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Supporting Information For Binding to Gold Nanocluster Alters the Hydrogen Bonding Interactions and Electronic Properties of Canonical and Size-Expanded DNA Base Pairs

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Contents

List of Tables

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List of Figures

Details on the calculation of properties

Energetics

E_{int} is calculated by considering the base pair as one unit which is interacting with the gold cluster. We also calculate the deformation energy of the base pair ($E_{def}^{base\,pair}$) as well as the cluster ($E_{def}^{cluster}$). The deformation energy (E_{def}) is defined as:

$$E_{def}^{base\,pair} = E_{base\,pair}^{complex} - E_{base\,pair}^{isolated} \tag{1}$$

where, $E_{base\,pair}^{complex}$ is the single point energy of the base pair when it forms a complex with gold cluster and $E_{base\,pair}^{isolated}$ is the electronic ground state energy of the base pair when it is optimized in isolation. Similarly, we define the deformation corresponding to the gold cluster as:

$$E_{def}^{cluster} = E_{cluster}^{complex} - E_{cluster}^{isolated} \tag{2}$$

where, $E_{cluster}^{complex}$ is the single point energy of the cluster in the complexed state, whereas, $E_{cluster}^{isolated}$ is the energy of ground state optimized geometry of gold cluster.
The total deformation energy is given as:

$$E_{def} = E_{def}^{base\,pair} + E_{def}^{cluster} \tag{3}$$

The total interaction energy (E_{int}) of the complex is now calculated as:

$$E_{int} = E_{complex} - (E_{base\,pair}^{isolated} + E_{cluster}^{isolated}) + E_{def} \tag{4}$$

where, $E_{complex}$ is the total electronic energy of the ground state optimized complex.

Table S1: Geometrical features of base pairs complexed with Au_3. All the bond distances are in Å and bond angles in degrees.

System	Site	Anchor bond	Atoms involved	$r_{complex}$	r_{free}	Δr	$\angle_{complex}$	$\angle_{complex}$	$\Delta\angle$
AT	N3	2.12	A(N1)-T(N3)	2.83	2.87	0.04	179.12	178.26	-0.85
			A(N6)-T(O2)	2.89	2.85	-0.04	174.54	176.30	1.77
			A(C2)-T(O4)	3.62	3.65	0.03	132.24	129.80	-2.44
	N7	2.10	A(N1)-T(N3)	2.89	2.86	-0.03	179.12	178.27	-0.85
			A(N6)-T(O2)	2.83	2.88	0.05	174.54	176.58	2.04
			A(C2)-T(O4)	3.62	3.64	0.03	132.24	133.17	0.93
	O2(T)	2.22	A(N1)-T(N3)	2.89	2.79	-0.11	179.12	179.55	0.44
			A(N6)-T(O2)	2.83	2.90	0.07	174.54	173.02	-1.51
			A(C2)-T(O4)	3.52	3.62	0.10	132.24	132.19	-0.05
A-xT	N3	2.13	A(N1)-T(N3)	2.83	2.87	0.04	179.15	178.60	-0.55
			A(N6)-T(O2)	2.91	2.88	-0.03	174.16	175.85	1.69
			A(C2)-T(O4)	3.61	3.61	0.00	132.33	130.09	-2.24
	N7	2.10	A(N1)-T(N3)	2.83	2.86	0.02	179.15	178.57	-0.58
			A(N6)-T(O2	2.91	2.90	0.00	174.16	176.21	2.05
			A(C2)-T(O4)	3.61	3.62	0.01	132.33	133.59	1.26
	O2(T)	2.18	A(N1)-T(N3)	2.83	2.79	-0.04	179.15	179.54	0.39
		3.02 (NH-Au)	A(N6)-T(O2)	2.91	2.91	0.00	174.16	172.75	-1.41
			A(C2)-T(O4)	3.61	3.49	-0.12	132.33	132.15	-0.18
xA-T	N3	2.12	A(N1)-T(N3)	2.82	2.84	0.02	178.81	177.88	-0.94
			A(N6)-T(O2)	2.88	2.90	0.02	177.32	179.30	1.98
			A(C2)-T(O4)	3.63	3.68	0.05	132.32	130.25	-2.06
	N7	2.10	A(N1)-T(N3)	2.82	2.84	0.02	178.81	178.03	-0.79
			A(N6)-T(O2)	2.88	2.87	-0.01	177.32	177.54	0.22
			A(C2)-T(O4)	3.63	3.68	0.05	132.32	131.85	-0.46
	O2(T)	2.22	A(N1)-T(N3)	2.82	2.78	-0.04	178.81	179.03	0.22
			A(N6)-T(O2)	2.88	2.89	0.01	177.32	176.06	-1.26
			A(C2)-T(O4)	3.63	3.53	-0.10	132.32	132.22	-0.09
GC	N3	2.13	G(O6)-C(N4)	2.76	2.78	0.03	179.87	177.76	-2.11
			G(N1)-C(N3)	2.91	2.89	-0.02	177.72	177.01	-0.70
			G(N2)-C(O2)	2.89	2.82	-0.07	179.96	179.20	-0.76
	N7	2.11	G(O6)-C(N4)	2.76	2.79	0.03	179.87	177.81	-2.06
			G(N1)-C(N3)	2.91	2.89	-0.02	177.72	176.86	-0.85
			G(N2)-C(O2)	2.89	2.84	-0.04	179.96	178.84	-1.13
	O2(C)	2.21(NP)	G(O6)-C(N4)	2.76	2.72	-0.04	179.87	178.64	-1.23
			G(N1)-C(N3)	2.91	2.97	0.05	177.72	175.59	-2.13
			G(N2)-C(O2)	2.89	3.01	0.13	179.96	176.77	-3.19
G-xC	N7	2.11	G(O6)-C(N4)	2.74	2.78	0.04	178.46	179.75	1.29
			G(N1)-C(N3)	2.89	2.89	0.00	176.41	176.86	0.45
			G(N2)-C(O2)	2.88	2.83	-0.05	178.40	179.19	0.79
	N3	2.13	G(O6)-C(N4)	2.74	2.77	0.03	178.46	179.30	0.83
			G(N1)-C(N3)	2.89	2.89	0.00	176.41	176.65	0.24
			G(N2)-C(O2)	2.88	2.80	-0.08	178.40	179.46	1.06
	O2(C)	2.17	G(O6)-C(N4)	2.74	2.71	-0.03	178.46	177.10	-1.37
		3.90(Nh-Au)	G(N1)-C(N3)	2.89	2.97	0.08	176.41	175.16	-1.25
			G(N2)-C(O2)	2.88	2.98	0.10	178.40	175.78	-2.62
xG-C	N7	2.10	G(O6)-C(N4)	2.78	2.80	0.02	178.96	178.29	-0.67
			G(N1)-C(N3)	2.90	2.89	-0.01	176.18	176.73	0.55
			G(N2)-C(O2)	2.92	2.88	-0.04	176.96	178.69	1.73
	N3	2.12	G(O6)-C(N4)	2.78	2.81	0.02	178.96	177.43	-1.53
			G(N1)-C(N3)	2.90	2.88	-0.02	176.18	176.72	0.54
			G(N2)-C(O2)	2.92	2.84	-0.08	176.96	179.80	2.84
	O2(C)	2.21	G(O6)-C(N4)	2.78	2.75	-0.04	178.96	179.01	0.05
			G(N1)-C(N3)	2.90	2.96	0.06	176.18	175.02	-1.15
			G(N2)-C(O2)	2.92	3.04	0.12	176.96	174.79	-2.17

