Electronic Supplementary Material (ESI) for Journal of Materials Chemistry

Supplementary Information

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

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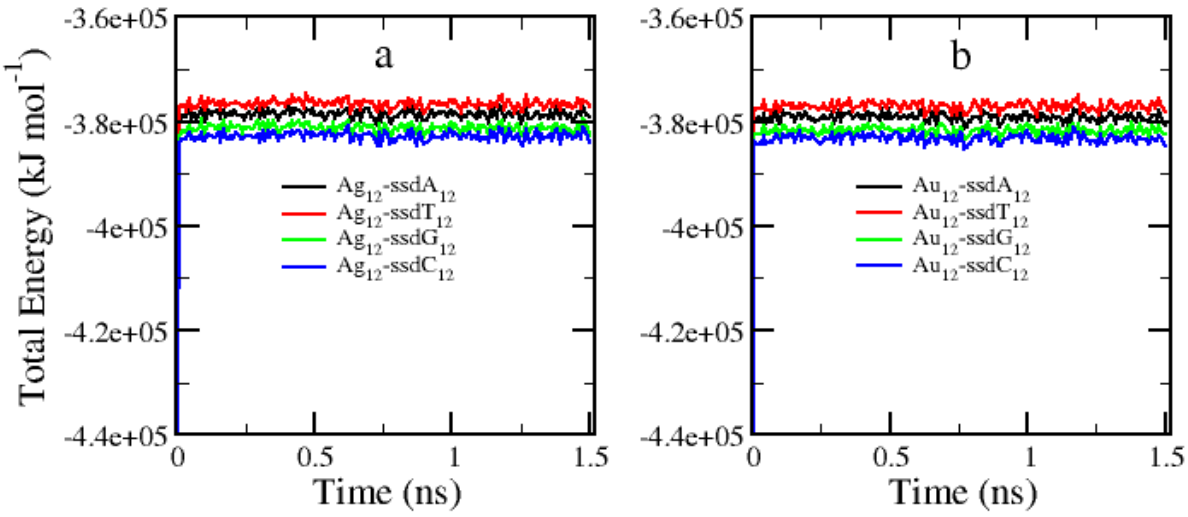

Figure S1. Total energies of (a) Ag_{12}-ssDNA and (b) Au_{12}-ssDNA composites during the NPT simulation.

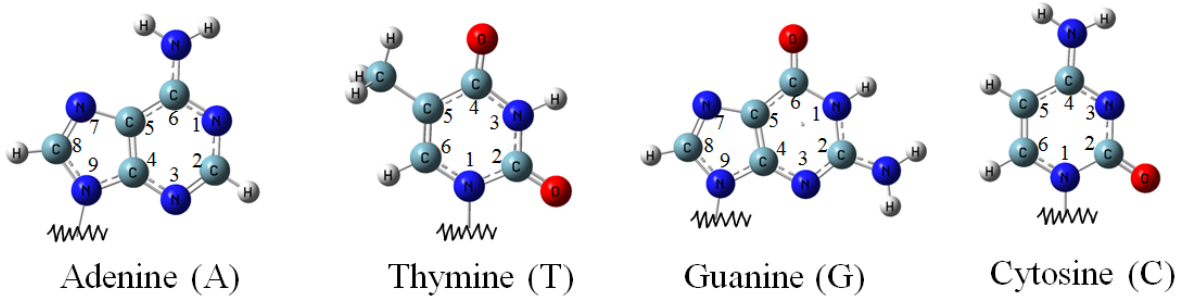

Figure S2. Optimized geometry of nucleobases (Adenine, Thymine, Guanine and Cytosine). The labeling used in this paper given here.

