Supporting Information

Detection of Mercury(II) by Quantum Dot-DNA-Gold Nanoparticle Ensemble Based Nanosensor Via Nanometal Surface Energy Transfer

Ming Li, [†] Qiaoyi Wang, [‡] Xiaodong Shi, [‡] Lawrence A. Hornak,[§] and Nianqiang Wu*,[†]

[†]Department of Mechanical and Aerospace Engineering, WVNano Initiative, [‡]Eugene Bennett Department of Chemistry, [§]Lane Department of Computer Science and Electrical Engineering, West Virginia University, Morgantown, WV 26506, USA

*Corresponding author: Tel: +1-304-293-3326, Fax: +1-304-293-6689, E-mail: nick.wu@mail.wvu.edu

DNA loadings of QDs and Au NPs

The loading of ssDNA onto the QDs was determined based on the UV-Vis absorption spectra before and after modification with ssDNA and the absorbance difference at 260 nm.[1] The molar extinction coefficient (ε) of QDs is 2.0×10^5 L/(mol·cm) according to the literature.[2] In addition, the exact DNA concentration can be determined by the absorbance at 260 nm, according to[3]

1 O.D. (260 nm)=50 ng DNA/μL

Therefore, since the resulting DNA-QD stock solution has a QD concentration of 0.9 μM ($C=A_{551nm}/(b\cdot\varepsilon)$), the average DNA loading can be calculated to be four DNAs per QD.

Similarly, we can obtain the DNA loading per Au NP. 3 nm Au NPs contain 976 Au atom (Au_{976}).[4] The average DNA loading was roughly estimated to be one DNA per Au NP. In the above calculation, we used the molecular weight 3043 g/mol and 2985 g/mol for 5'-HS-CAGTTTGGAC-3' and 5'-HS-GTCCTTTCTG-3', respectively.

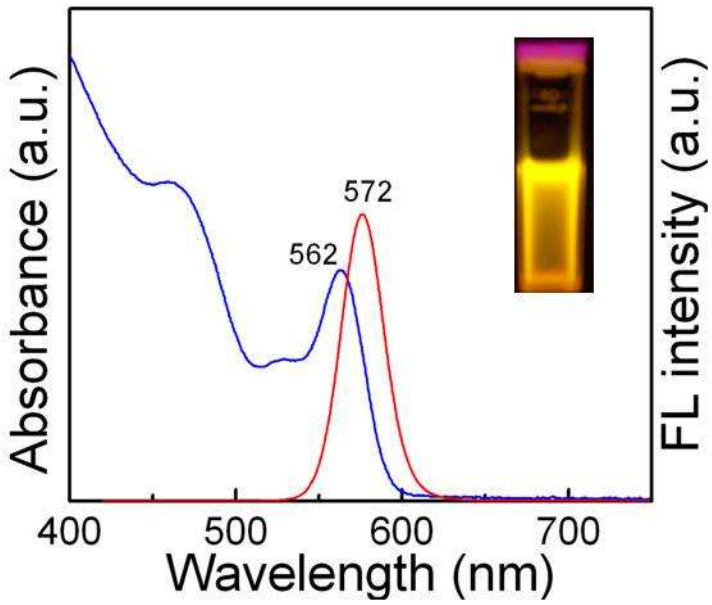

Figure S1. UV-Visible absorption and fluorescence emission spectra of the TOPO-capped quantum dots (QDs) in CH_2Cl_2. The TOPO-capped QDs show a fluorescence emission peak at 572 nm and the first absorption peak at 562 nm. The inset is the photo of the TOPO-capped QDs in CH_2Cl_2 under 365 nm light.

