Electronic Supplementary Material (ESI) for Nanoscale Advances.


# *Electronic Supplementary Information*

*Optical, structural, and biological properties of silver nanoclusters formed within the loop of C-12 hairpin sequence.*

Akhilesh Kumar Gupta[1], Nolan Marshall[1], Liam Yourston[1], Lewis Rolband[2], Damian Beasock[2], Leyla Danai[2], Elizabeth Skelly[2], Kirill A. Afonin[2], and Alexey V. Krasnoslobodtsev[1*]

[1] Department of Physics, University of Nebraska at Omaha, Omaha, NE 68182, USA.
[2] Nanoscale Science Program, Department of Chemistry, University of North Carolina at Charlotte, Charlotte, NC 28223, USA.
* Correspondence: akrasnos@unomaha.edu; Tel.: +1-402-554-3723.

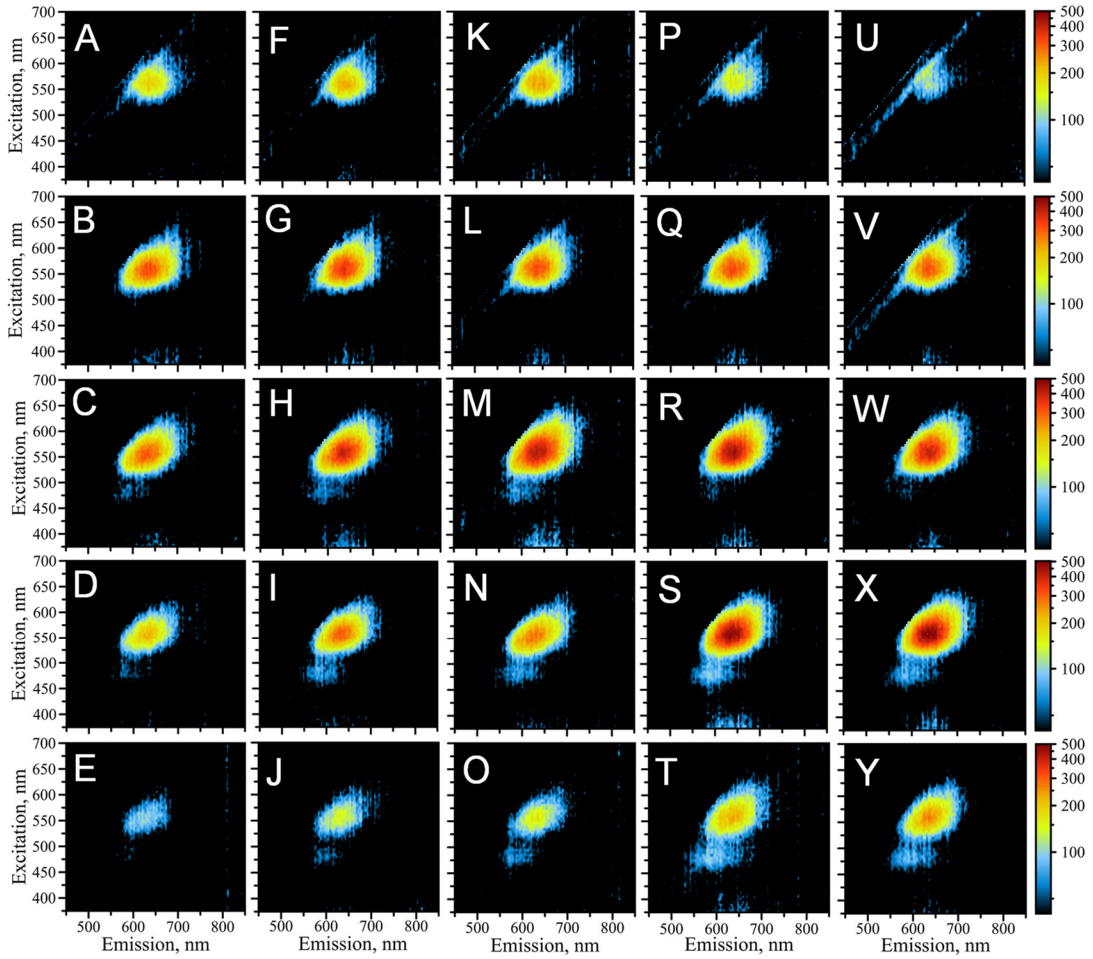


**Figure S1.** EEM patterns of AgNC@hpC$_{12}$ obtained during optimization of AgNC synthesis conditions. Concentrations of $AgNO_3$ and DNA were varied for $AgNO_3$ from 80 μM to 160 μM and for DNA from 2 μM to 40 μM. **(A)** $C_{AgNO3}$= 80 μM and $C_{DNA}$= 2 μM, **(B)** $C_{AgNO3}$= 80 μM and $C_{DNA}$= 5 μM, **(C)** $C_{AgNO3}$= 80 μM and $C_{DNA}$= 10 μM, **(D)** $C_{AgNO3}$= 80 μM and $C_{DNA}$= 20 μM, **(E)** $C_{AgNO3}$= 80 μM and $C_{DNA}$= 40 μM, **(F)** $C_{AgNO3}$= 100 μM and $C_{DNA}$= 2 μM, **(G)** $C_{AgNO3}$= 100 μM and $C_{DNA}$= 5 μM, **(H)** $C_{AgNO3}$= 100 μM and $C_{DNA}$= 10 μM, **(I)** $C_{AgNO3}$= 100 μM and $C_{DNA}$= 20 μM, **(J)** $C_{AgNO3}$= 100 μM and $C_{DNA}$= 40 μM, **(K)** $C_{AgNO3}$= 120 μM and $C_{DNA}$= 2 μM, **(L)** $C_{AgNO3}$= 120 μM and $C_{DNA}$= 5 μM, **(M)** $C_{AgNO3}$= 120 μM and $C_{DNA}$= 10 μM, **(N)** $C_{AgNO3}$= 120 μM and $C_{DNA}$= 20 μM, **(O)** $C_{AgNO3}$= 120 μM and $C_{DNA}$= 40 μM, **(P)** $C_{AgNO3}$= 140 μM and $C_{DNA}$= 2 μM, **(Q)** $C_{AgNO3}$= 140 μM and $C_{DNA}$= 5 μM, **(R)** $C_{AgNO3}$= 140 μM and $C_{DNA}$= 10 μM, **(S)** $C_{AgNO3}$= 140 μM and $C_{DNA}$= 20 μM, **(T)** $C_{AgNO3}$= 140 μM and $C_{DNA}$= 40 μM, **(U)** $C_{AgNO3}$= 160 μM and $C_{DNA}$= 2 μM, **(V)** $C_{AgNO3}$= 160 μM and $C_{DNA}$= 5 μM, **(W)** $C_{AgNO3}$= 160 μM and $C_{DNA}$= 10 μM, **(X)** $C_{AgNO3}$= 160 μM and $C_{DNA}$= 20 μM, **(Y)** $C_{AgNO3}$= 160 μM and $C_{DNA}$= 40 μM. The intensity of the "red" fluorescence reaches maximum for ratios $C_{AgNO3}$ / $C_{DNA}$ between 10 and 12. We therefore used the following combination in this study: $C_{AgNO3}$= 120 μM and $C_{DNA}$= 10 μM.

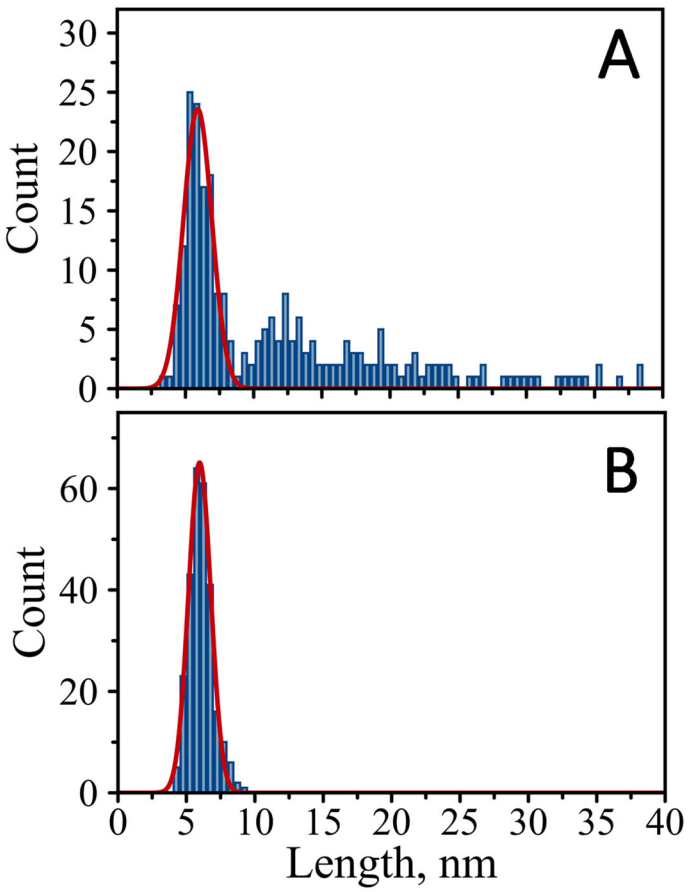


