule is introduced subsequently. The peaks at 457.8eV and 463.4eV are assigned to Ti2p3/2 and 2p1/2(Figure S4f).

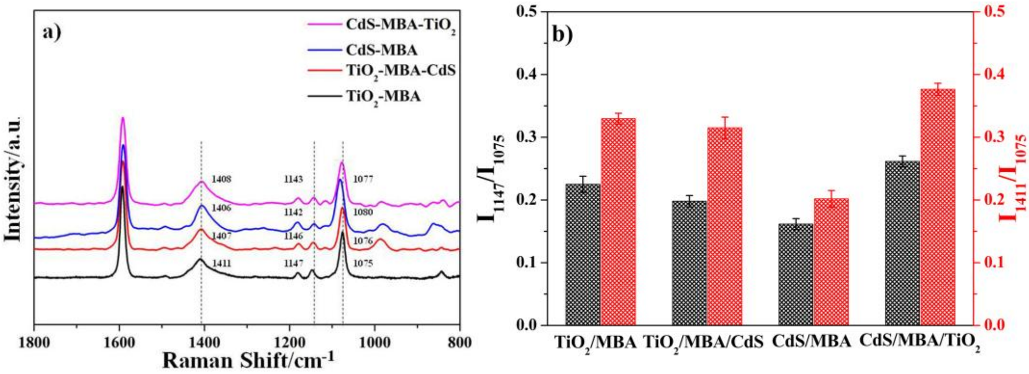

Figure S5. a) SERS spectra of TiO_2/MBA, TiO_2/MBA/CdS, CdS/MBA and CdS/MBA/TiO_2 systems at 785 nm excitation; b) The SERS intensity ratio of the modes 1147 and 1075 cm^{-1} as well as 1411 and 1075 cm^{-1} in four systems.

Figure S5. presents the SERS spectrum of TiO_2-MBA, TiO_2-MBA-CdS, CdS-MBA and CdS-MBA-TiO_2 under the excitation of 785 nm laser. The histogram showed the peak intensities at 1147 cm^{-1} and 1411 cm^{-1} (b2 mode) relative to 1075 cm^{-1} (a1 mode) in these four kinds of assemblies. Similar to the situation of 633 nm excitation, in CdS-MBA-TiO_2 system, the b2 mode greatly enhanced compared to TiO_2-MBA-CdS system.

References

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3. H. Zhang, X. Y. Ma, J. Xu, Directional CdS nanowires fabricated by chemical bath deposition, *Journal of Crystal Growth*, 2002,**246,** 108-112.