Electronic Supplementary Material (ESI) for Nanoscale.

Electronic Supplementary Information for

Nanoclusters with Specific DNA-Overhangs: Modifying Configurability, Engineering Contrary Logic Pairs and Parity Generator/Checker for Error Detection

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Figures and tables:

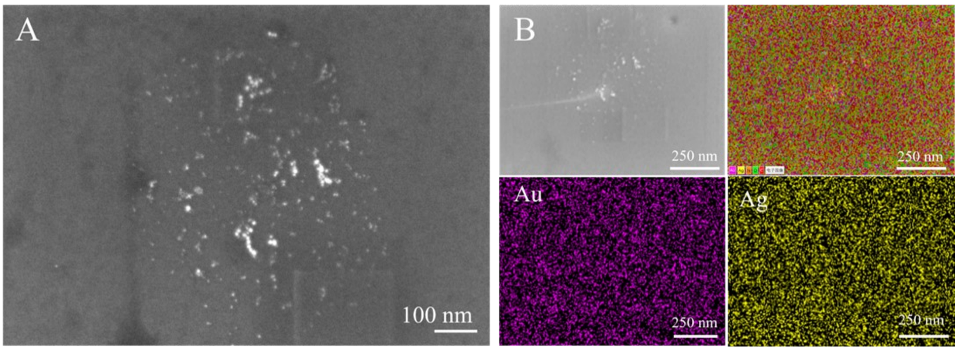


Fig. S1 (A) SEM image (scale: 100 nm)and (B) SEM-EDS elemental mapping images of Au and Ag in T-Au/Ag NCs (scale: 250 nm).

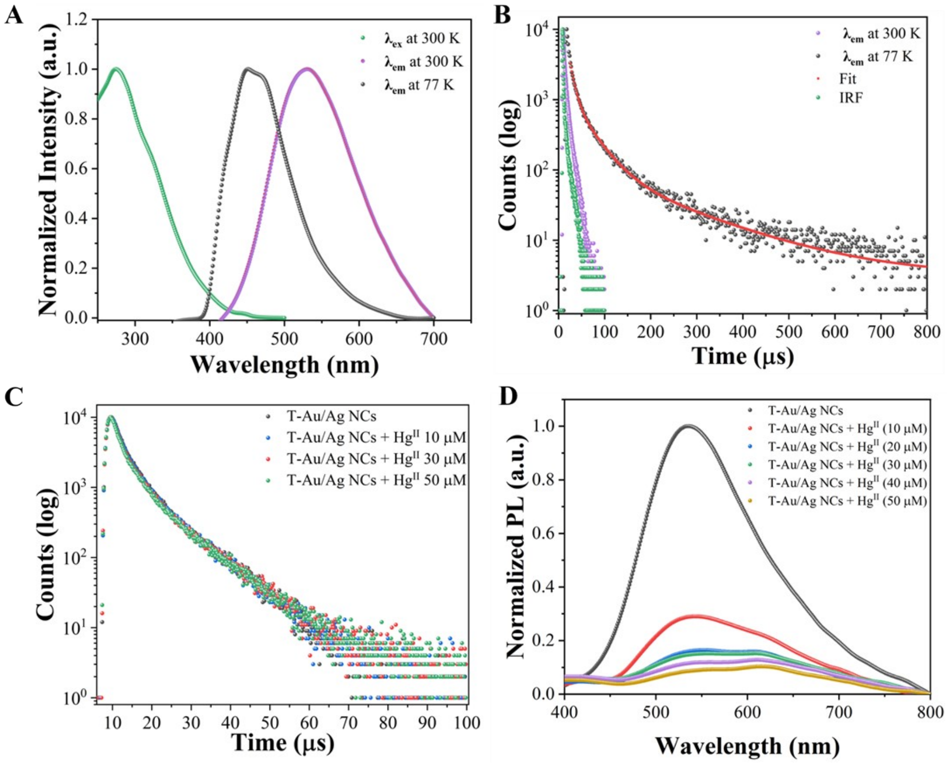


Fig. S2 (A) Temperature-dependent solid-state emission intensity of T-Au/Ag NCs at 300 K and 77 K upon excitation at 275 nm. (B) Temperature dependence of the excited-state lifetimes of T-Au/Ag NCs at 300 K and 77 K, IRF: instrument response function. (C) Lifetime decay plot of T-Au/Ag NCs and sequential addition of Hg^{II} in increasing concentration. (D) Difference in emission intensity of T-Au/Ag NCs upon addition Hg^{II} with increasing concentration (10 - 50 μM).