**Figure S2.** Results of AFM image analysis presented in **Figure 1**. **(A)** Statistical distribution of sizes for AgNC@ssC$_{12}$, D, measured along the longest axis of observed structures. Fitting the histogram with Gaussian function produces $D_{AV}$=5.9±0.2 nm for the most intense peak. Bigger structures are also evident as indicated by the peaks at greater length. **(B)** Statistical distribution of sizes for AgNC@hpC$_{12}$ producing only one peak at $D_{AV}$=6.0±0.2 nm. The real size of the AgNC is expected to be less than 6 nm due to convolution effect of the AFM tip.

***Cytosine-rich hairpin-loop DNA templates:*** The single C->T replacement results in change of the fluorescence pattern in EEM but it also reduces the number of templating cytosines in the 12-base long loop. Previously, our group[1] and others[2] have reported that various sizes of $hpC_N$ loops generate AgNCs@$hpC_N$ with distinct fluorescence patterns. Thus, we looked at how the reduction of the loop size by 1, 2, and 3 cytosines affects the cluster's properties. Figure 4 shows excitation-emission plots (EEM) for AgNCs templated on hairpins with $C_9$, $C_{10}$, $C_{11}$, and $C_{12}$ loop sizes. The EEM maps were recorded in the 350-700 nm range for the excitation and in the 400-800 nm range for the emission. The EEMs show various patterns of multiple-peaked fluorescence with up to 3 distinct peaks per sample in different parts of the visible spectrum. These observations are in a good agreement with previously published data on hpDNA templates.{O'Neill, 2009 #153} We classify the observed peaks as red I (RI), red II (RII), orange (O), and green (G) with the following positions of lambda maximum: RI=> $\lambda_{EXC}/\lambda_{EM}$=565/640 nm, RII=> $\lambda_{EXC}/\lambda_{EM}$=550/625 nm, O=> $\lambda_{EXC}/\lambda_{EM}$=480/600 nm, and G=> $\lambda_{EXC}/\lambda_{EM}$=405/525 nm. These peaks are similar to the ones observed in T-scanning. The peaks are quite reproducible but present with different intensities for various loop sizes. For example, "orange" is quite strong for $hpC_9$ and $hpC_{11}$ and is present only faintly for $hpC_{10}$. Red peak is RII for smaller loop sizes $hpC_9$, $hpC_{10}$, and $hpC_{11}$ but red-shifts to RI for $hpC_{12}$. Interestingly, the excitation-emission pattern of $hpC_{11}$ loop (Fig. S1, D) where the size of the loop is one less cytosine resembles the pattern observed for T1, T2, T3, and T9 replacements, further substantiating our hypothesis that these positions are critical for nanocluster's stability and optical properties.

