Supplemental Material for

Structural Insights into DNA-Stabilized Silver Clusters

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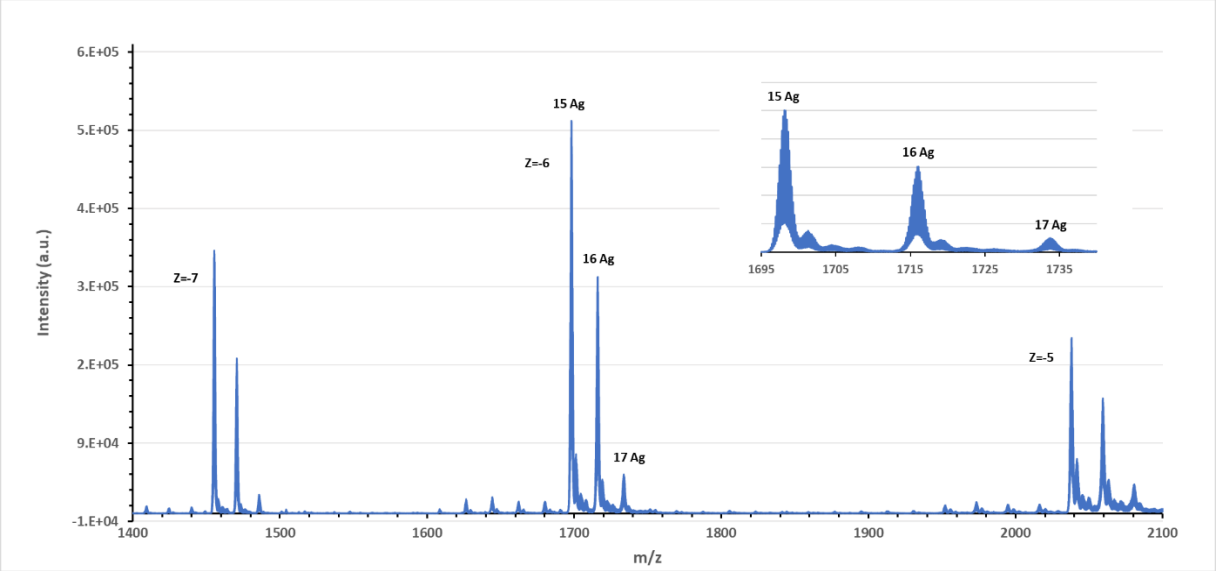
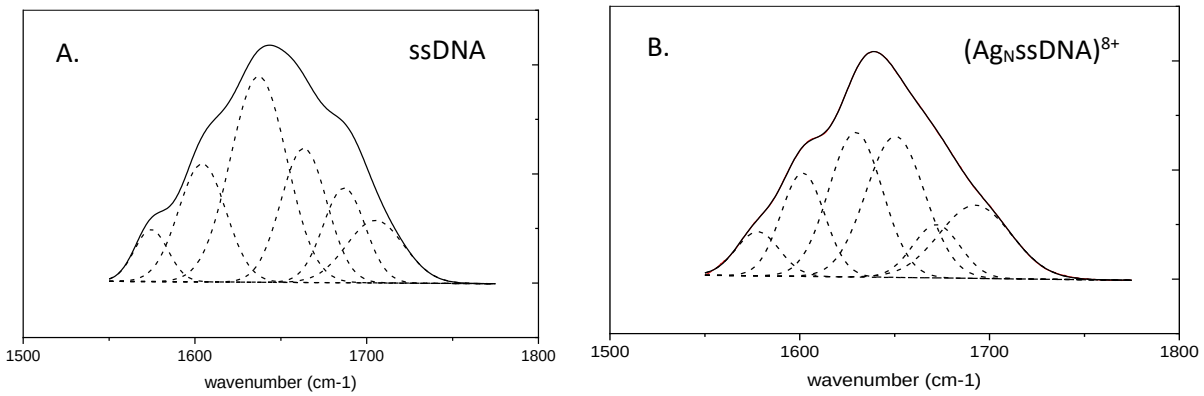


