

## Nitrilotriacetate Stabilized Gold Nanoparticles: A Novel Strategy for Colorimetric Detection of Cr(III)/Cr(VI) and Mechanistic Aspect

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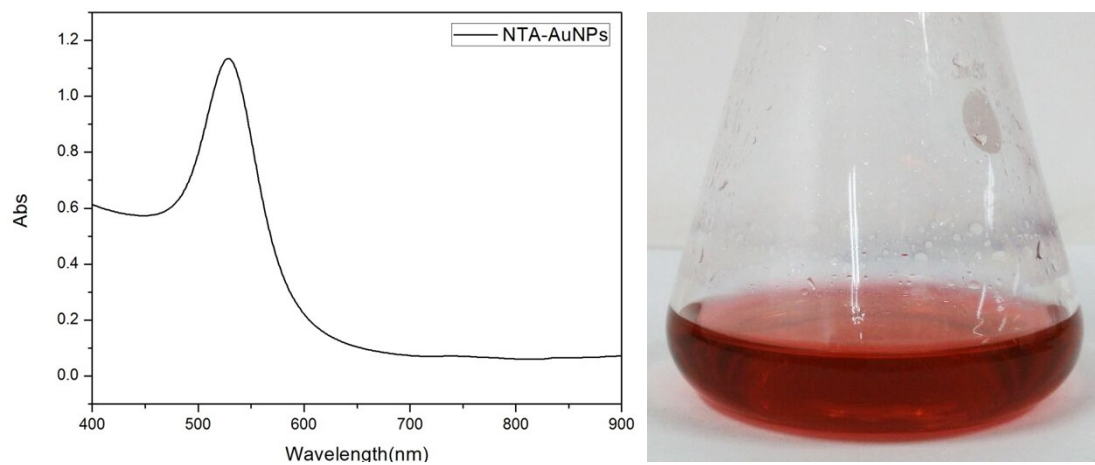
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### Supporting Information

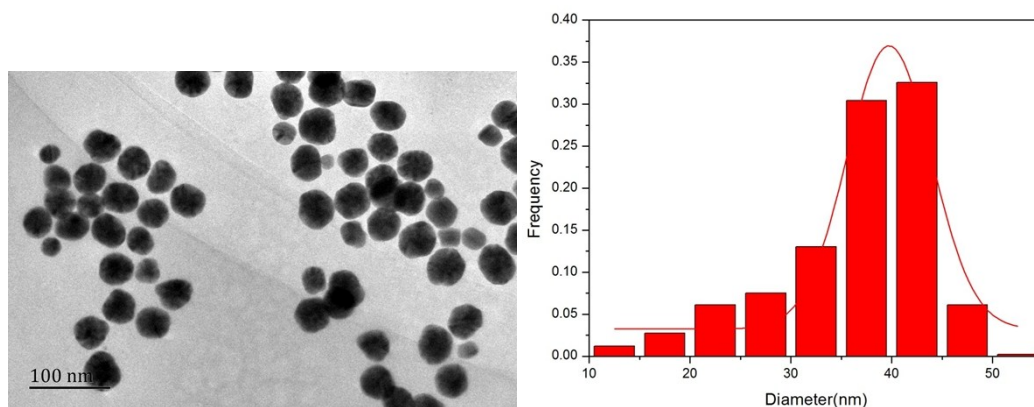
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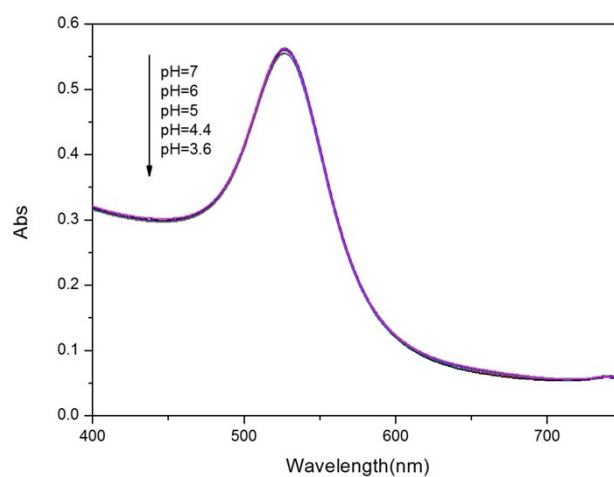
## The characterization of NTA-AuNPs