Table S2: Frequency analysis of base pairs complexed with Au_3. All frequency values are reported in cm^{-1} and I in atomic units.

System	Site	Atoms	ν_{free}	$\nu_{complex}$	$\Delta\nu$	I_{free}	$I_{complex}$	$I_{complex}/I_{free}$
AT	N3	N6-O4	3397.46	3333.99	-63.47	1326.50	1951.80	1.47
		N1-N3	2929.37	3128.87	199.50	2596.64	1871.08	0.72
		C2-O2	3190.43	3213.17	22.74	1.98	1.71	0.86
	N7	N6-O4	3397.46	3341.43	-56.03	1326.50	1380.58	1.04
		N1-N3	2929.37	3053.13	123.76	2596.64	2034.72	0.78
		C2-O2	3190.43	3191.13	0.70	1.98	1.89	0.95
	N1(T)	N6-O4	3397.46	3435.69	38.23	1326.50	1024.20	0.77
		N1-N3	2929.37	2696.23	-233.14	2596.64	3076.11	1.18
		C2-O2	3190.43	3194.34	3.91	1.98	2.55	1.29
A-xT	N3	N6-O4	3422.66	3353.87	-68.79	1403.71	2042.32	1.45
		N1-N3	2927.09	3107.50	180.41	3105.29	2348.47	0.76
		C2-O2	3191.64	3212.99	21.35	1.79	3.90	2.18
	N7	N6-O4	3422.66	3369.47	-53.19	1403.71	1115.22	0.79
		N1-N3	2927.09	3041.82	114.73	3105.29	2104.63	0.68
		C2-O2	3191.64	3179.88	-11.76	1.79	2.65	1.48
	N1(T)	N6-O4	3422.66	3447.64	24.98	1403.71	1219.98	0.87
		N1-N3	2927.09	2735.13	-191.96	3105.29	3876.22	1.25
		C2-O2	3191.64	3196.81	5.17	1.79	1.88	1.05
xA-T	N3	N6-O4	3368.71	3289.36	0.76	1702.99	2485.71	1.46
		N1-N3	2904.10	3066.76	137.72	3099.16	1950.27	0.63
		C2-O2	3178.18	3205.00	1.70	4.65	5.36	1.15
	N7	N6-O4	3368.71	3342.32	-26.39	1702.99	1562.94	0.92
		N1-N3	2904.10	2971.61	67.51	3099.16	2426.68	0.78
		C2-O2	3178.18	3166.06	-12.12	4.65	7.94	1.71
	N1(T)	N6-O4	3368.71	3405.91	37.20	1702.99	1373.15	0.81
		N1-N3	2904.10	2661.46	-242.64	3099.16	3818.49	1.23
		C2-O2	3178.18	3181.36	3.18	4.65	6.84	1.47
GC	N3	N2-O2	3394.38	3287.59	-106.79	1539.67	2857.16	1.86
		N1-N3	3200.93	3091.83	-109.10	2139.15	962.99	0.45
		O6-N4	3111.15	3224.36	113.21	898.40	1098.91	1.22
	N7	N2-O2	3394.38	3342.78	-51.60	1539.67	1790.12	1.16
		N1-N3	3200.93	3090.02	-110.91	2139.15	896.23	0.42
		O6-N4	3111.15	3242.82	131.67	898.40	1473.53	1.64
	O2(C)	N2-O2	3394.38	3517.54	123.16	1539.67	740.27	0.48
		N1-N3	3200.93	3293.00	92.07	2139.15	1311.48	0.61
		O6-N4	3111.15	3027.76	-83.39	898.40	1885.75	2.10
G-xC	N3	N2-O2	3382.60	3266.57	-116.03	1791.57	3503.82	1.96
		N1-N3	3192.51	3085.90	-106.61	2056.45	956.16	0.46
		O6-N4	3068.32	3187.77	119.45	1488.18	1805.37	1.21
	N7	N2-O2	3382.60	3315.46	-67.14	1791.57	2593.60	1.45
		N1-N3	3192.51	3095.97	-96.54	2056.45	852.51	0.41
		O6-N4	3068.32	3199.80	131.48	1488.18	2351.03	1.58
	O2(C)	N2-O2	3382.60	3516.43	133.83	1791.57	1014.47	0.57
		N1-N3	3192.51	3279.04	86.53	2056.45	1708.14	0.83
		O6-N4	3068.32	3004.41	-63.91	1488.18	2515.94	1.69
xG-C	N3	N2-O2	3425.42	3319.12	-106.30	1476.91	2730.79	1.85
		N1-N3	3200.93	3087.64	-113.29	3504.92	1302.11	0.37
		O6-N4	3200.93	3258.60	57.67	3504.92	1266.59	0.36
	N7	N2-O2	3425.42	3394.11	-31.31	1476.91	1614.26	1.09
		N1-N3	3200.93	3111.61	-89.32	3504.92	1028.73	0.29
		O6-N4	3200.93	3242.58	41.65	3504.92	1957.57	0.56
	O2(C)	N2-O2	3425.42	3533.11	107.69	1476.91	770.10	0.52
		N1-N3	3200.93	3286.79	85.86	3504.92	1758.95	0.50
		O6-N4	3200.93	3084.21	-116.72	3504.92	1886.87	0.54