Figure S1. Mass spectrum of the $(Ag_N ssDNA)^{8+}$ complex showing the DNA complex with Ag_{15}:Ag_{16}:Ag_{17} abundances of 7.1:4.9:1. The predominant species has a net charge of +8.



ssDNA (cm^{-1})	$(Ag_N ssDNA)^{8+}$ (cm^{-1})
1700	1692
1689	1672
1661	1650
1634	1629
1604	1601
1574	1577

Figure S2: Gaussian peak fit to base region and resulting peak positions of liquid ssDNA (A) and $(Ag_N ssDNA)^{8+}$ (B). There are theoretically a minimum of 14 vibrational modes in this region. However, only 6 unique peaks were fit that could contain multiple modes. Addition of Ag resulted in red shift of all peaks and changes in relative intensities.

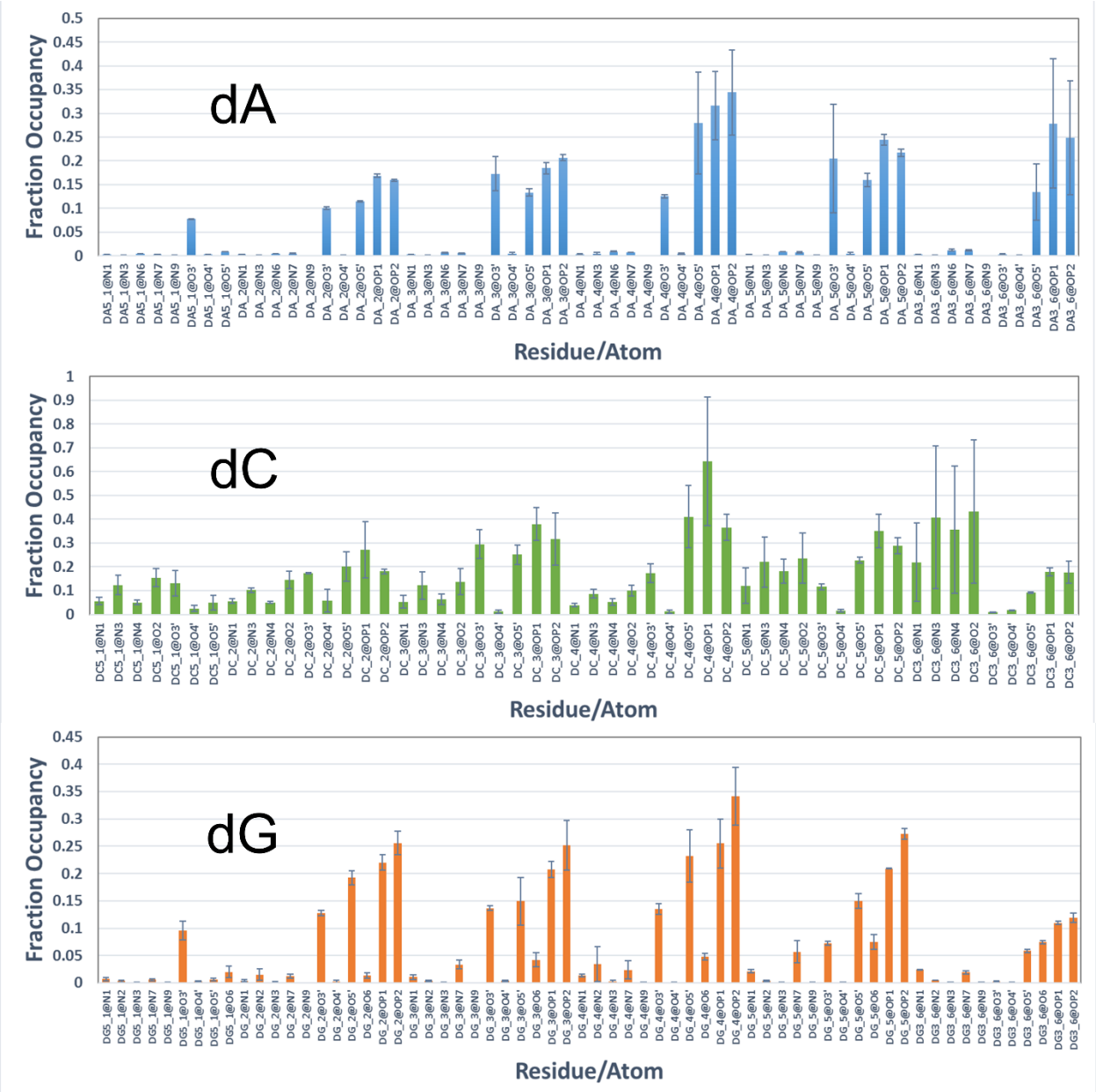