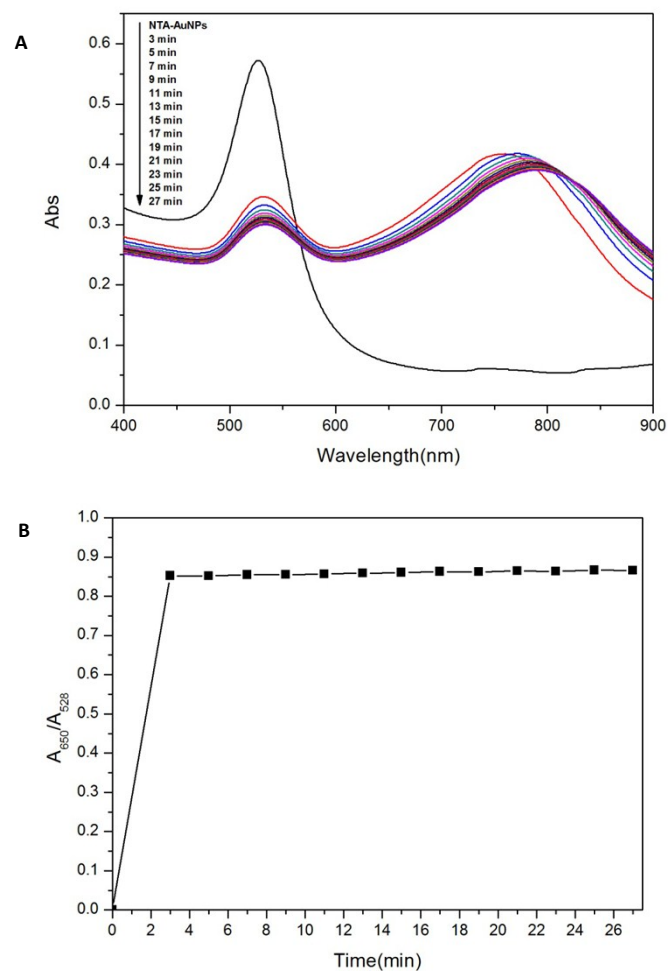
**Fig. S1** UV-vis spectroscopy (left) and photographic image (right) of NTA-AuNPs.



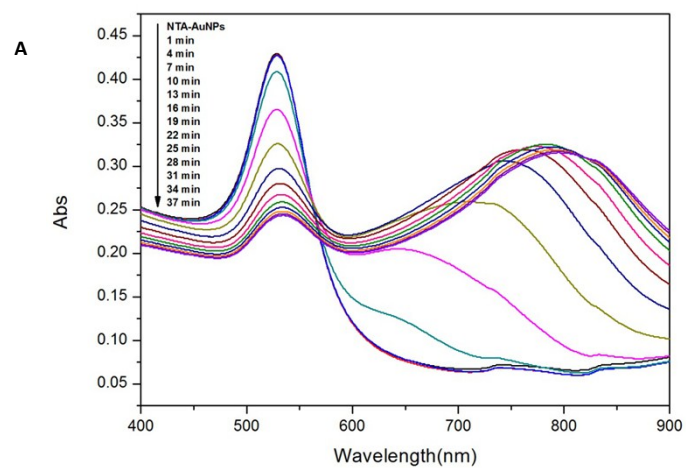
**Fig. S2** TEM image (left) and diameter histogram distribution (right) of NTA-AuNPs ( $d = 36.5$  nm).