NBO and AIM calculations

Energies of second order stabilization, $E^{(2)}$, resulting from transfer of electron cloud from donor NBO(i) to acceptor NBO(j), which is a consequence of interactions between filled Lewis and empty non-Lewis orbitals, are obtained using the equation:

$$E^{(2)} = q_i \left[\frac{(F(i,j))^2}{E_j - E_i} \right] \tag{5}$$

where q_i is donor orbital occupancy, E_i and E_j are energies of the orbitals i, j respectively, and F(i,j) is the off diagonal NBO Fock matrix element. In AIM analysis, the nature of interaction is studied in terms of properties of electron density and its derivatives. The term $\nabla^2\rho(\mathrm{r})$ is related to bond interaction energy. A positive value represents a depletion of electronic charge density along the bond, a case of ionic interaction. A negative value indicates a charge density concentrated at the center of the inter nuclear region, a case of covalent interaction. The electronic energy density (H(r)) at the bond critical point (BCP) is given as:

$$H(\mathbf{r}) = G(\mathbf{r}) + V(\mathbf{r}) \tag{6}$$

where G(r) represents the kinetic energy density and V(r) the potential energy density. The negative H(r) indicates a stabilization effect due to accumulation of charge at $\mathbf{r}$, as in case of covalent interactions.

Table S3 (a): Natural charge analysis of AT and their derivatives complexed with Au_3.

System	Site		q_{free}	$q_{complex}$
AT	N3	A-N1	-0.286	-0.606
		A-N3	-0.992	-0.615
		A-N6	-0.797	-0.754
		A-N7	-0.779	-1.061
		T-N3	-0.663	-0.648
		T-O2	-0.651	-0.641
		TO4	-0.669	-0.673
	N7	A-N1	-0.286	-1.246
		A-N3	-0.992	-1.416
		A-N6	-0.797	-1.595
		A-N7	-0.779	-0.56
		T-N3	-0.663	-0.661
		T-O2	-0.651	-0.651
		TO4	-0.669	-0.662
	O2(T)	A-N1	-0.286	-0.625
		A-N3	-0.992	-0.532
		A-N6	-0.797	-0.766
		A-N7	-0.779	-0.502
		T-N3	-0.663	-0.636
		T-O2	-0.651	-0.712
		TO4	-0.669	-0.65
A-xT	N3	A-N1	-0.64	-0.627
		A-N3	-0.873	-0.65
		A-N6	-0.778	-0.754
		A-N7	-0.688	-1.837
		T-N3	-0.182	-0.652
		T-O2	-1.098	-0.641
		TO4	-1.731	-0.674
	N7	A-N1	-0.64	-0.583
		A-N3	-0.873	-0.504
		A-N6	-0.778	-1.557
		A-N7	-0.688	-0.536
		T-N3	-0.182	-1.066
		T-O2	-1.098	-0.626
		TO4	-1.731	-1.516
	O2(T)	A-N1	-0.64	-0.642
		A-N3	-0.873	-0.549
		A-N6	-0.778	-0.833
		A-N7	-0.688	-0.753
		T-N3	-0.182	-0.74
		T-O2	-1.098	-0.691
		TO4	-1.731	0.8
XA-T	N3	A-N1	-0.632	-0.741
		A-N3	-0.552	-0.713
		A-N6	-0.772	-0.894
		A-N7	-0.496	-0.576
		T-N3	-0.659	-0.789
		T-O2	-0.646	-0.755
		TO4	-0.672	-0.776
	N7	A-N1	-0.632	-0.627
		A-N3	-0.552	-0.775
		A-N6	-0.772	-0.751
		A-N7	-0.496	-0.557
		T-N3	-0.659	-0.654
		T-O2	-0.646	-0.646
		TO4	-0.672	-0.667
	O2(T)	A-N1	-0.632	-0.637
		A-N3	-0.552	-0.514
		A-N6	-0.772	-0.768
		A-N7	-0.496	-0.495
		T-N3	-0.659	-0.636
		T-O2	-0.646	-0.71
		TO4	-0.672	-0.653

Table S3 (b): Natural charge analysis of GC and their derivatives complexed with Au_3.