Figure S3. Average fraction occupancies per atom for Ag(I) associated with dA, dC, and dG ssDNA. Averages and standard deviations are reported for two independent simualtions with different starting conformations of ssDNA and different (randomized) ion positions. Note the different y-axis scales for fraction occupancy.

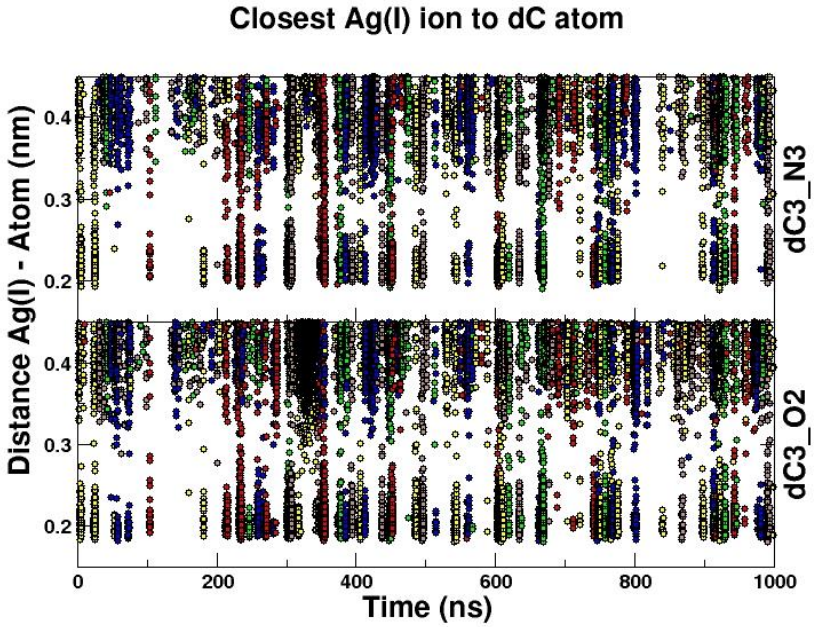


Figure S4. Plot showing distance between Ag(I) and N3 (top) or O2 (bottom) of dC3 vs. time. Distances less than 0.45 nm (where 0.4 nm cutoff for "bound" ions) are shown. Different colors indicate different Ag(I) ions in the simulation. It is clear that for some binding events, the same ion is bound to O2 and N3, and for other binding events there is only one ion associated with the dC atom.