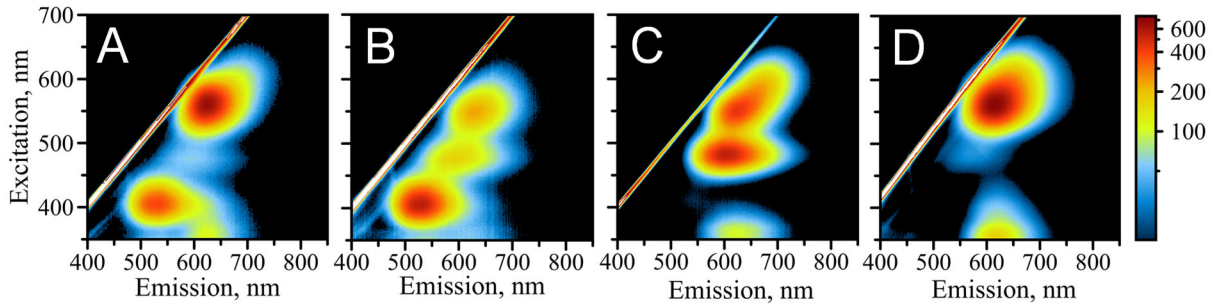


**Figure S3.** EEM patterns of AgNCs@hpDNA for the following hairpin loop sizes: **(A)** $C_9$, **(B)** $C_{10}$, **(C)** $C_{11}$, and **(D)** $C_{12}$.

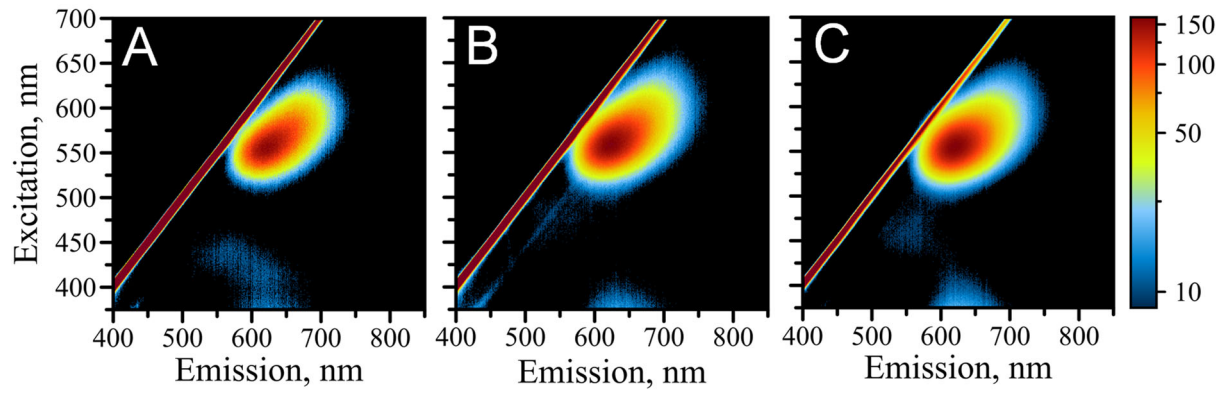


**Figure S4.** EEM patterns of AgNCs@hpC$_{12}$ with the following stem sequences of the hairpin lool structure: **(A)** TAAGACG - C$_{12}$ - CGTCTTA, **(B)** TAAGGCA - C$_{12}$ - TGCCTTA, and **(C)** A$_6$A$_{12}$.