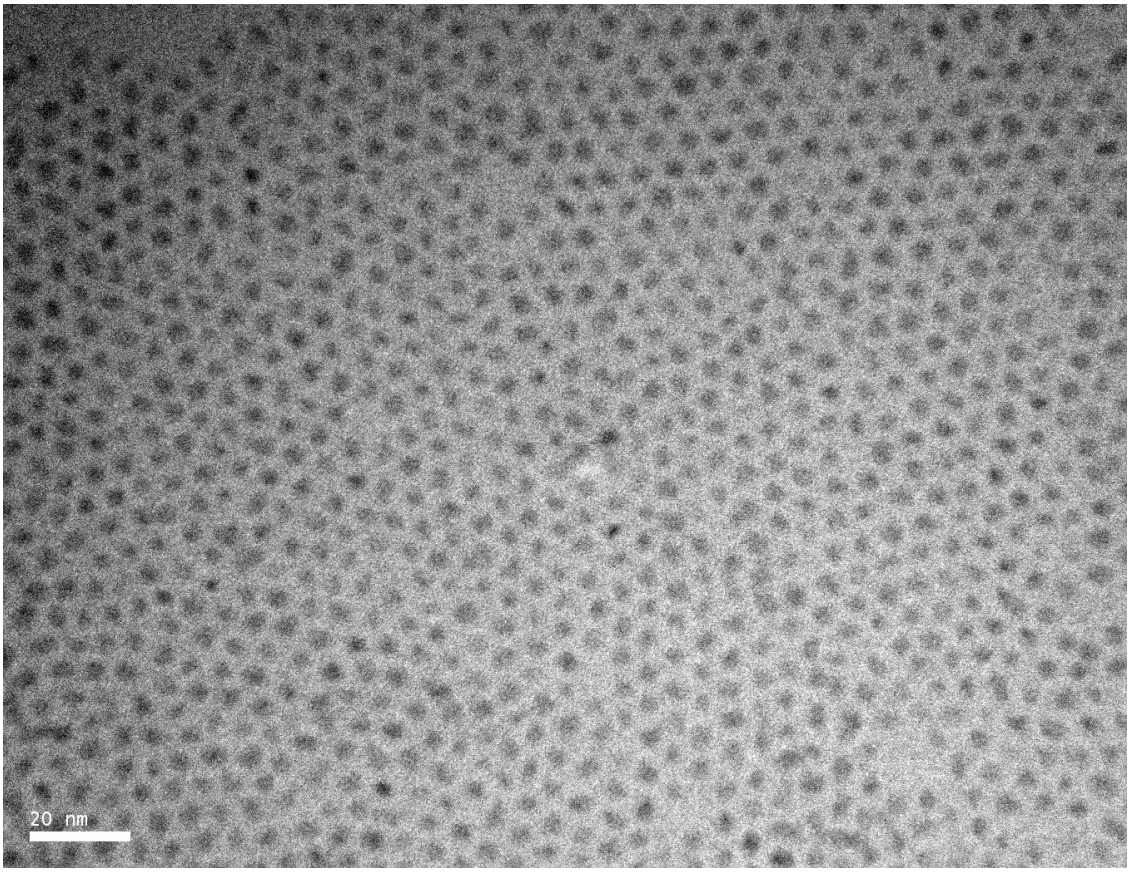

Figure S2. TEM image of the TOPO-capped quantum dots (QDs) used for the QD-DNA-Au ensemble based nanosensor, showing the particle size of 3.8 nm and the narrow size distribution.