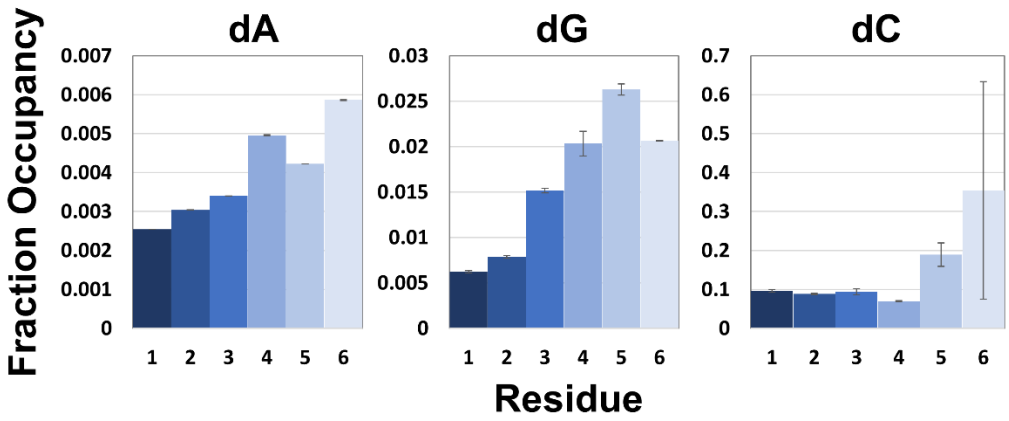


Figure S5. Average base atom occupancies per residue (1-6) for Ag(I) associated with dA, dC, and dG ssDNA. Averages are over all base oxygen and nitrogen atoms for two simualtions. Error bars represent the sum of squares of base atom standard deviations between two runs. Note the different scales for the y-axis values.

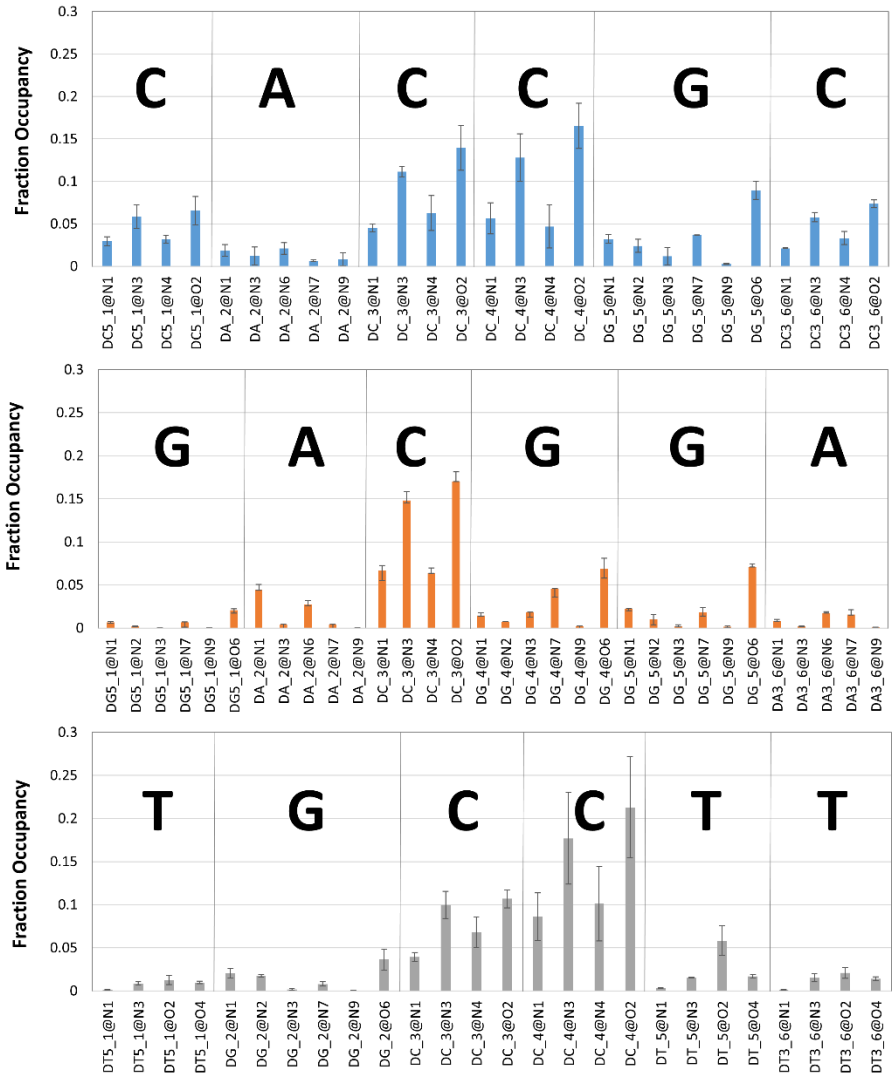


Figure S6. Average base atom occupancies for Ag(I) associated with CACCGC, GACGGA, and TGCCTT oligomers of ssDNA. Averages are over all base oxygen and nitrogen atoms for two simualtions. Error bars represent the standard deviations between two runs.