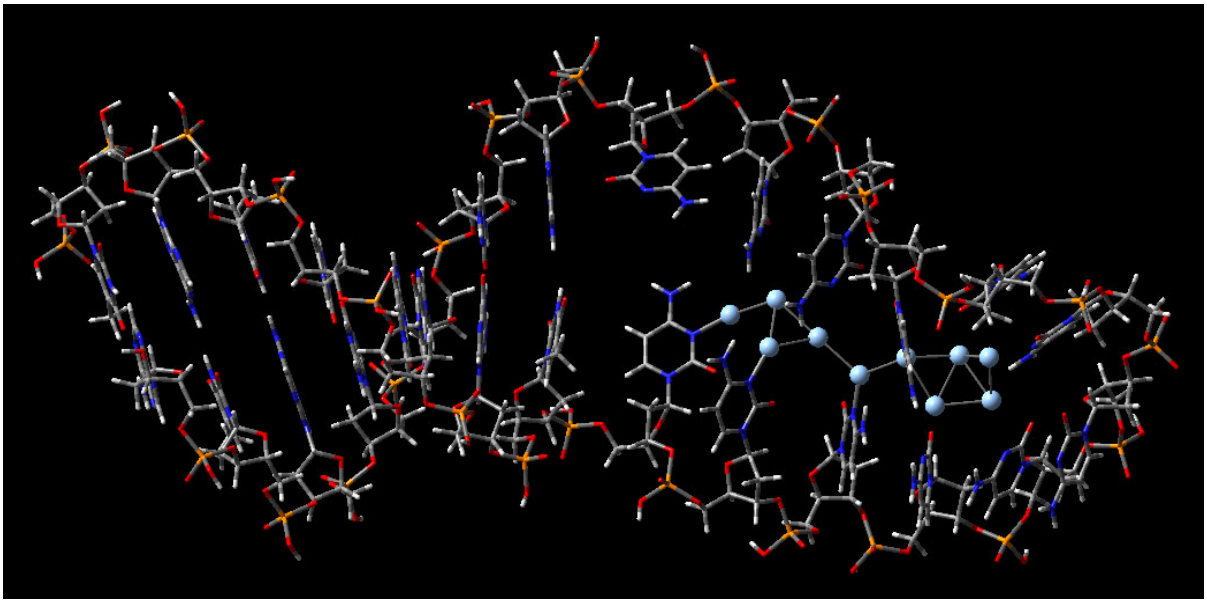

**Figure S5.** Full final optimized structure of Ag$_{10}$NC@hpC$_{12}$.

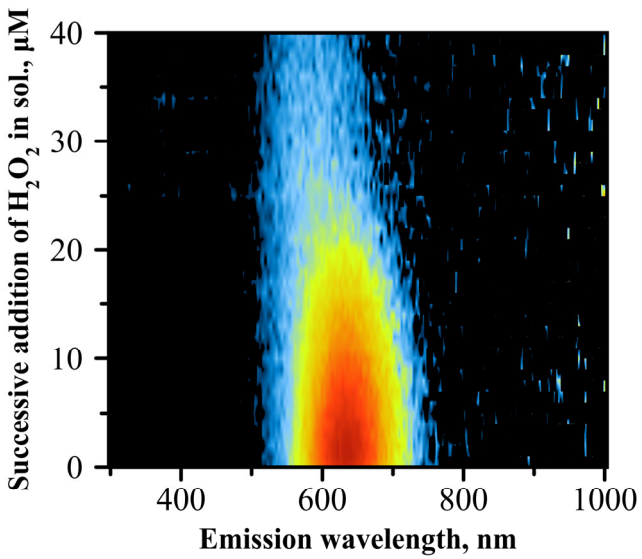


**Figure S6.** The evolution of emission spectrum for AgNC@hpC$_{12}$ in response to successive addition of oxidizing agent, $H_2O_2$.

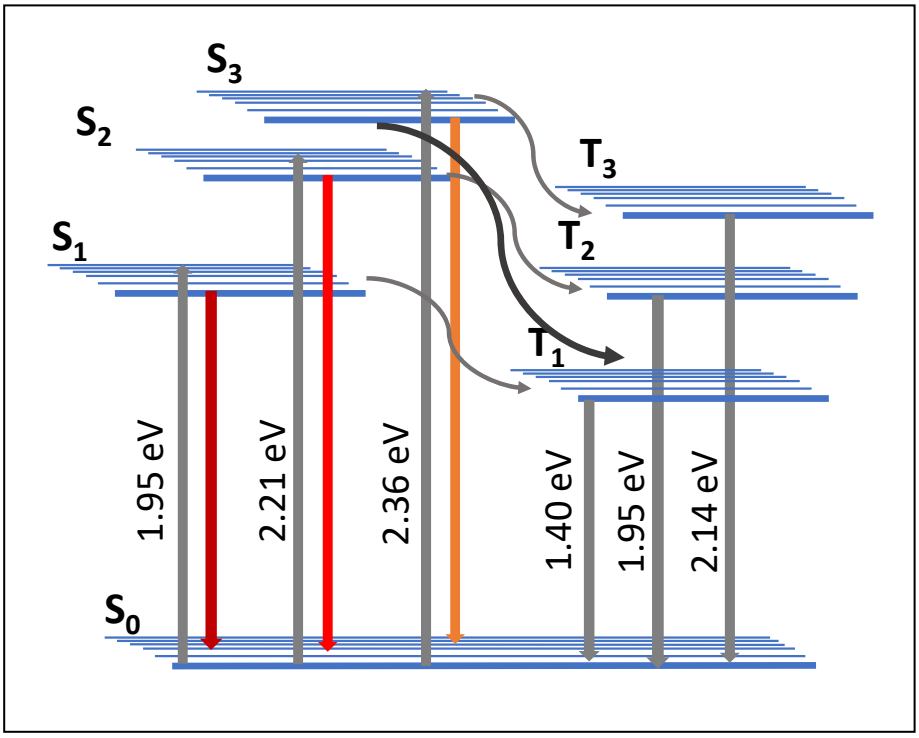


**Figure S7.** Schematic representation of energy levels for 3 singlet and 3 triplet excited states of Ag$_{10}$NC@hpC$_{12}$ computed using TD-DFT analysis. The transition *$S_3$ to *$T_1$ is depicted with a bold arrow.