System	Site		q_{free}	$q_{complex}$
G-C	N3	G-N1	0.27	-0.695
		G-N2	-0.803	-0.776
		G-N3	-0.641	-0.663
		G-O6	-0.714	-1.416
		G-N7	-0.754	-1.193
		C-O2	-0.698	-0.695
		C-N3	-0.661	-0.662
		C-N4	-0.751	-0.75
	N7	G-N1	0.27	-0.697
		G-N2	-0.803	-0.77
		G-N3	-0.641	-0.575
		G-O6	-0.714	-0.957
		G-N7	-0.754	-0.53
		C-O2	-0.698	-0.671
		C-N3	-0.661	-0.632
		C-N4	-0.751	-0.73
	O2(C)	G-N1	0.27	-0.653
		G-N2	-0.803	-0.789
		G-N3	-0.641	-0.613
		G-O6	-0.714	-0.699
		G-N7	-0.754	-0.719
		C-O2	-0.698	-0.755
		C-N3	-0.661	-0.626
		C-N4	-0.751	-0.736
G-xC	N3	G-N1	-0.652	-0.719
		G-N2	-0.79	-0.774
		G-N3	-0.627	-0.645
		G-O6	-0.708	0.574
		G-N7	-0.753	-0.455
		C-O2	-0.695	-0.703
		C-N3	-0.658	0.277
		C-N4	-0.743	-0.813
	N7	G-N1	-0.652	-0.632
		G-N2	-0.79	-0.77
		G-N3	-0.627	-0.569
		G-O6	-0.708	-0.629
		G-N7	-0.753	-0.518
		C-O2	-0.695	-0.669
		C-N3	-0.658	-0.705
		C-N4	-0.743	-0.753
	O2(C)	G-N1	-0.652	-0.657
		G-N2	-0.79	-0.796
		G-N3	-0.627	-0.62
		G-O6	-0.708	-0.766
		G-N7	-0.753	-0.734
		C-O2	-0.695	-1.014
		C-N3	-0.658	-0.933
		C-N4	-0.743	-0.726
XG-C	N3	G-N1	0.269	-0.629
		G-N2	-0.81	-0.775
		G-N3	-0.607	-0.633
		G-O6	0.097	-0.676
		G-N7	-0.488	-0.817
		C-O2	-0.694	-0.692
		C-N3	-0.662	-0.661
		C-N4	-0.785	-0.748
	N7	G-N1	0.269	-0.664
		G-N2	-0.81	-0.803
		G-N3	-0.607	-1.414
		G-O6	0.097	-0.743
		G-N7	-0.488	-0.545
		C-O2	-0.694	-0.665
		C-N3	-0.662	-0.632
		C-N4	-0.785	-0.745
	O2(C)	G-N1	0.269	
		G-N2	-0.81	
		G-N3	-0.607	
		G-O6	0.097	
		G-N7	-0.488	
		C-O2	-0.694	
		C-N3	-0.662	
		C-N4	-0.785	

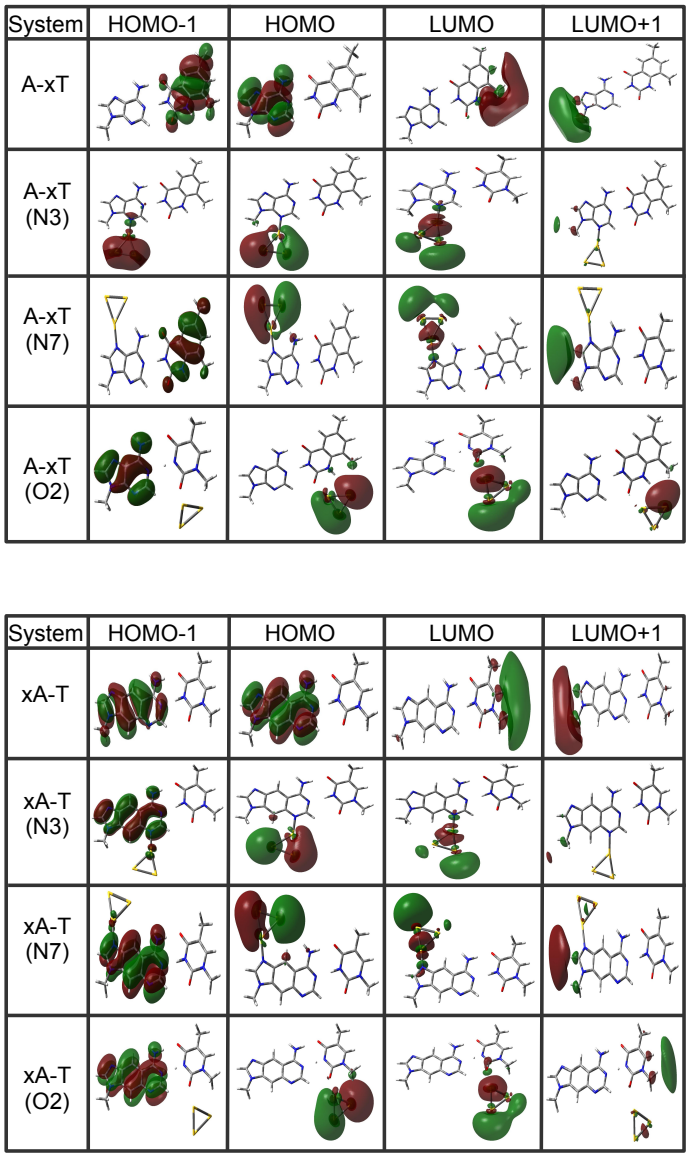

Figure S1: The distribution of the HOMO-1, HOMO, LUMO and LUMO+1 levels of the complexed and uncomplexed AT base pairs calculated at UHF level of theory using 6-31+G(2d,2p)∪SDD basis set.