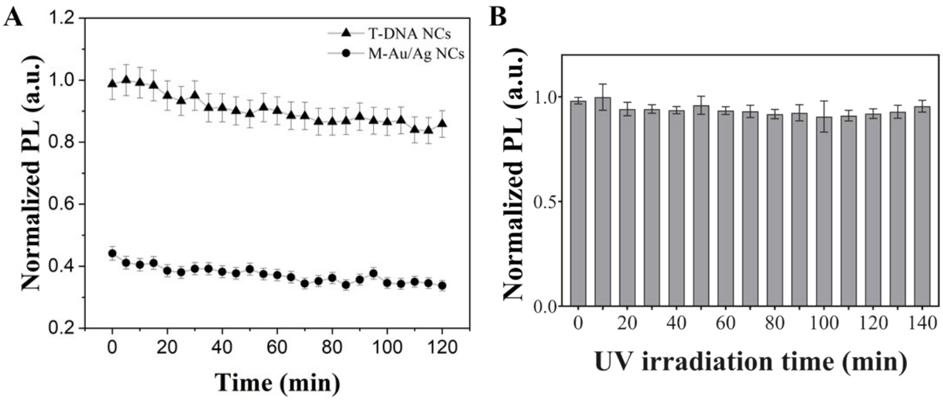


Fig. S3 (A) Time dependent emission spectra of T-Au/Ag NCs and M-Au/Ag NCs. (B) Time dependent normalized PL spectra of T-Au/Ag NCs under UV light (365 nm).

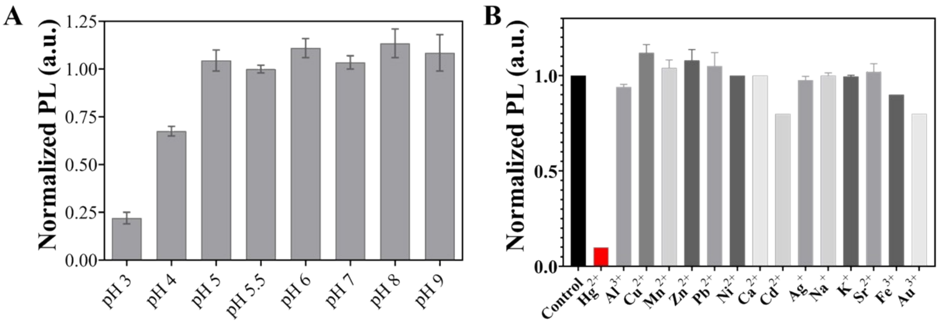


Fig. S4 (A) Normalized PL spectra of T-Au/Ag NCs under different pH windows. (B) Normalized PL spectra of T-Au/Ag NCs as control in the presence of different metal ions of 30 μM.

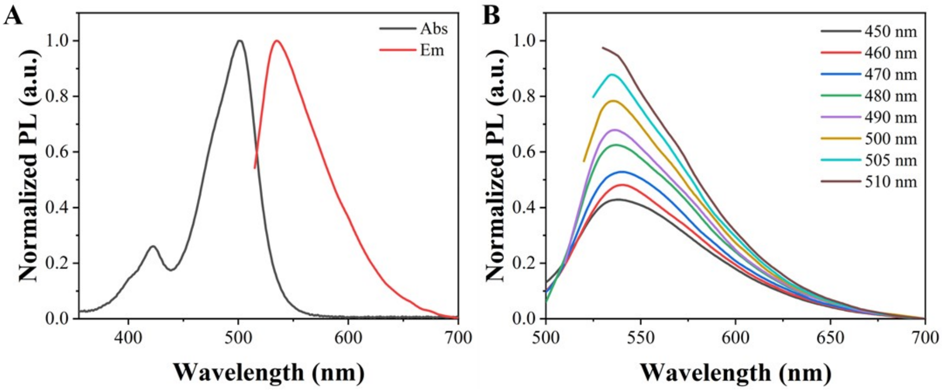


Fig. S5 (A) Absorption and emission of TO. (B) Different excitation measurement from 450 to 510 nm of blank TO.

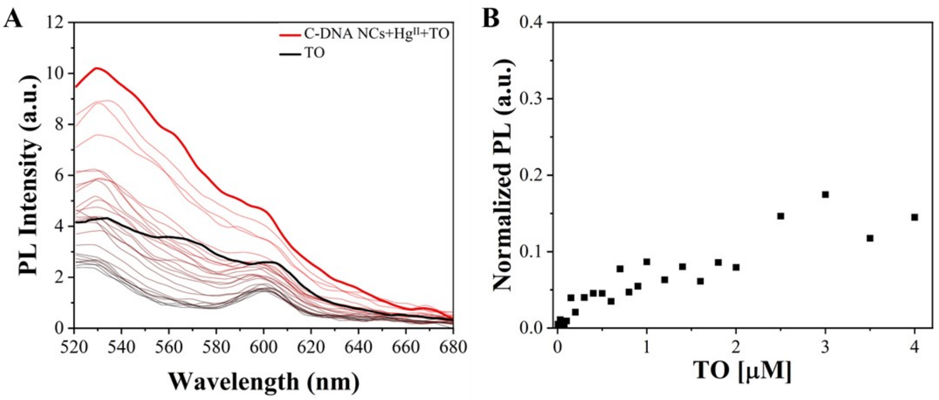


Fig. S6 (A) PL spectra and (B) normalized PL intensities of TO incorporated C-DNA NCs upon increasing the concentration.