**Table S1**. List of the atomic percentage of the silicon substrate, phosphorous, and silver detected during the SEM-EDS scans. Based on the known number of phosphorus atoms for the sequence of $hpC_{12}$, the number of silver atoms is calculated using the ratio of signal intensity between phosphorus and silver.

| Exp # | P % | Ag % | P/Ag | # of P | # of Ag |
|---|---|---|---|---|---|
| **1** | 4.45 | 1.71 | 2.60 | 25 | 9.61 |
| **2** | 5.62 | 2.72 | 2.07 | 25 | 12.07 |
| **3** | 4.85 | 2.46 | 1.97 | 25 | 12.69 |
| **4** | 5.63 | 2.92 | 1.93 | 25 | 12.95 |
| **5** | 3.85 | 1.55 | 2.48 | 25 | 10.08 |
| **6** | 3.59 | 1.25 | 2.87 | 25 | 8.71 |
| **7** | 4.54 | 2.27 | 2.00 | 25 | 12.50 |
| **8** | 4.39 | 1.40 | 3.14 | 25 | 7.96 |
| **9** | 4.24 | 1.52 | 2.79 | 25 | 8.96 |
| **10** | 3.52 | 1.48 | 2.38 | 25 | 10.50 |
| **11** | 3.94 | 0.96 | 4.10 | 25 | 6.09 |
| **12** | 4.55 | 2.00 | 2.28 | 25 | 10.96 |
| **13** | 4.63 | 1.92 | 2.41 | 25 | 10.37 |
| **Average** | **4.45** | **1.86** | **2.54** | **25** | **10.26** |
| **STDEV** | **0.66** | **0.59** | **0.60** | **0** | **2.06** |
| **SEM** | **0.18** | **0.16** | **0.17** | **0** | **0.57** |

**Table S2.** Calculated optical transitions for the $Ag_{10}NC@hpC_{12}$ nanoclusters of +2 charge using different Density Functionals and different basis sets.

| **DFT Level of Theory** | | **Peak I (red I)** | | **Peak II (red II)** | | **Peak III (orange)** | |
|---|---|---|---|---|---|---|---|
| Exchange Density Functional | Basis Set | Position, eV | Oscillator strength, f | Position, eV | Oscillator strength, f | Position, eV | Oscillator strength, f |
| B3lYP | LANL2DZ | 1.77 | 0.1537 | 2.11 | 0.0199 | 2.15 | 0.0669 |
| B3PW91 | LANL2DZ | 1.81 | 0.1485 | 2.21 | 0.0311 | 2.26 | 0.0628 |
| M06-2X | LANL2DZ | 1.95 | 0.1494 | 2.19 | 0.0088 | 2.40 | 0.2589 |
| M06-2X | LANL2MB | 1.83 | 0.4319 | 2.00 | 0.0866 | 2.29 | 0.1140 |
| M06-2X | def2TZVPP | 1.91 | 0.4195 | 2.22 | 0.1059 | 2.34 | 0.0469 |
| M06-2X | def2QZVPP | 1.90 | 0.4180 | 2.22 | 0.1164 | 2.33 | 0.0356 |

**Table S3.** Calculated optical transitions for the charged $Ag_{10}NC@hpC_{12}$ nanoclusters using TD-DFT and M06-2X/LANL2DZ combination of functional/basis set.

| | **Peak I (red I)** | | **Peak II (red II)** | | **Peak III (orange)** | |
|---|---|---|---|---|---|---|
| Total Charge | Position, eV | Oscillator strength, f | Position, eV | Oscillator strength, f | Position, eV | Oscillator strength, f |
| 0 | 1.97 | 0.6571 | 2.17 | 0.2351 | - | - |
| +2 | 1.95 | 0.4184 | 2.19 | 0.0710 | 2.36 | 0.0932 |
| +4 | 2.00 | 0.1494 | 2.20 | 0.0088 | 2.40 | 0.2589 |
| +6 | 2.04 | 0.1514 | 2.20 | 0.0068 | 2.40 | 0.2865 |
| +8 | 2.04 | 0.0805 | 2.27 | 0.0396 | 2.44 | 0.2806 |
| +10 | - | - | 2.22 | 0.0317 | 2.65 | 0.1220 |

***Additional computational details:*** Multiple runs using Universal Force Field (UFF) at molecular mechanics level of theory to achieve energy minimum with a convergence factor for energy change tolerance of $10E^{-7}$. Further optimization was achieved via a single geometry optimization run with DFT utilizing M06-2X/LANL2DZ combination of functional/basis set. The DFT optimization was done for $Ag_{10}$ cluster only, while DNA template was frozen (using 0 and -1 input for respective atoms in Gaussian16). The optimization result and the input list of atoms for Gaussian16 are given below. TD-DFT computation only used Ag atoms and atoms of cytosine bases, while sugar-phosphate backbone and stem of the hairpin were completely removed to save computational time.

***Atomic list of geometrically optimized $Ag_{10}$NC@hp$C_{12}$ as Gaussian input for TD-DFT calculations of excited states:***

| | | | | | |
|---|---|---|---|---|---|
| C-C_3 | 0 | 7.93025 | 6.85446 | 0.55102 | L |
| N-N_R | 0 | 8.47293 | 5.86544 | -0.4084 | L |
| C-C_R | 0 | 7.71476 | 4.77839 | -0.80998 | L |
| O-O_R | 0 | 6.58273 | 4.6134 | -0.38945 | L |
| N-N_R | 0 | 8.22792 | 3.85909 | -1.68479 | L |
| C-C_R | 0 | 9.48195 | 3.98223 | -2.18495 | L |
| N-N_R | 0 | 9.98258 | 3.01173 | -3.08378 | L |
| C-C_R | 0 | 10.26405 | 5.07481 | -1.80694 | L |
| C-C_R | 0 | 9.73683 | 6.0106 | -0.91468 | L |
| H-H_ | 0 | 10.35427 | 6.85216 | -0.63155 | L |
| H-H_ | 0 | 11.26722 | 5.20027 | -2.19477 | L |
| C-C_3 | 0 | 3.37542 | 6.81936 | 2.13613 | L |
| N-N_R | 0 | 4.20687 | 5.64082 | 2.47942 | L |
| C-C_R | 0 | 4.12974 | 4.47778 | 1.73193 | L |
| O-O_R | 0 | 3.37427 | 4.3925 | 0.77853 | L |
| N-N_R | 0 | 4.91281 | 3.39954 | 2.04569 | L |
| C-C_R | 0 | 5.77663 | 3.42903 | 3.0893 | L |
| N-N_R | 0 | 6.57234 | 2.29673 | 3.38157 | L |
| C-C_R | 0 | 5.87321 | 4.58529 | 3.86078 | L |
| C-C_R | 0 | 5.07763 | 5.68371 | 3.53521 | L |
| H-H_ | 0 | 5.16756 | 6.56803 | 4.14478 | L |