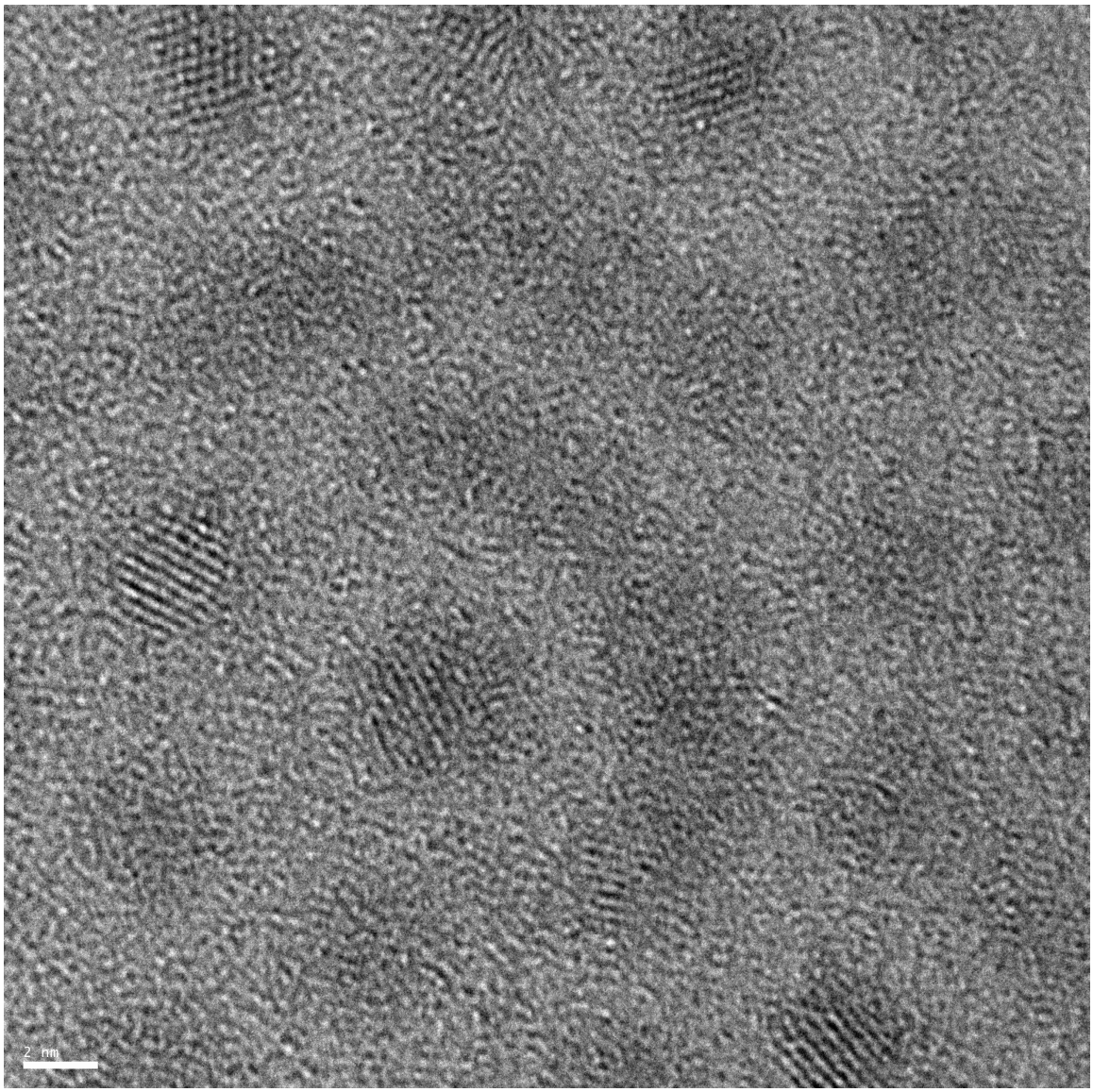

Figure S3. HRTEM image of the TOPO-capped quantum dots used for the QD-DNA-Au ensemble based nanosensor (scale bar: 2 nm).

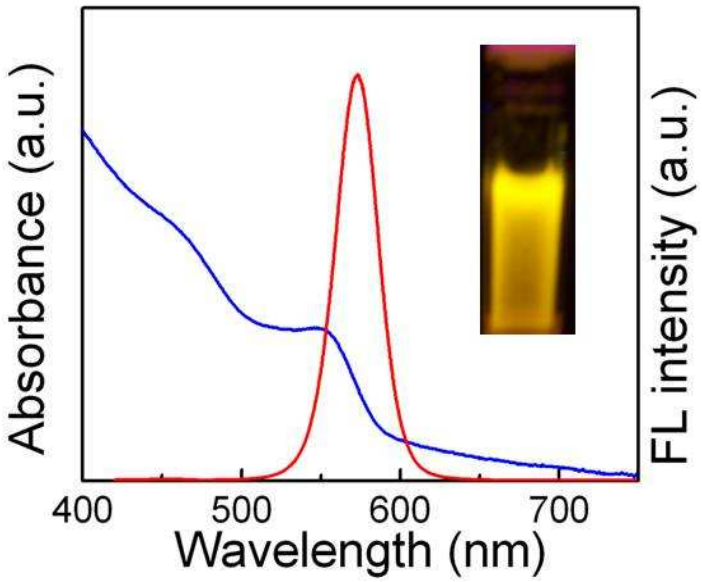

Figure S4. UV-Visible absorption and fluorescence emission spectra of DNA-functionalized quantum dots (QDs) in 0.3 M PBS buffer solution. The inset is the photo of the DNA-functionalized QDs in 0.3 M PBS buffer under 365 nm light. The DNA functionalized QDs show a fluorescence emission peak at 572 nm and an absorption peak at 556 nm in 0.3 M PBS solution.