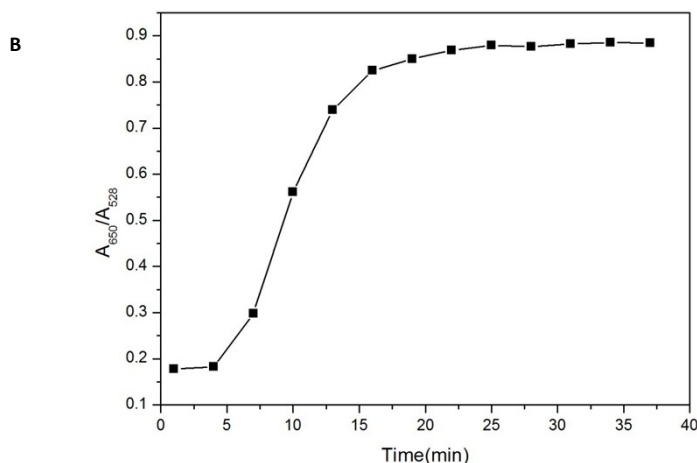


**Fig. S3** UV-vis spectroscopy of NTA-AuNPs with 1h incubation after adjusting pH value from 7 to 3.6.

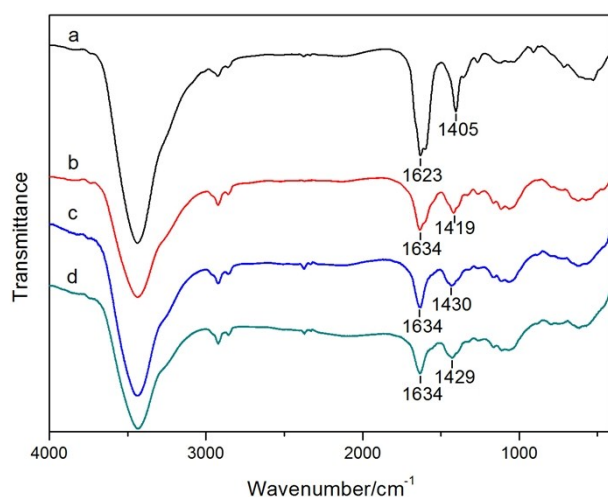


**Fig. S4** Time-course measurements of (A) UV-vis spectroscopy and (B)  $A_{650}/A_{528}$  ratio of NTA-AuNPs after the addition of Cr(III) ( $C_f = 4.0 \mu\text{M}$ ) at pH 3.6.





**Fig. S5** Time-course measurements of (A) UV-vis spectroscopy and (B)  $A_{650}/A_{528}$  ratio of NTA-AuNPs after the addition of Cr(VI) ( $C_f = 1.0 \mu\text{M}$ ) at pH 3.6.



**Fig. S6** The FT-IR spectra of (a) NTA, (b) NTA-AuNPs, (c) NTA-AuNPs with with Cr(III) ( $C_f = 5 \mu\text{M}$ ) and (d) Cr(VI) ( $C_f = 4 \mu\text{M}$ ) at pH 3.6.

#### Procedure for the sensitivity investigation of Cr(III) detection using NTA-AuNPs

1.5 mL NTA-AuNPs was mixed with 1.5 mL different concentrations of  $\text{CrCl}_3$  ( $C_i = 1 \mu\text{M}$ ,  $2 \mu\text{M}$ ,  $3 \mu\text{M}$ ,  $4 \mu\text{M}$ ,  $5 \mu\text{M}$ ,  $6 \mu\text{M}$ ,  $7 \mu\text{M}$ ,  $8 \mu\text{M}$ ,  $10 \mu\text{M}$ ,  $15 \mu\text{M}$ ) ( $C_f = C_i/2 \approx 0.5\text{--}7.5 \mu\text{M}$  for Cr(III)) respectively. Subsequently, 100  $\mu\text{L}$  HAc-NaAc buffer solution (0.2M, pH 3.6) was added to the mixture solution, which was incubated at room temperature for 3 min. And then the photographic images and UV-vis spectroscopy measurements were recorded. The value of  $\lg[(A_0 - A)/A_0]$  and the concentration of Cr(III) showed good linear relationship,  $y = -1.66122 + 0.36075x$ , over the range of  $0.5 \mu\text{M}$ – $3 \mu\text{M}$ , with the correlation coefficient of 0.99396.