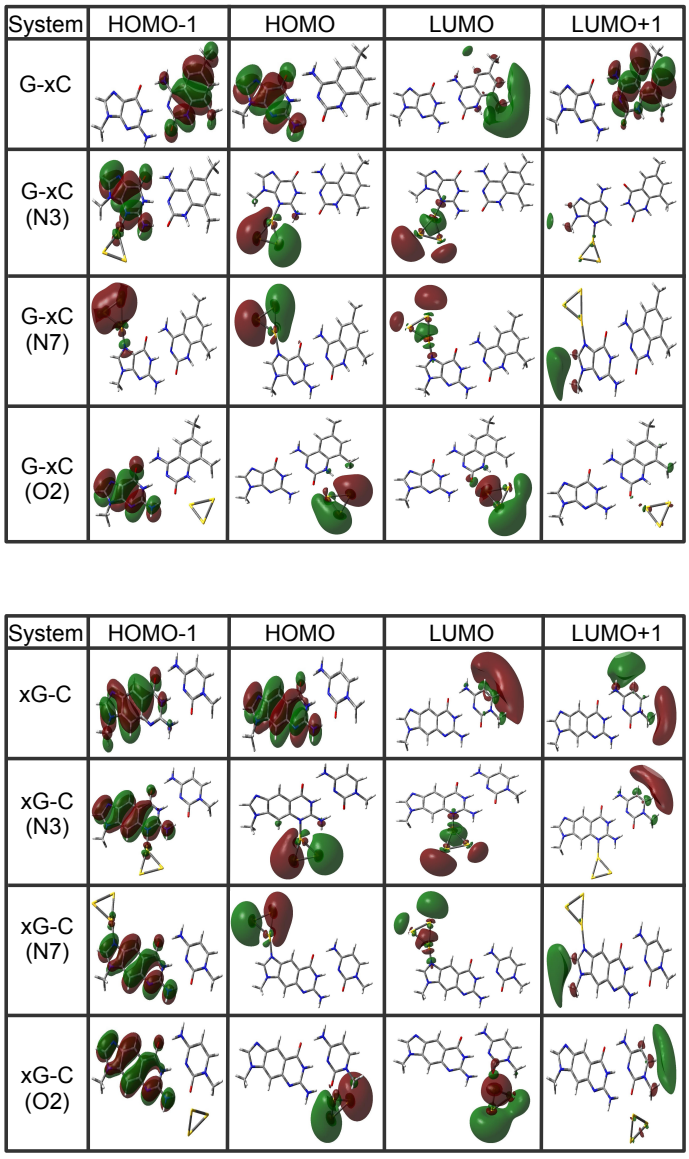

Figure S2: The distribution of the HOMO-1, HOMO, LUMO and LUMO+1 levels of the complexed and uncomplexed GC base pairs calculated at UHF level of theory using 6-31+G(2d,2p)∪SDD basis set.

Table S4: Electric properties of base pairs complexed with Au_3.

System	Site	μ	β	ω
AT	N3	7.96	423.98	3.51
	N7	7.13	447.38	3.66
	O2(T)	4.98	381.34	5.04
A-xT	N3	9.16	541.30	3.65
	N7	6.16	488.76	3.63
	O2(T)	4.71	451.17	4.76
xA-T	N3	7.72	495.05	4.65
	N7	5.92	550.97	4.50
	O2(T)	5.48	491.54	4.95
GC	N3	8.66	430.34	3.68
	N7	13.67	452.67	3.43
	O2(C)	5.24	403.16	5.24
G-xC	N3	10.28	565.08	4.38
	N7	12.34	531.70	4.80
	O2(C)	4.30	489.49	4.82
xG-C	N3	9.00	481.39	3.31
	N7	12.75	579.48	3.40
	O2(C)	5.26	523.55	5.17

Table S5 (a): Second order perturbation energy analysis of AT and their derivatives complexed with Au_3.