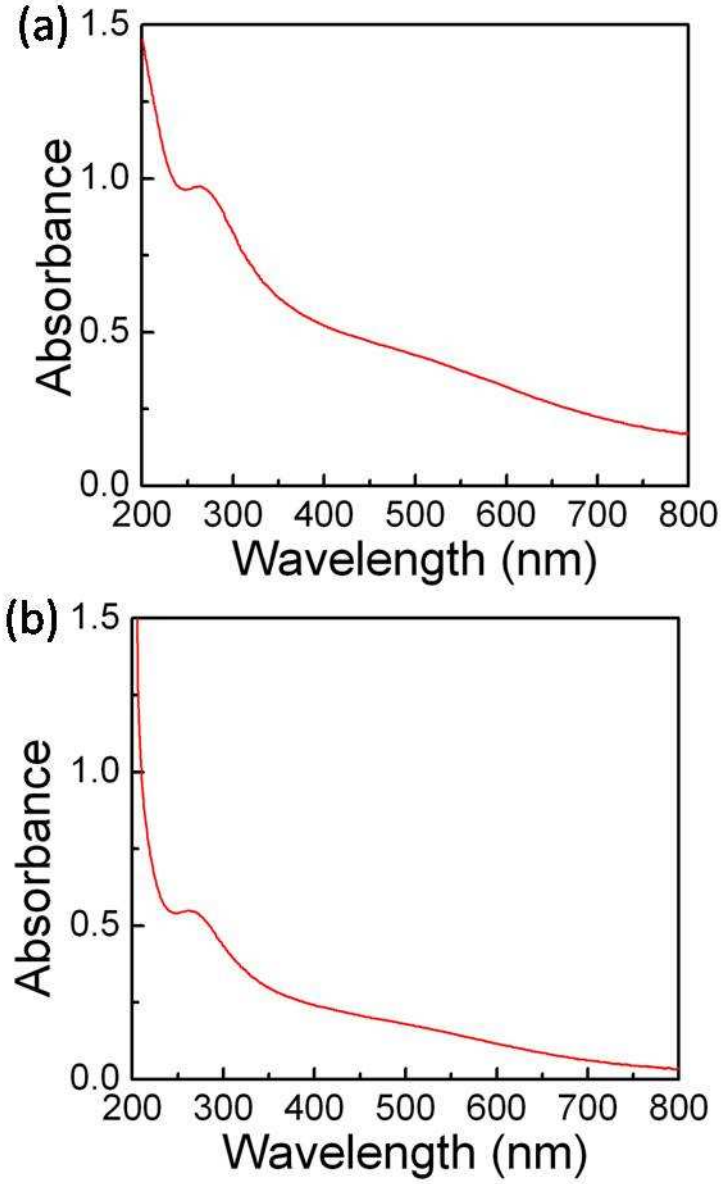

Figure S5. UV-Visible absorption spectra of (a) as-made 3 nm Au nanoparticles (NPs), and (b) DNA-functionalized Au NPs in 0.3 M PBS solution. Both the UV-Visible absorption spectra show no surface plasmon resonance absorption band.

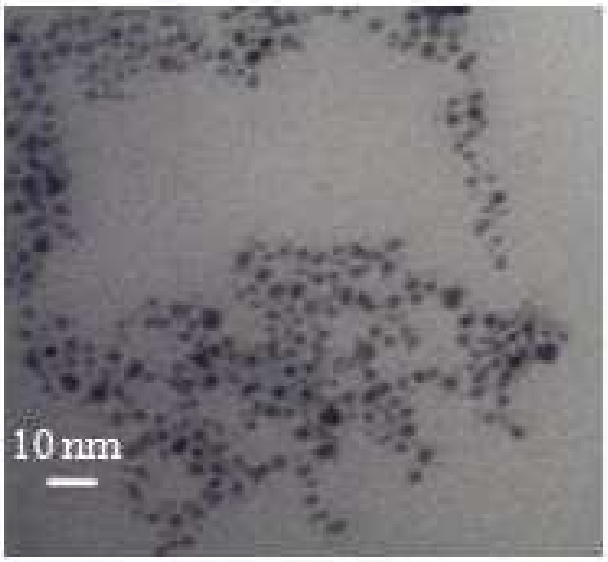

Figure S6. TEM image of the as-made Au nanoparticles used for the QD-DNA-Au ensemble based nanosensor

