Supplementary Information

Computational Studies on Structural and Optical Properties of Single-stranded DNA Encapsulated Silver/Gold cluster

Pralok K. Samanta*a, Ganga Periyasamy*a, Arun K. Mannaa and Swapan K. Pati*a,b

*aTheoretical Sciences Unit, bNew Chemistry Unit
Jawaharlal Nehru Center for Advanced Scientific Research
Jakkur P. O., Bangalore 560064, India
Email: pati@jncasr.ac.in

Figure S1. Total energies of (a) Ag12-ssDNA and (b) Au12-ssDNA composites during the NPT simulation.

Figure S2. Optimized geometry of nucleobases (Adenine, Thymine, Guanine and Cytosine). The labeling used in this paper given here.
Figure S3. Interaction Energies ($E_{\text{int}}$) between $M_{12}$ ($M=$Ag or Au) and ssDNA of (a) Ag$_{12}$-ssDNA and (b) Au$_{12}$-ssDNA composites during NPT simulation.

Figure S4. Electronic total density of states (DOS) and projected density of states (pDOS) of (a) ssdA$_{12}$, (b) ssdT$_{12}$, (c) ssdG$_{12}$ and (d) ssdC$_{12}$ (black, red and green denote DOS, pDOS of nucleobase and backbone respectively). The energy ($E$) is scaled with respect to the Fermi energy ($E_F$).
Figure S5. Electronic total density of states (DOS) and projected density of states (pDOS) of (a) Ag$_{12}$-ssdA$_{12}$, (b) Ag$_{12}$-ssdT$_{12}$, (c) Ag$_{12}$-ssdG$_{12}$ and (d) Ag$_{12}$-ssdC$_{12}$ (black, red, green and blue lines denote total DOS, pDOS of base, backbone and metal respectively). The energy (E) is scaled with respect to the Fermi energy ($E_F$).

Figure S6. Electronic total density of states (DOS) and projected density of states (pDOS) of (a) Au$_{12}$-ssdA$_{12}$, (b) Au$_{12}$-ssdT$_{12}$, (c) Au$_{12}$-ssdG$_{12}$ and (d) Au$_{12}$-ssdC$_{12}$ (black, red, green and blue lines denote total DOS, pDOS of base, backbone and metal respectively). The energy (E) is scaled with respect to the Fermi energy ($E_F$).