System	site of int	Donor	Acceptor	E(2)	$\Delta q_{cluster}$
AT	isolated	n_{N1} A	$\sigma*_{N3-H}$ T	19.57	
		n_{O4} T	$\sigma*_{N6-H}$ A	9.83	
		n_{O2} T	$\sigma*_{C2-H}$ A	0.37	
	N3	n_{N1} A	$\sigma*_{N3-H}$ T	16.24	-0.57912
		n_{O4} T	$\sigma*_{N6-H}$ A		
		n_{O2} T	$\sigma*_{C2-H}$ A	12.53	
		n_{N3} A	n_{Au1}	40.62	
		n_{Au1} A	$\sigma*_{N3-C4}$ A	31.3	
	N7	n_{N1} A	$\sigma*_{N3-H}$ T	17.06	-0.56701
		n_{O4} T	$\sigma*_{N6-H}$ A	4.75	
		n_{O2} T	$\sigma*_{C2-H}$ A	0.4	
		n_{N7} A	$\sigma*_{Au1-Au2}$	8.85	
		n_{Au1} A	$\sigma*_{N7-C5}$ A	1.42	
		n_{Au3} A	$\sigma*_{N6-H}$ A	1.89	
	O2(T)	n_{N1} A	$\sigma*_{N3-H}$ T	24.54	-0.53779
		n_{O4} T	$\sigma*_{N6-H}$ A	9.41	
		n_{O2} T	$\sigma*_{C2-H}$ A	0.32	
		n_{O2} T	$\sigma*_{Au1-Au2}$	6.26	
		n_{Au1} A	$\sigma*_{C2-O2}$	0.13	
A-xT	isolated	n_{N1} A	$\sigma*_{N3-H}$ T	15.96	
		n_{O4} T	$\sigma*_{N6-H}$ A	8.69	
		n_{O2} T	$\sigma*_{C2-H}$ A	0.44	
	N3	n_{N1} A	$\sigma*_{N3-H}$ T	15.84	-0.58021
		n_{O4} T	$\sigma*_{N6-H}$ A	4.96	
		n_{O2} T	$\sigma*_{C2-H}$ A	0.31	
		n_{N3}	$\sigma*_{Au1-Au2}$	37.27	
		n_{Au1}	$\sigma*_{C2-N3}$ A	7.04	
	N7	n_{N1} A	$\sigma*_{N3-H}$ T	17.44	-0.56475
		n_{O4} T	$\sigma*_{N6-H}$ A		
		n_{O2} T	$\sigma*_{C2-H}$ A	0.62	
		n_{N7} A	$\sigma*_{Au1-Au2}$	39.87	
		n_{Au1}	$\sigma*_{C2-N3}$ A	2.4	
	O2(T)	n_{N1} A	$\sigma*_{N3-H}$ T	28.99	-0.53804
		n_{O4} T	$\sigma*_{N6-H}$ A	0.67	
		n_{O2} T	$\sigma*_{C2-H}$ A	0.38	
		n_{O2} T	$\sigma*_{Au1-Au2}$	4.71	
		n_{Au1}	$\sigma*_{C1-O2}$	0.25	
		n_{Au3} A	$\sigma*_{N1-H}$ A	19.08	
xA-T	isolated	n_{N1} A	$\sigma*_{N3-H}$ T	20.07	
		n_{O4} T	$\sigma*_{N6-H}$ A	10.5	
		n_{O2} T	$\sigma*_{C2-H}$ A	0.22	
	N3	n_{N1} A	$\sigma*_{N3-H}$ T	16.85	-0.56903
		n_{O4} T	$\sigma*_{N6-H}$ A	12.43	
		n_{O2} T	$\sigma*_{C2-H}$ A	0.27	
		n_{N3}	$\sigma*_{Au1-Au2}$	13.26	
		n_{Au1}	$\sigma*_{N3-C4}$	2.44	
		n_{Au3}	$\sigma*_{C(benz)-H}$	2.05	
	N7	n_{N1} A	$\sigma*_{N3-H}$ T	18.22	-0.56335
		n_{O4} T	$\sigma*_{N6-H}$ A	11.39	
		n_{O2} T	$\sigma*_{C2-H}$ A	0.33	
		n_{N7} A	$\sigma*_{Au1-Au2}$	36.96	
		n_{Au1}	$\sigma*_{N7-C8}$	4.13	
		n_{Au3}	$\sigma*_{C(benz)-H}$	3.25	
	O2(T)	n_{N1} A	$\sigma*_{N3-H}$ T	25.03	0.45844
		n_{O4} T	$\sigma*_{N6-H}$ A	10.18	
		n_{O2} T	$\sigma*_{C2-H}$ A	0.3	
		n_{O2}	$\sigma*_{Au1-Au2}$	6.15	
		n_{Au1}	$\sigma*_{C2-O2}$	0.13	

Table S5 (b): Second order perturbation energy analysis of GC and their derivatives complexed with Au_3.