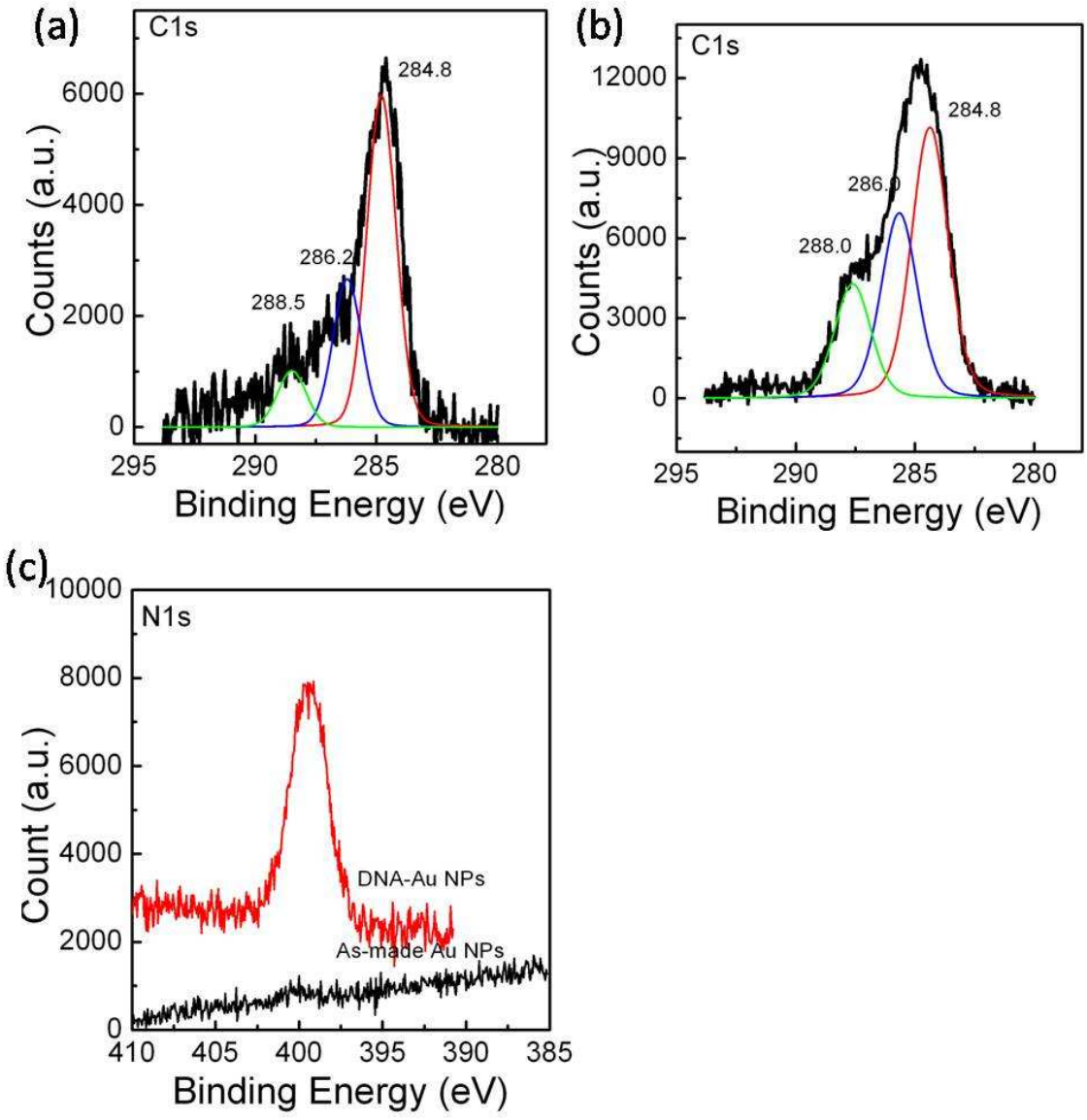

Figure S7. XPS spectra: (a) the C 1s core level of the as-made Au nanoparticles. (b) the C 1s core level of the DNA functionalized Au nanoparticles. (c) the N 1s core level of the as-made Au nanoparticles and the DNA-functionalized Au nanoparticles.

