Electronic Supplementary Information

Section I: Microscope images of TiO_2 thin films, DNA-CdTe (CA as ligands) and DNA-CdTe (TGA as ligands)

Silanized glass slides were immersed into an anhydrous toluene solution containing 0.1 M TDD for 30 min at room temperature under a N_2 atmosphere. Fig. S1 (A) is a bright-field microscope image of TiO_2 thin films on a silanized slide.

DNA (1.0 μM, 10 mL) and CA-capped CdTe (10.0 *m*M, 0.1 mL) were mixed for 20 min, spread evenly on the surface of TiO_2 thin films, and observed with an inverted fluorescence microscope at a dark-field condition. A long luminescent chain (Fig. S1B) appeared. However, when CA-capped CdTe NCs were replaced by CA-thioglycolic acid-capped CdTe NCs, no similar phenomenon were observed (Fig. S1C).

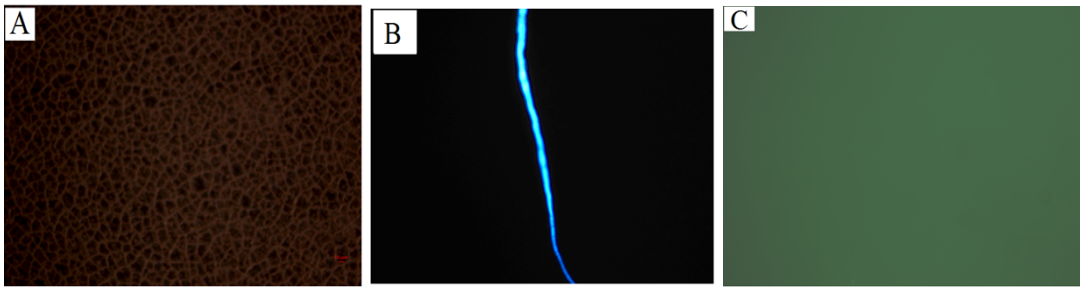
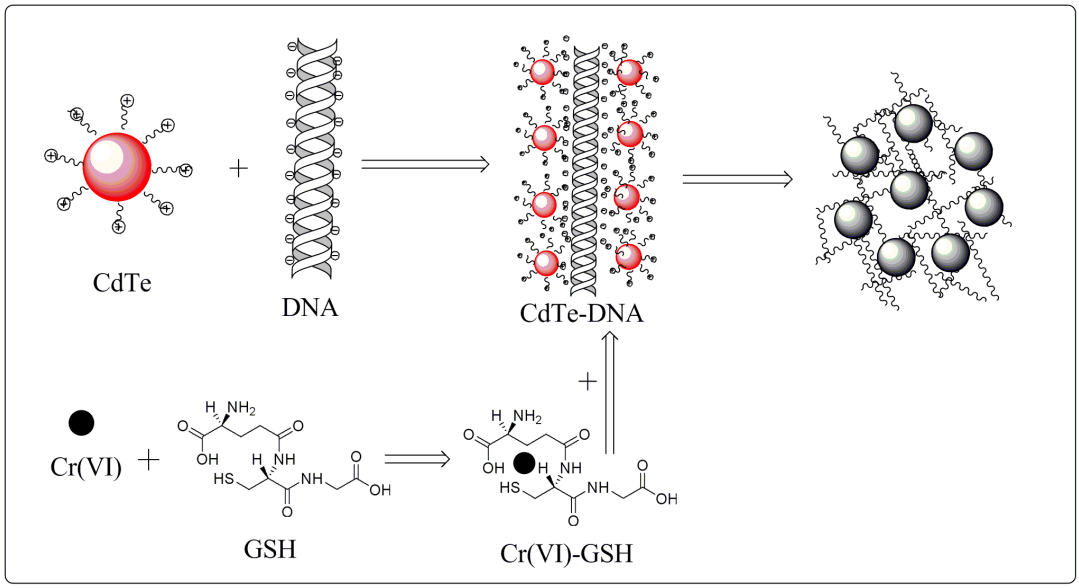


Fig. S1 (A) Bright-field microscope image of TiO_2 thin films on silanized slides; (B) Fluorescence microscope image of DNA-CdTe (CA as ligands); (C) Fluorescence microscope image of DNA-CdTe (TGA as ligands).

Section II: The possible mechanism of DNA damage induced by Cr(V)-GSH complexes



Section III: AFM images of DNA damage induced by Cr(V)-GSH complexes

AFM can generate high-resolution images at a single molecule level, which was employed to visualize Cr(V)-induced DNA damage in this study. AFM images of Cr(V)-induced DNA damaged were obtained similar to the literature (P. H. Yang, W. H. Zhang, et al. *Chinese Journal of Inorganic Chemistry*, 2006.3.113). AFM imaging was performed using a multimode with a Nanoscopy IIIa controller. Cr(V)-GSH (10.0 μM, 2.0 L) and DNA-CdTe solution (50.0 μM, 10.0 mL) were mixed, and deposited on freshly cut mica substrates and was imaged in air at room temperature. Commercially available NCH-100 silicon micro-cantilevers were used for tapping mode scanning with an E-scanner. Images were captured at a scan rate of 0.5 Hz and flattened to remove the background slop.