| | | | | | |
|---|---|---|---|---|---|
| H-H_ | 0 | 6.55548 | 4.63899 | 4.69993 | L |
| H-H_ | 0 | 6.4982 | 1.4462 | 2.80496 | L |
| H-H_ | 0 | 7.2347 | 2.30652 | 4.17107 | L |
| C-C_3 | 0 | -0.48106 | 6.67387 | -1.8469 | L |
| N-N_R | 0 | -0.67539 | 5.70075 | -0.74176 | L |
| C-C_R | 0 | -0.31639 | 4.36993 | -0.90799 | L |
| O-O_R | 0 | 0.12407 | 3.96599 | -1.9708 | L |
| N-N_R | 0 | -0.4499 | 3.48213 | 0.12618 | L |
| C-C_R | 0 | -0.92341 | 3.87261 | 1.33447 | L |
| N-N_R | 0 | -1.03839 | 2.93206 | 2.38438 | L |
| C-C_R | 0 | -1.29513 | 5.19946 | 1.52848 | L |
| C-C_R | 0 | -1.16568 | 6.09876 | 0.4736 | L |
| H-H_ | 0 | -1.43739 | 7.12104 | 0.66314 | L |
| H-H_ | 0 | -1.67338 | 5.53668 | 2.48539 | L |
| H-H_ | 0 | -0.75728 | 1.95229 | 2.23702 | L |
| H-H_ | 0 | -1.40021 | 3.212 | 3.30774 | L |
| C-C_3 | 0 | -5.5566 | 6.11149 | -3.31389 | L |
| N-N_R | 0 | -5.30295 | 5.71859 | -1.90138 | L |
| C-C_R | 0 | -4.70296 | 4.49856 | -1.60945 | L |
| O-O_R | 0 | -4.39668 | 3.71994 | -2.49614 | L |
| N-N_R | 0 | -4.44722 | 4.14728 | -0.32304 | L |
| C-C_R | 0 | -4.75596 | 4.96346 | 0.71253 | L |
| N-N_R | 0 | -4.46597 | 4.56143 | 2.03679 | L |
| C-C_R | 0 | -5.35138 | 6.19417 | 0.45807 | L |
| C-C_R | 0 | -5.61705 | 6.5534 | -0.86121 | L |
| H-H_ | 0 | -6.05408 | 7.5194 | -1.02251 | L |
| H-H_ | 0 | -5.60123 | 6.86925 | 1.26697 | L |
| H-H_ | 0 | -4.0269 | 3.64694 | 2.21633 | L |

| | | | | | |
|---|---|---|---|---|---|
| H-H_ | 0 | -4.68955 | 5.17245 | 2.83585 | L |
| C-C_3 | 0 | -9.80045 | 2.71085 | -2.98341 | L |
| N-N_R | 0 | -9.12568 | 2.87054 | -1.67299 | L |
| C-C_R | 0 | -8.55567 | 1.78439 | -1.02527 | L |
| O-O_R | 0 | -8.57389 | 0.67428 | -1.5265 | L |
| N-N_R | 0 | -7.96937 | 1.94113 | 0.18931 | L |
| C-C_R | 0 | -7.91589 | 3.14777 | 0.80353 | L |
| N-N_R | 0 | -7.31438 | 3.26297 | 2.07738 | L |
| C-C_R | 0 | -8.46181 | 4.26168 | 0.17311 | L |
| C-C_R | 0 | -9.06345 | 4.09967 | -1.07181 | L |
| H-H_ | 0 | -9.48625 | 4.97246 | -1.53938 | L |
| H-H_ | 0 | -8.42952 | 5.23848 | 0.63943 | L |
| H-H_ | 0 | -6.91253 | 2.43386 | 2.53811 | L |
| H-H_ | 0 | -7.27641 | 4.17125 | 2.5628 | L |
| C-C_3 | 0 | -11.0162 | -1.80442 | -0.98661 | L |
| N-N_R | 0 | -11.04191 | -0.68449 | -0.01954 | L |
| C-C_R | 0 | -10.3476 | -0.74783 | 1.17928 | L |
| O-O_R | 0 | -9.70232 | -1.73772 | 1.47939 | L |
| N-N_R | 0 | -10.37257 | 0.30328 | 2.04034 | L |
| C-C_R | 0 | -11.06643 | 1.43526 | 1.76142 | L |
| N-N_R | 0 | -11.06254 | 2.51006 | 2.68042 | L |
| C-C_R | 0 | -11.7747 | 1.52791 | 0.56654 | L |
| C-C_R | 0 | -11.74766 | 0.44938 | -0.3134 | L |
| H-H_ | 0 | -12.29644 | 0.53173 | -1.2361 | L |
| H-H_ | 0 | -12.33588 | 2.42006 | 0.3177 | L |
| H-H_ | 0 | -10.53416 | 2.4373 | 3.56168 | L |
| H-H_ | 0 | -11.58219 | 3.37752 | 2.48091 | L |
| C-C_3 | 0 | -8.4014 | -6.65378 | -0.22698 | L |