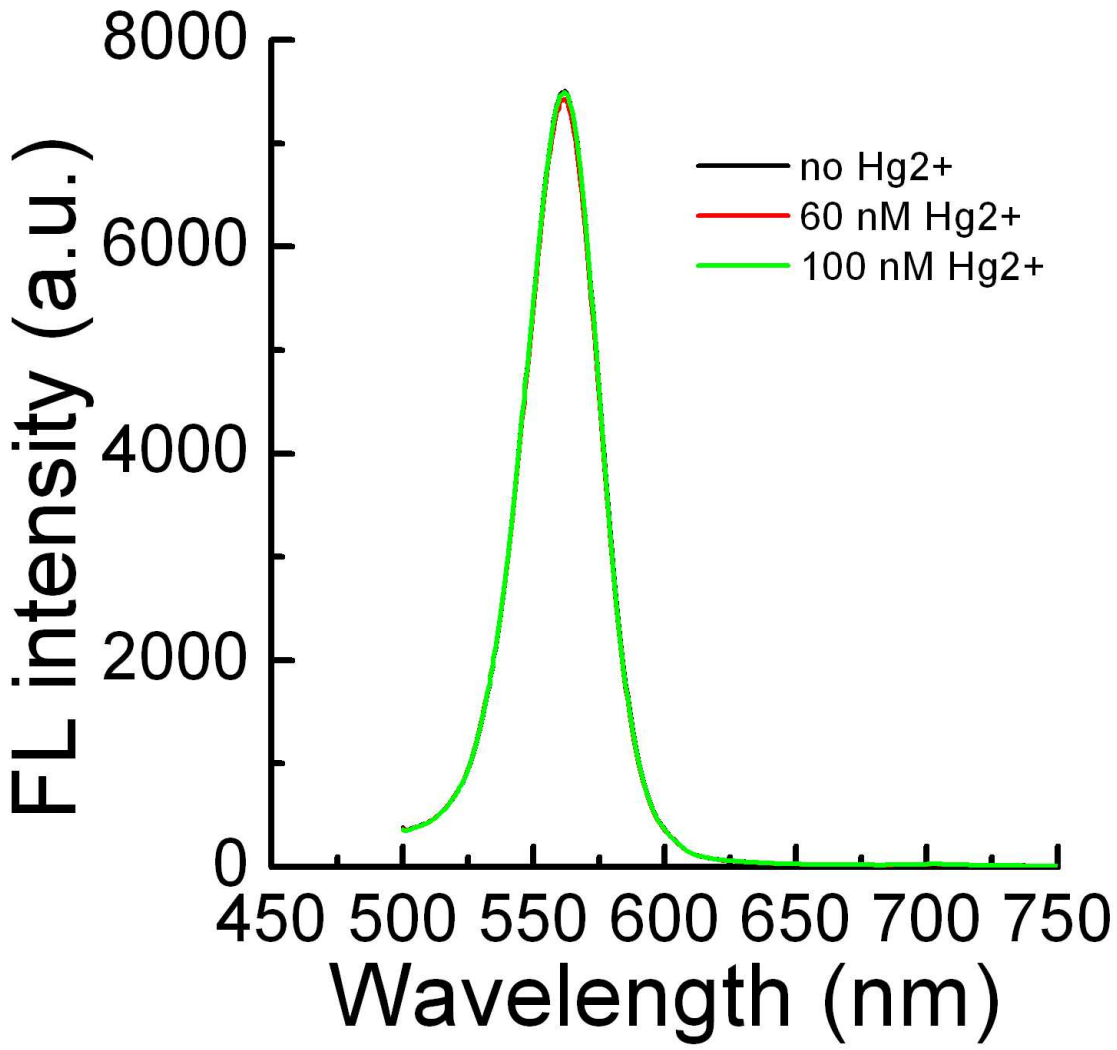

Figure S8. Fluorescence spectra of DNA-functionalized quantum dots (QDs) in the absence and presence of 60 nM and 100 nM. The FL intensity shows no observable change after addition 60 nM and 100 nM Hg^{2+}, indicating that Hg^{2+} makes negligible contribution to quenching of fluorescence from QDs in the present work.