System	site of int	Donor	Acceptor	E(2)	$\Delta q_{cluster}$
GC	isolated	n_{N3} C	$\sigma*_{N1-H}$ G	13.89	
		n_{O2} C	$\sigma*_{N2-H}$ G	10.36	
		n_{O6} G	$\sigma*_{N4-H}$ C	18.11	
	N3	n_{N3} C	$\sigma*_{N1-H}$ G	14.21	-0.57788
		n_{O2} C	$\sigma*_{N2-H}$ G	10.27	
		n_{O6} G	$\sigma*_{N4-H}$ C	13.45	
		n_{N3}	$\sigma*_{Au1-Au2}$	33.12	
		n_{Au1}	$\sigma*_{N3-C4}$	4.37	
		n_{Au3}	$\sigma*_{N2-H}$	2.19	
	N7	n_{N3} C	$\sigma*_{N1-H}$ G	15.63	-0.57581
		n_{O2} C	$\sigma*_{N2-H}$ G	12.35	
		n_{O6} G	$\sigma*_{N4-H}$ C	15.02	
		n_{N7} A	$\sigma*_{Au1-Au2}$		
		n_{Au1} A	$\sigma*_{N7-C5}$ A		
		n_{Au3} A	$\sigma*_{N6-H}$ A		
	O2(C)	n_{N3} C	$\sigma*_{N1-H}$ G	12.54	-0.54227
		n_{O2} C	$\sigma*_{N2-H}$ G	4.6	
		n_{O6} G	$\sigma*_{N4-H}$ C	21.06	
		n_{O2}	$\sigma*_{Au1-Au2}$	8.58	
		n_{Au1}	$\sigma*_{C2-O2}$	0.14	
G-xC	isolated	n_{N3} C	$\sigma*_{N1-H}$ G	22.71	
		n_{O2} C	$\sigma*_{N2-H}$ G	6.07	
		n_{O6} G	$\sigma*_{N4-H}$ C	19.97	
	N3	n_{N3} C	$\sigma*_{N1-H}$ G	14.27	-0.57819
		n_{O2} C	$\sigma*_{N2-H}$ G	10.08	
		n_{O6} G	$\sigma*_{N4-H}$ C	16.31	
		n_{Au1}	$\sigma*_{N3-C4}$	35.41	
		n_{Au3}	$\sigma*_{N2-H}$	6.04	
	N7	n_{N3} C	$\sigma*_{N1-H}$ G	15.83	-0.57593
		n_{O2} C	$\sigma*_{N2-H}$ G	3.49	
		n_{O6} G	$\sigma*_{N4-H}$ C	3.09	
		n_{N7} A	$\sigma*_{Au1-Au2}$	12.51	
		n_{Au1}	$\sigma*_{N7-C8}$	3.18	
	O2(C)	n_{N3} C	$\sigma*_{N1-H}$ G	30.25	-0.54517
		n_{O2} C	$\sigma*_{N2-H}$ G	11.88	
		n_{O6} G	$\sigma*_{N4-H}$ C	14.44	
		n_{O2}	$\sigma*_{Au1-Au2}$	35.92	
		n_{Au1}	$\sigma*_{C2-O2}$	0.23	
XG-C	isolated	n_{N3} C	$\sigma*_{N1-H}$ G	14.52	
		n_{O2} C	$\sigma*_{N2-H}$ G	8.88	
		n_{O6} G	$\sigma*_{N4-H}$ C	15.96	
	N3	n_{N3} C	$\sigma*_{N1-H}$ G	16.19	-0.57867
		n_{O2} C	$\sigma*_{N2-H}$ G	12.76	
		n_{O6} G	$\sigma*_{N4-H}$ C	32.72	
		n_{N3}	$\sigma*_{Au1-Au2}$	23.63	
		n_{Au1}	$\sigma*_{N3-C4}$	1.73	
	N7	n_{N3} C	$\sigma*_{N1-H}$ G	15.51	-0.57612
		n_{O2} C	$\sigma*_{N2-H}$ G	10.67	
		n_{O6} G	$\sigma*_{N4-H}$ C	18.04	
		n_{N7} A	$\sigma*_{Au1-Au2}$	48.55	
		n_{Au1}	$\sigma*_{N7-C8}$	3.2	
	O2(C)	n_{N3} C	$\sigma*_{N1-H}$ G	11.64	
		n_{O2} C	$\sigma*_{N2-H}$ G	4.17	
		n_{O6} G	$\sigma*_{N4-H}$ C	19.23	
		n_{O2}	$\sigma*_{Au1-Au2}$	4.26	
		n_{Au1}	$\sigma*_{C2-O2}$	0.2	

Table S6 (a): AIM analysis of AT and their derivatives complexed with Au_3.

System	Site	Atoms	$\Delta^2\rho$	G(r)	V(r)	H
AT	isolated	A(N1)-T(N3)	0.0868	0.0283	-0.035	-6.65E-3
		A(N6)-T(O2)	0.0926	0.0228	-0.0225	3.27E-4
		A(C2)-T(O4)	0.0164	0.00345	-0.00279	6.60E-4
	N3	Au-N3	0.372	0.123	-0.153	-3.01E-2
		A(N1)-T(N3)	0.109	0.0298	-0.0324	-2.64E-3
		A(N6)-T(O2)	0.118	0.0288	-0.028	7.20E-4
		A(C2)-T(O4)	0.0141	0.00285	-0.00217	6.74E-4
	N7	Au-N7	0.388	0.13	-0.163	-3.32E-2
		A(N1)-T(N3)	0.0867	0.0265	-0.0314	-4.86E-3
		A(N6)-T(O2)	0.0946	0.0236	-0.0236	2.26E-5
		A(C2)-T(O4)	0.0158	0.0033	-0.00264	6.53E-4
	O2(T)	Au-O2	0.327	0.0891	-0.0965	-7.42E-3
		A(N1)-T(N3)	0.0845	0.0315	-0.0419	-1.04E-2
		A(N6)-T(O2)	0.0921	0.0224	-0.0219	5.75E-4
		A(C2)-T(O4)	0.0206	0.00441	-0.00369	7.28E-4
A-xT	isolated	A(N1)-T(N3)	0.0865	0.0283	-0.035	-6.69E-3
		A(N6)-T(O2)	0.0898	0.0219	-0.0213	5.77E-4
		A(C2)-T(O4)	0.0166	0.00348	-0.00282	6.63E-4
	N3	Au-N3	0.366	0.121	-0.15	-2.93E-2
		A(N1)-T(N3)	0.0868	0.026	-0.0302	-4.26E-3
		A(N6)-T(O2)	0.0945	0.0236	-0.0236	1.29E-5
		A(C2)-T(O4)	0.0146	0.00301	-0.00235	6.52E-4
	N7	Au-N7	0.409	0.131	-0.159	-2.85E-2
		A(N1)-T(N3)	0.117	0.0333	-0.0372	-3.94E-3
		A(N6)-T(O2	0.111	0.0264	-0.0251	1.37E-3
		A(C2)-T(O4)	0.0177	0.00365	-0.00287	7.81E-4
	O2(T)	Au-O2	0.37	0.104	-0.114	-1.10E-2
		A(N1)-T(N3)	0.085	0.0311	-0.0411	-9.91E-3
		A(N6)-T(O2)	0.0895	0.0216	-0.0209	7.43E-4
		A(C2)-T(O4)	0.0209	0.0045	-0.00376	7.35E-4
xA-T		A(N1)-T(N3)	0.0869	0.0288	-0.036	-7.12E-3
		A(N6)-T(O2)	0.0946	0.0236	-0.0236	6.53E-6
		A(C2)-T(O4)	0.0162	0.00339	-0.00274	6.51E-4
	N3	Au-N3	0.364	0.121	-0.151	-3.02E-2
		A(N1)-T(N3)	0.087	0.0265	-0.0312	-4.72E-3
		A(N6)-T(O2)	0.102	0.0263	-0.0272	-8.61E-4
		A(C2)-T(O4)	0.014	0.00287	-0.00223	6.38E-4
		Au44-CH	0.0489	0.0109	-0.00952	1.35E-3
	N7	Au-N7	0.39	0.13	-0.163	-3.29E-2
		A(N1)-T(N3)	0.0867	0.0275	-0.0333	-5.82E-3
		A(N6)-T(O2)	0.0974	0.0246	-0.0248	-2.39E-4
		A(C2)-T(O4)	0.0147	0.00304	-0.00241	6.33E-4
		Au44-CH	0.0169	0.0039	-0.00358	3.22E-4
	O2(T)	Au-O2	0.325	0.0886	-0.096	-7.38E-3
		A(N1)-T(N3)	0.084	0.0321	-0.0432	-1.11E-2
		A(N6)-T(O2)	0.0943	0.0233	-0.0231	2.36E-4
		A(C2)-T(O4)	0.0202	0.00435	-0.00364	7.11E-4