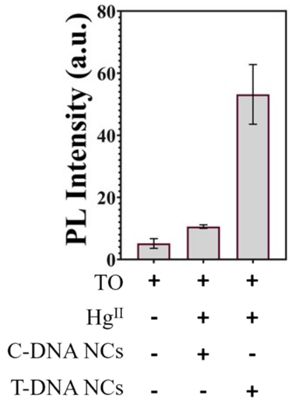


Fig. S7 Column representation PL intensity of TO incorporated C-DNA NCs and T-Au/Ag NCs in the presence of Hg^{II}.

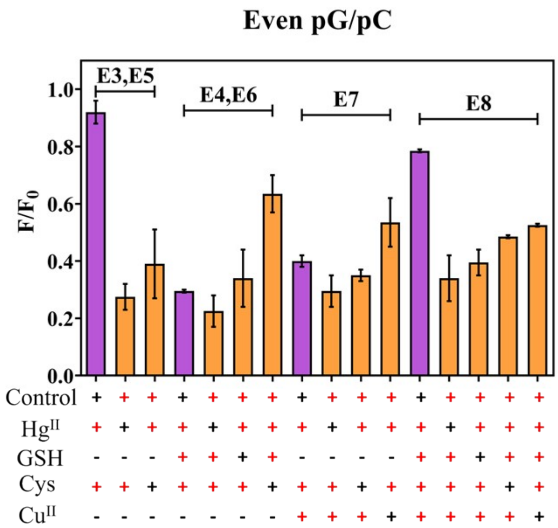


Fig. S8 The study of PL spectra in the order of addition in the preincubation of the M-Au/Ag NCs (when P = 1) with different analytes in different entries (E3, E4, E5, E6, E7, E8) for even pG/pC. The "+" (plus icon in red color) in Y-axis represents those which analytes are undergo for 10 min preincubation.

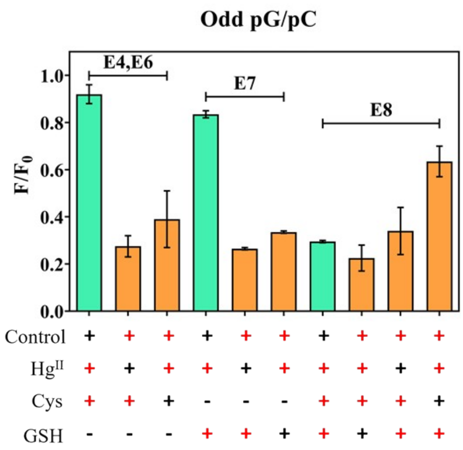


Fig. S9 The study of PL spectra in the order of addition in the preincubation of the DNA-Au/Ag NCs (when P = 1) with different analytes in different entries (E4, E6, E7, E8) for odd pG/pC. The "+" (plus icon in red color) in Y-axis represents those which analytes are undergo for 10 min preincubation.

Table S1. Truth tables of different types of CLPs, such as (A) YES^NOT, (B) OR^NOR and (C) INH^IMP.

A

Inputs	Outputs (YES^NOT)	
IN1	M-Au/Ag NCs	T-Au/Ag NCs
0	0	1
1	1	0

B

Inputs		Outputs (OR^NOR)	
IN1	IN2	M-Au/Ag NCs	T-Au/Ag NCs
0	0	0	1
0	1	1	0
1	0	1	0
1	1	1	0

C

Inputs		Outputs (INH^IMP)	
IN3	IN4	M-Au/Ag NCs	T-Au/Ag NCs
0	0	0	1
0	1	0	0
1	0	1	1
1	1	0	1

Table S2. Summary of phosphorescence decay profiles of T-Au/Ag NCs in Solid-state.

	$\lambda_{exc.}$ (nm)	$\lambda_{monitored}$ (nm)	t_1 (μs)	t_2 (μs)	t_3 (μs)	$\langle t_{avg.} \rangle$ (μs)
T-DNA NCs at 300 K	275	530	2.6 (40 %)	9.0 (59 %)	-	**6.3**
T-DNA NCs at 77 K	275	450	9.01 (29 %)	38.1 (47 %)	165.8 (23 %)	**58.6**

Table S3. Summary of phosphorescence decay of T-Au/Ag NCs and various Hg^{II} concentration in solution (citrate buffer).