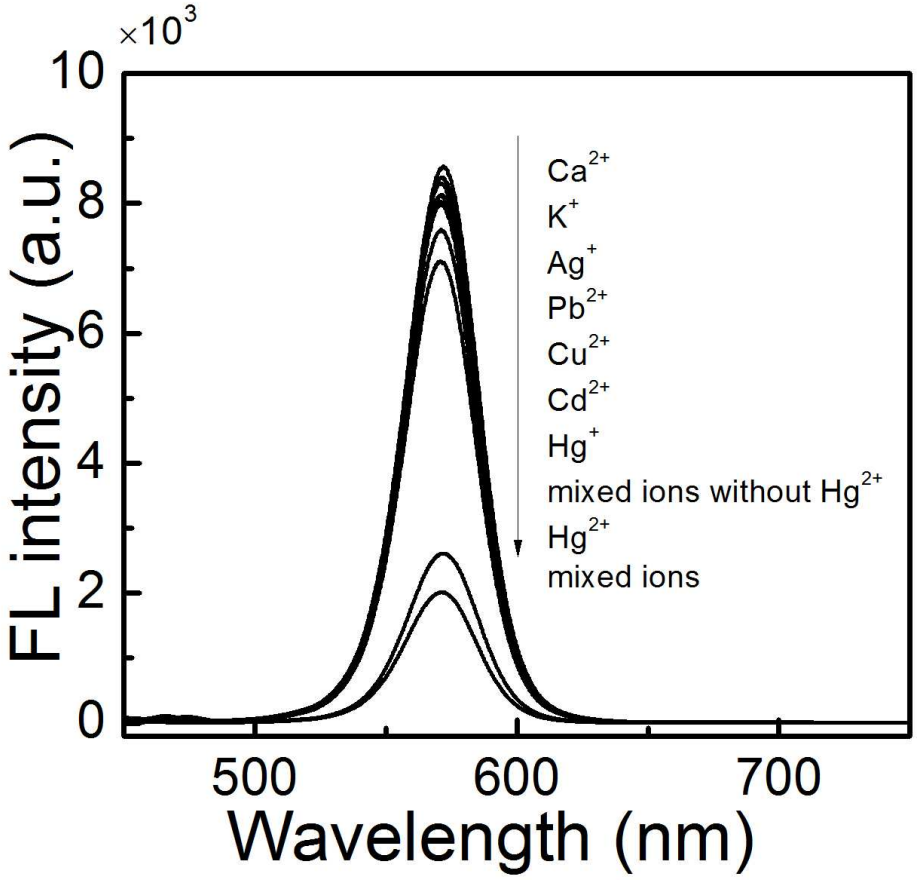

Figure S9. Fluorescence spectra of the QD/DNA/Au NP system in 0.3 M PBS buffer solution after addition of various metal ions at the concentration of 100 nM (96 nM QDs, 104 nM Au NPs and 0.1 mM ethylenediamine in 0.3 M PBS).

References

1. Freeman, R.; Finder, T.; Willner, I. Multiplexed Analysis of Hg^{2+} and Ag^{+} Ions by Nucleic Acid Functionalized CdSe/ZnS Quantum Dots and Their Use for Logic Gate Operations. *Angew. Chem. Int. Ed.* **2009**, *48*, 7818–7821.
2. Yu, W. W.; Qu, L.; Guo, W.; Peng, X. Formation and Stability of Size-, Shape-, and Structure-Controlled CdTe Nanocrystals: Ligand Effects on Monomers and Nanocrystals. *Chem. Mater.* **2003,** *15,* 2854-2860.
3. Molecular Techniques and Methods, Construction of Genomic Library, http://www.molecularinfo.com/MTM/A/A2/A2-3/A2-3-1.html, (accessed on January 12, 2011).
4. Hostetler, M. J.; Wingate, J. E.; Zhong, C.-J.; Harris, J. E.; Vachet, R. W.; Clark, M. R.; Londono, J. D.; Green, S. J.; Stokes, J. J.; Wignall, G. D.; Glish, G. L.; Porter, Marc D.; Evans, N. D.; Murray, R. W. Alkanethiolate Gold Cluster Molecules with Core Diameters from 1.5 to 5.2 nm: Core and Monolayer Properties as a Function of Core Size. *Langmuir* **1998**, *14*, 17-30.