#### Procedure for the sensitivity investigation of Cr(VI) detection using NTA-AuNPs

1.5 mL NTA-AuNPs was mixed with 1.5 mL different concentrations of potassium dichromate ( $C_i = 0.1 \mu\text{M}$ ,  $0.2 \mu\text{M}$ ,  $0.3 \mu\text{M}$ ,  $0.4 \mu\text{M}$ ,  $0.5 \mu\text{M}$ ,  $0.6 \mu\text{M}$ ,  $0.7 \mu\text{M}$ ,  $0.8 \mu\text{M}$ ,  $1 \mu\text{M}$ ,  $1.5 \mu\text{M}$ ,  $2 \mu\text{M}$ ) ( $C_f = C_i = 0.1\text{--}2 \mu\text{M}$  for Cr(VI)) respectively. Subsequently, 100  $\mu\text{L}$  HAc-NaAc buffer solution

(0.2M, pH 3.6) was added to the mixture solution, which was incubated at room temperature for 25 min. And then the photographic images and UV-vis spectroscopy measurements were recorded. The value of  $\lg(A_{650}/A_{528})$  and the concentration of Cr(VI) showed good linear relationship,  $y=-1.05607+1.19042X$ , over the range of 0.2  $\mu\text{M}$ -0.8  $\mu\text{M}$ , with the correlation coefficient of 0.99632.

### Procedure for the detection of real tap water samples using NTA-AuNPs

1) Cr(III) ( $C_i = 5 \mu\text{M}$ ) standard solution was prepared using tap water and divided into two groups. One group is brought to boiling for 20 min in the present of excess amount (10 fold of Cr(III)) of  $\text{K}_2\text{CO}_3$  and followed by re-adjusting of the sample volume after cooling, while the other is not treated. Then 1.5 mL NTA-AuNPs was mixed with 1.5 mL of the above two groups of Cr(III) ( $C_f = C_i/2 \approx 2.5 \mu\text{M}$ ) respectively. Subsequently, 100  $\mu\text{L}$  HAc-NaAc buffer solution (0.2M, pH 3.6) was added to the mixture solution, which was incubated at room temperature for 3 min. And then the UV-vis spectroscopy measurements were recorded. The value of  $\lg[(A_0-A)/A_0]$  was fitted into the above linear equation to calculate the concentration of Cr(III). The experiments were repeated for 3 times.

2) Potassium dichromate ( $C_i = 0.5 \mu\text{M}$ ) standard solution was prepared using tap water and divided into two groups. One group is brought to boiling for 20 min in the present of excess amount (10 fold of Cr(VI)) of  $\text{K}_2\text{CO}_3$  and followed by re-adjusting of the sample volume after cooling, while the other is not treated. Then 1.5 mL NTA-AuNPs was mixed with 1.5 mL of the above two groups of Cr(VI) ( $C_f = C_i/2 = 0.25 \mu\text{M}$ ) respectively. Subsequently, 100  $\mu\text{L}$  HAc-NaAc buffer solution (0.2M, pH 3.6) was added to the mixture solution, which was incubated at room temperature for 25 min. And then the UV-vis spectroscopy measurements were recorded. The value of  $\lg(A_{650}/A_{528})$  was fitted into the above linear equation to calculate the concentration of Cr(VI). The experiments were repeated for 3 times.

### The mechanism data

**Table S1** ICP-MS determination of the concentration of Cr and  $\text{Cu}^{2+}$  in the control group and experimental group.

Samples	Ions	Control group ( $\mu\text{M}$ )	Experimental group ( $\mu\text{M}$ )	Changed (%)
<b>1</b>	Cr(III)	0.882	0.793	-10.1
	$\text{Cu}^{2+}$	0.891	0.886	-0.6
<b>2</b>	Cr(VI)	1.099	0.988	-10.1
	$\text{Cu}^{2+}$	0.839	0.854	+1.8