Table S6 (b): AIM analysis of GC and their derivatives complexed with Au_3.

System	Site	Atoms	$\Delta^2\rho$	G(r)	V(r)	H
GC	isolated	G(O6)-C(N4)	0.119	0.0328	-0.0359	-3.13E-3
		G(N1)-C(N3)	0.0825	0.0232	-0.0258	-2.58E-3
		G(N2)-C(O2)	0.0941	0.0234	-0.0232	1.65E-4
	N3	Au-N3	0.358	0.119	-0.149	-2.98E-2
		G(O6)-C(N4)	0.114	0.0303	-0.0321	-1.80E-3
		G(N1)-C(N3)	0.0831	0.0243	-0.0279	-3.55E-3
		G(N2)-C(O2)	0.107	0.0279	-0.0291	-1.15E-3
	N7	Au-N7	0.405	0.128	-0.155	-2.69E-2
		G(O6)-C(N4)	0.141	0.0361	-0.037	-9.48E-4
		G(N1)-C(N3)	0.112	0.0305	-0.0329	-2.38E-3
		G(N2)-C(O2)	0.127	0.0313	-0.0309	3.69E-4
	O2(C)	Au-O2	0.331	0.0911	-0.0995	-8.40E-3
		G(O6)-C(N4)	0.126	0.0363	-0.041	-4.69E-3
		G(N1)-C(N3)	0.0771	0.0203	-0.0213	-1.01E-3
		G(N2)-C(O2)	0.075	0.0173	-0.0159	1.42E-3
G-xC	isolated	G(O6)-C(N4)	0.122	0.0343	-0.0381	-3.86E-3
		G(N1)-C(N3)	0.0828	0.0234	-0.026	-2.67E-3
		G(N2)-C(O2)	0.0952	0.0236	-0.0235	1.66E-4
	N3	Au-N3	0.358	0.119	-0.149	-2.98E-2
		G(O6)-C(N4)	0.117	0.0315	-0.0339	-2.38E-3
		G(N1)-C(N3)	0.0832	0.0244	-0.0281	-3.63E-3
		G(N2)-C(O2)	0.109	0.0288	-0.0302	-1.41E-3
	N7	Au-N7	0.385	0.128	-0.159	-3.15E-2
		G(O6)-C(N4)	0.115	0.031	-0.0333	-2.25E-3
		G(N1)-C(N3)	0.0838	0.0246	-0.0283	-3.67E-3
		G(N2)-C(O2)	0.105	0.027	-0.0278	-7.95E-4
	O2(C)	Au-O2	0.38	0.107	-0.119	-1.22E-2
		G(O6)-C(N4)	0.128	0.0372	-0.0424	-5.22E-3
		G(N1)-C(N3)	0.0767	0.0203	-0.0213	-1.07E-3
		G(N2)-C(O2)	0.0797	0.0185	-0.0172	1.39E-3
xG-C	isolated	G(O6)-C(N4)	0.113	0.0306	-0.0329	-2.34E-3
		G(N1)-C(N3)	0.0837	0.0239	-0.0268	-2.94E-3
		G(N2)-C(O2)	0.0881	0.0213	-0.0207	6.80E-4
	N3	Au-N3	0.355	0.119	-0.15	-3.07E-2
		G(O6)-C(N4)	0.109	0.0286	-0.0299	-1.32E-3
		G(N1)-C(N3)	0.084	0.0249	-0.0288	-3.88E-3
		G(N2)-C(O2)	0.103	0.0264	-0.0271	-6.71E-4
	N7	Au-N7	0.409	0.131	-0.159	-2.84E-2
		G(O6)-C(N4)	0.137	0.0351	-0.0359	-8.55E-4
		G(N1)-C(N3)	0.113	0.0307	-0.033	-2.35E-3
		G(N2)-C(O2)	0.117	0.028	-0.0269	1.11E-3
	O2(C)	Au-O2	0.329	0.0906	-0.099	-8.35E-3
		G(O6)-C(N4)	0.12	0.0338	-0.0375	-3.69E-3
		G(N1)-C(N3)	0.0785	0.0209	-0.0221	-1.24E-3
		G(N2)-C(O2)	0.07	0.016	-0.0144	1.52E-3