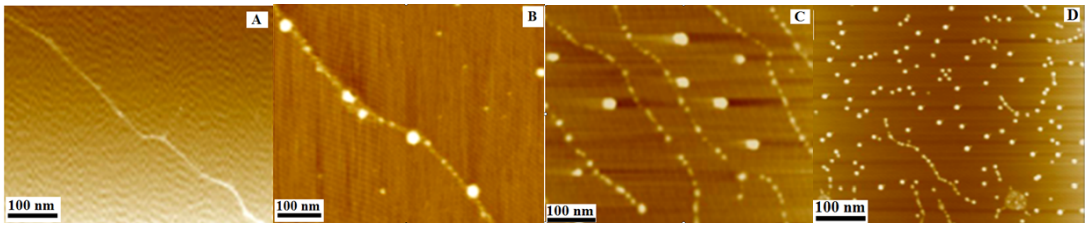


Fig. S2 AFM images of DNA damage induced by Cr(V)-GSH complexes. (A) DNA molecule; (B) Incubation for 20 min. (C) Incubation for 40 min. (D) Incubation for 60 min.

Section IV: Comet assay

A human B lymphoblastoid cell line (Cell Bank, Chinese Academy of Sciences) were cultured in IMDM (HyClone, USA) supplemented with 10% fetal bovine serum at 37 °C in a fully humidified atmosphere with 5% CO_2. The cells were subcultured every three days. Human B lymphoblastoid cells were exposed to Cr(VI)-GSH complexes at

the doses of 0, 0.5, 1.0, 2.0, 5.0, and 10.0 μM for 24 h.

Comet assay is a simple, sensitive and rapid technique for detection of DNA damage in individual cells and can be very useful in studies of genetic toxicology. The comet assay was performed under alkaline conditions according to the procedure of Singh et al. (*Experimental cell research*, 175, 184-191.) with slight modifications. The lymphocytes were embedded in 0.65% low melting point agarose at a final concentration of 10^4 cells/ml; 75 μL of this cellular suspension was then spread onto a frosted slide that had previously been covered with 100 μL of 1% normal melting point agarose (as the first layer). The slides were immersed in freshly prepared lysis solution (1% sodium sarcosinate, 2.5 M NaCl, 100 *m*M Na_2EDTA, 10 *m*M Tris-HCl pH 10, 1% Triton X-100 and 10% DMSO) at 4 °C for 1 h. Then the slides were placed in a horizontal electrophoresis unit covered with fresh buffer (1 *m*M Na_2EDTA; 300 *m*M NaOH, pH 13) for 20 min. Electrophoresis was performed for 20 min at 1.5 V/cm and 300 *m*A. Subsequently, the slides were washed gently twice in neutralization buffer (0.5 M Tris-HCl, pH 7.5). Each slide was stained with 50 μL of ethidium bromide (25 μg /ml). All the above steps were conducted under yellow light (580 nm) to avoid additional DNA damage.

Observations were made using a fluorescence microscope equipped with a 530 nm excitation filter, a 590 nm emission filter, and a camera. Fifty cells from each of the two replicate slides per sample were selected for data analysis, and the CASP software was used to analyze the comets and the percentage of DNA tails was calculated.

Section V: Zeta potential of DNA-CdTe solution

Zeta potential (ζ) was measured by dynamic light scattering analysis with a 633 nm laser. Three rounds of assays were performed, and the average data were reported. As seen from Fig. S3, ζ of DNA-CdTe NCs reached 30.5 mV (A). When Cr(VI)-GSH complexes were added, the ζ of the NC's solution decreased 20.2 mV (B) and 4.63 mV (C), respectively.

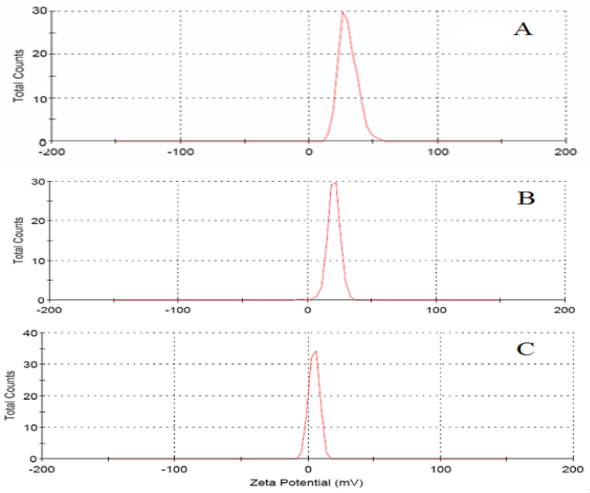


Fig. S3 Zeta potential of DNA-CdTe with different concentration of Cr(VI)-GSH complexes. B: 2.0 μM; C: 10.0 μM.