	$\lambda_{exc.}$ (nm)	$\lambda_{collected}$ (nm)	t_1 (ms)	t_2 (ms)	$<t_{avg.}>$ (ms)
T-DNA NCs	320	535	2.5 (51 %)	9.0 (48 %)	5.6
T-DNA NCs +Hg^{II} (10 mM)	320	535	2.4 (44 %)	8.9 (55 %)	5.9
T-DNA NCs +Hg^{II} (20 mM)	320	535	2.6 (43 %)	9.4 (56 %)	6.2
T-DNA NCs +Hg^{II} (30 mM)	320	535	2.8 (42 %)	9.8 (57 %)	6.7
T-DNA NCs +Hg^{II} (40 mM)	320	535	2.9 (42 %)	9.9 (57 %)	6.8
T-DNA NCs +Hg^{II} (50 mM)	320	535	2.8 (39 %)	9.7 (60 %)	6.9

Table S4. Truth table of the 2-bit even/odd pG (D1' = Cys, D2' = GSH, [a] number of 1's in the D1'D2'P' string for even pG; D1" = Hg^{II}, D2" = Cys, [a] number of 1's in the D1"D2"P" string for odd pG)

Entry	Inputs		M-Au/Ag NCs (Even pG)		DNA-Au/Ag NCs (Odd pG)	
	D1	D2	Outputs(P')	∑ [a]	Outputs(P")	∑ [a]
1	0	0	0	0; even	1	1; odd
2	0	1	1	2; even	0	1; odd
3	1	0	1	2; even	0	1; odd
4	1	1	0	2; even	1	3; odd

Table S5. A molecular perspective representation of chemical structures illustrating all possible interactions leading to different outputs.

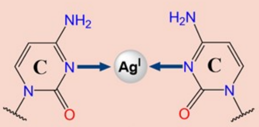
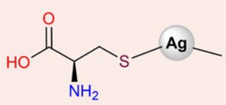
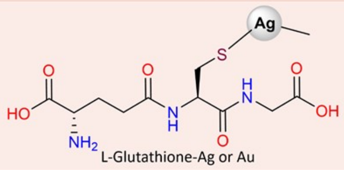
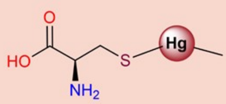
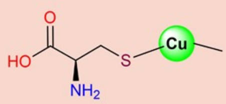
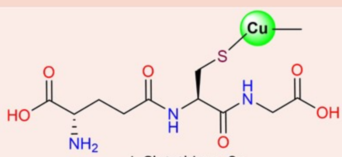
Molecular interaction	Operation	Molecular interaction	Operation
 Cytosine-Ag^{I}-Cytosine	Nanoclusters formation	 Thymine-Hg^{II}-Thymine	Nanoclusters ensemble formation, even pG (entry 1), odd pG (entry 3), odd pC (entry 5)
 L-Cysteine-Ag or Au	YES-NOT, OR-NOR, odd pG (entry 2)	 L-Glutathione-Ag or Au	Even pG (entry 2)
 L-Cysteine-Hg	YES-NOT, OR-NOR, even pG (entry 3, 4), even pC (entry 5, 6, 8), odd pG (entry 4), odd pC (6, 8)	 L-Cysteine-Cu	Even pC (entry 7, 8)
 L-Glutathione-Hg	OR-NOR, even pG (entry 4), even pC (entry 6, 8), odd pC (entry 7, 8)	 L-Glutathione-Cu	Even pC (entry 8)

Table S6. Comparison of the proposed method in error detection using DNA computing with the previously reported methods.

Platform	No. of DNA utilized in the study			Assay	Even/Odd	Ref
	Platform	Input entry	Total			
TP/NMM/TMB	1	3	4	Fluorescence, Colorimetric	Even	1
Polydopamine nanosphere	1	3	4	Fluorescence	Even	2
SH-DNA, MCH	1	3	4	Electrochemical	Even	3
H-AgNCs, IN2/Xaux	3	3	6	Fluorescence	Even/Odd	4
GCNNs, $Ru(phen)_3^{2+}$, GCE	4	3	7	ECL-RET	Even/Odd	5
H1, H2, H3, Exo III, MB, IN1/AX1	5	3	8	Electrochemical	Even/Odd	6
M-Au/Ag NCs, T-DNA NCs	**1**	**0**	**1**	**Photoluminescence**	**Even/Odd**	**Present work**

References

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