| | | | | | |
|---|---|---|---|---|---|
| N-N_R | 0 | -8.07934 | -5.40371 | -0.95482 | L |
| C-C_R | 0 | -7.33325 | -4.40776 | -0.34517 | L |
| O-O_R | 0 | -6.93498 | -4.53996 | 0.79695 | L |
| N-N_R | 0 | -7.02797 | -3.26782 | -1.01634 | L |
| C-C_R | 0 | -7.42411 | -3.07078 | -2.29678 | L |
| N-N_R | 0 | -7.08021 | -1.87238 | -2.96344 | L |
| C-C_R | 0 | -8.15973 | -4.05916 | -2.94489 | L |
| C-C_R | 0 | -8.48305 | -5.22284 | -2.25108 | L |
| H-H_ | 0 | -9.05362 | -5.97749 | -2.77527 | L |
| H-H_ | 0 | -8.4769 | -3.93372 | -3.97158 | L |
| H-H_ | 0 | -6.53018 | -1.149 | -2.47803 | L |
| H-H_ | 0 | -7.37428 | -1.7059 | -3.9369 | L |
| C-C_3 | 0 | -3.52435 | -6.3819 | 1.69168 | L |
| N-N_R | 0 | -3.96813 | -6.0834 | 0.31273 | L |
| C-C_R | 0 | -3.6458 | -4.86862 | -0.27143 | L |
| O-O_R | 0 | -3.0022 | -4.03367 | 0.33994 | L |
| N-N_R | 0 | -4.0244 | -4.59894 | -1.54692 | L |
| C-C_R | 0 | -4.71889 | -5.49832 | -2.28633 | L |
| N-N_R | 0 | -5.0941 | -5.17851 | -3.61148 | L |
| C-C_R | 0 | -5.05399 | -6.73112 | -1.73033 | L |
| C-C_R | 0 | -4.66448 | -7.00696 | -0.42078 | L |
| H-H_ | 0 | -4.93049 | -7.97075 | -0.00672 | L |
| H-H_ | 0 | -5.60712 | -7.46689 | -2.30029 | L |
| H-H_ | 0 | -5.62503 | -5.84841 | -4.1869 | L |
| H-H_ | 0 | -4.84533 | -4.26315 | -4.01364 | L |
| C-C_3 | 0 | 0.66238 | -5.01033 | 2.71609 | L |
| N-N_R | 0 | -0.14182 | -3.77626 | 2.91055 | L |
| C-C_R | 0 | -0.39584 | -2.91078 | 1.85613 | L |

| | | | | | |
|---|---|---|---|---|---|
| O-O_R | 0 | 0.03631 | -3.14023 | 0.73994 | L |
| N-N_R | 0 | -1.16108 | -1.78731 | 2.04812 | L |
| C-C_R | 0 | -1.67475 | -1.48449 | 3.26625 | L |
| N-N_R | 0 | -2.45887 | -0.32012 | 3.4364 | L |
| C-C_R | 0 | -1.43411 | -2.33457 | 4.34088 | L |
| C-C_R | 0 | -0.6704 | -3.48036 | 4.13823 | L |
| H-H_ | 0 | -0.50482 | -4.122 | 4.98578 | L |
| H-H_ | 0 | -1.83768 | -2.11872 | 5.32234 | L |
| H-H_ | 0 | -2.85631 | -0.0803 | 4.35652 | L |
| H-H_ | 0 | -2.63747 | 0.30735 | 2.64119 | L |
| C-C_3 | 0 | 3.28841 | -5.65278 | -1.52741 | L |
| N-N_R | 0 | 3.58473 | -4.5618 | -0.5635 | L |
| C-C_R | 0 | 2.96962 | -3.32258 | -0.69496 | L |
| O-O_R | 0 | 2.20119 | -3.09601 | -1.61411 | L |
| N-N_R | 0 | 3.21823 | -2.33309 | 0.20092 | L |
| C-C_R | 0 | 4.05668 | -2.51647 | 1.24869 | L |
| N-N_R | 0 | 4.28148 | -1.46227 | 2.16363 | L |
| C-C_R | 0 | 4.68261 | -3.74745 | 1.41556 | L |
| C-C_R | 0 | 4.43427 | -4.75939 | 0.49285 | L |
| H-H_ | 0 | 4.91481 | -5.70464 | 0.66422 | L |
| H-H_ | 0 | 5.34894 | -3.92521 | 2.25011 | L |
| H-H_ | 0 | 3.80982 | -0.55545 | 2.03526 | L |
| H-H_ | 0 | 4.91512 | -1.58581 | 2.96684 | L |
| C-C_3 | 0 | 8.22448 | -4.90676 | -4.03651 | L |
| N-N_R | 0 | 8.06976 | -4.34547 | -2.68379 | L |
| C-C_R | 0 | 7.53334 | -3.0878 | -2.5015 | L |
| O-O_R | 0 | 7.17616 | -2.41223 | -3.45523 | L |
| N-N_R | 0 | 7.41119 | -2.55701 | -1.25341 | L |