Section VI: Circular dichroism spectra of DNA

Circular dichroism (CD) spectra were measured in a rectangular quartz cell (1.00 mm path length) at 200 nm/min scanning speed. CD spectra were obtained after different concentration of Cr(VI)-GSH complexes were added to the DNA solution (10.0 μM).

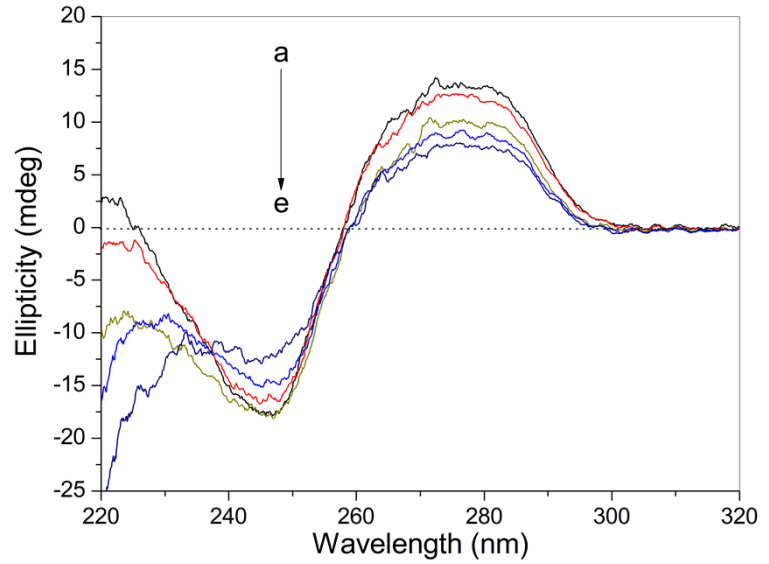


Fig. S4 CD spectra of DNA (100 μM) showing conformational change in the presence of Cr(VI)-GSH complexes. a-e ($C_{Cr(VI)-GSH}$, μM): 0, 5 , 10, 20, 40.

Section VII: Fluorescence and time-resolved fluorescent spectra of DNA-CdTe

Fluorescence and time-resolved spectra were performed on FLS920 combined fluorescence lifetime andsteady statespectrometer with a R928-P photomultiplier detector, and excited by 405 nm picosecond laser diode pulses. Fluorescence spectra were obtained from 420 to 680 nm with a fixed-width slit. Time-resolved spectra were obtained using time-correlated single-photon counting technique.

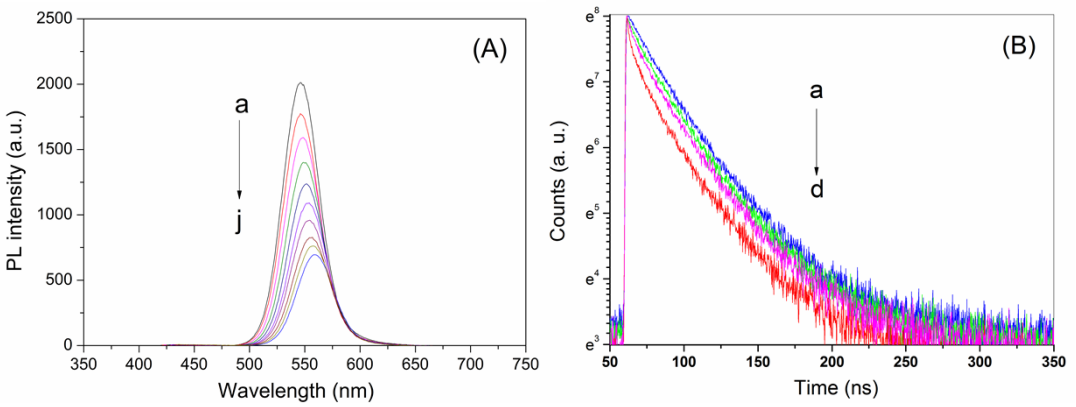


Fig. S5 Fluorescence (Fig. A; $C_{Cr(VI)\text{-}GSH}$, μM, a-j: 0, 0.4, 0.8, 1.6, 2.4, 3.2, 4.0, 4.8, 5.6, 6.4) and time-resolved fluorescence (Fig. B; $C_{Cr(VI)\text{-}GSH}$, μM, a-d: 0, 1.0, 2.0, 5.0) spectra of DNA-CdTe with Cr(VI)-GSH complexes.