| | | | | | |
|---|---|---|---|---|---|
| C-C_R | 0 | 7.76952 | -3.19358 | -0.1894 | L |
| N-N_R | 0 | 7.63024 | -2.58008 | 1.07953 | L |
| C-C_R | 0 | 8.3169 | -4.55925 | -0.29955 | L |
| C-C_R | 0 | 8.45082 | -5.09335 | -1.51792 | L |
| H-H_ | 0 | 8.82677 | -6.10058 | -1.58229 | L |
| H-H_ | 0 | 8.5971 | -5.12183 | 0.58578 | L |
| H-H_ | 0 | 7.24372 | -1.6281 | 1.15925 | L |
| H-H_ | 0 | 7.91001 | -3.07917 | 1.93624 | L |
| C-C_3 | 0 | 14.94938 | -4.38827 | -0.85597 | L |
| N-N_R | 0 | 14.05967 | -4.42821 | 0.32448 | L |
| C-C_R | 0 | 14.35257 | -3.70412 | 1.47054 | L |
| O-O_R | 0 | 15.35965 | -3.02036 | 1.54157 | L |
| N-N_R | 0 | 13.51573 | -3.74852 | 2.53937 | L |
| C-C_R | 0 | 12.37902 | -4.4883 | 2.52264 | L |
| N-N_R | 0 | 11.53411 | -4.50563 | 3.65649 | L |
| C-C_R | 0 | 12.05467 | -5.22282 | 1.3839 | L |
| C-C_R | 0 | 12.91451 | -5.17777 | 0.28888 | L |
| H-H_ | 0 | 12.64932 | -5.74563 | -0.59117 | L |
| H-H_ | 0 | 11.15149 | -5.81877 | 1.34299 | L |
| H-H_ | 0 | 11.78057 | -3.9597 | 4.49481 | L |
| H-H_ | 0 | 10.66593 | -5.06087 | 3.66049 | L |
| Ag- | 0 | 6.97309 | 2.27161 | -2.16331 | H |
| Ag- | 0 | 5.29389 | 0.21671 | -1.4337 | H |
| Ag- | 0 | 4.71665 | 1.74253 | 0.81794 | H |
| Ag- | 0 | 2.68935 | 0.85734 | -0.80362 | H |
| Ag- | 0 | 0.09697 | 1.50178 | -0.17625 | H |
| Ag- | 0 | -1.566 | -0.58176 | 0.39772 | H |
| Ag- | 0 | -3.83474 | 1.02697 | 0.6015 | H |

| | | | | | |
|---|---|---|---|---|---|
| Ag- | 0 | -3.93141 | -1.34475 | -0.80571 | H |
| Ag- | 0 | -6.23147 | -0.34139 | 0.28767 | H |
| Ag- | 0 | -5.18741 | -2.75221 | 1.24424 | H |
| H-H_ | 0 | 10.93338 | 3.0927 | -3.47285 | L |
| H-H_ | 0 | 9.39817 | 2.20981 | -3.36084 | L |
| H-H_ | 0 | 14.54677 | -5.01109 | -1.62727 | L |
| H-H_ | 0 | 15.92118 | -4.74265 | -0.5823 | L |
| H-H_ | 0 | 15.02395 | -3.38218 | -1.21252 | L |
| H-H_ | 0 | 8.65513 | -5.884 | -3.97006 | L |
| H-H_ | 0 | 8.86465 | -4.27341 | -4.61439 | L |
| H-H_ | 0 | 7.26604 | -4.97066 | -4.50791 | L |
| H-H_ | 0 | 3.85242 | -6.52339 | -1.26513 | L |
| H-H_ | 0 | 3.55568 | -5.33872 | -2.51475 | L |
| H-H_ | 0 | 2.24369 | -5.88195 | -1.49658 | L |
| H-H_ | 0 | 0.74087 | -5.535 | 3.64531 | L |
| H-H_ | 0 | 1.64059 | -4.74789 | 2.37095 | L |
| H-H_ | 0 | 0.18484 | -5.63684 | 1.99198 | L |
| H-H_ | 0 | -3.86305 | -7.35738 | 1.97209 | L |
| H-H_ | 0 | -3.93307 | -5.6558 | 2.36297 | L |
| H-H_ | 0 | -2.45585 | -6.34848 | 1.73761 | L |
| H-H_ | 0 | -8.98012 | -7.29512 | -0.85838 | L |
| H-H_ | 0 | -8.96234 | -6.41943 | 0.65353 | L |
| H-H_ | 0 | -7.49426 | -7.14939 | 0.0494 | L |
| H-H_ | 0 | -11.6127 | -1.55357 | -1.83876 | L |
| H-H_ | 0 | -11.40908 | -2.6851 | -0.52299 | L |
| H-H_ | 0 | -10.00822 | -1.98432 | -1.29729 | L |
| H-H_ | 0 | -10.17037 | 3.65956 | -3.31205 | L |
| H-H_ | 0 | -10.61586 | 2.02525 | -2.88349 | L |

| | | | | | |
|---|---|---|---|---|---|
| H-H_ | 0 | -9.10214 | 2.33248 | -3.70041 | L |
| H-H_ | 0 | -6.02104 | 7.07513 | -3.33816 | L |
| H-H_ | 0 | -6.20228 | 5.39268 | -3.77359 | L |
| H-H_ | 0 | -4.62888 | 6.14918 | -3.84572 | L |
| H-H_ | 0 | -0.81389 | 7.64114 | -1.53303 | L |
| H-H_ | 0 | -1.04603 | 6.36186 | -2.70034 | L |
| H-H_ | 0 | 0.55671 | 6.71966 | -2.10345 | L |
| H-H_ | 0 | 3.5775 | 7.61165 | 2.8263 | L |
| H-H_ | 0 | 2.34035 | 6.55382 | 2.19107 | L |
| H-H_ | 0 | 3.60834 | 7.14317 | 1.14326 | L |
| H-H_ | 0 | 8.66233 | 7.61318 | 0.73351 | L |
| H-H_ | 0 | 7.6883 | 6.36375 | 1.47057 | L |
| H-H_ | 0 | 7.04802 | 7.30105 | 0.1422 | L |

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