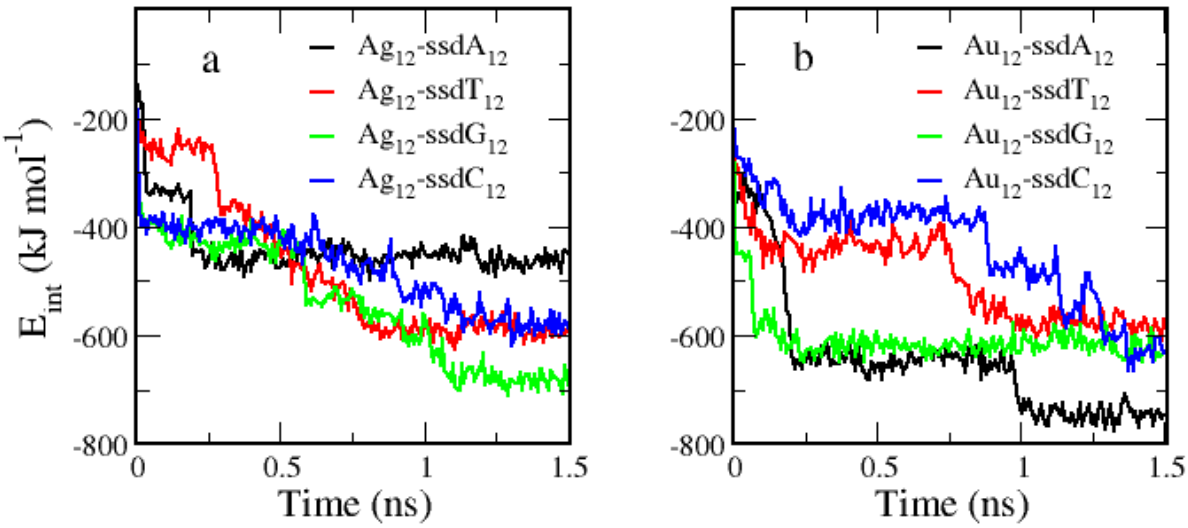

Figure S3. Interaction Energies (E_{int}) between M_{12} (M=Ag or Au) and ssDNA of (a) Ag_{12}-ssDNA and (b) Au_{12}-ssDNA composites during NPT simulation.

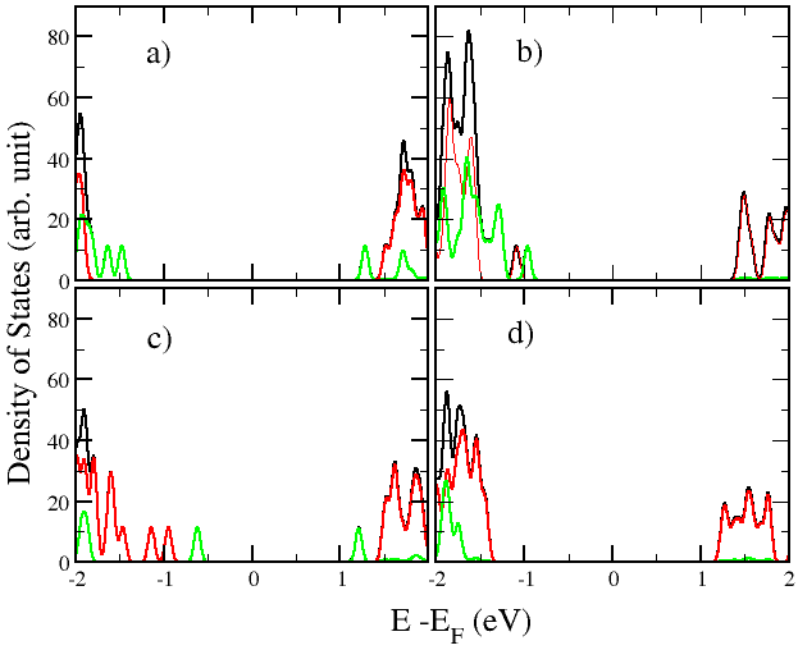

Figure S4. Electronic total density of states (DOS) and projected density of states (pDOS) of (a) ssdA_{12}, (b) ssdT_{12}, (c) ssdG_{12} and (d) ssdC_{12} (black, red and green denote DOS, pDOS of nucleobase and backbone respectively). The energy (E) is scaled with respect to the Fermi energy (E_F).

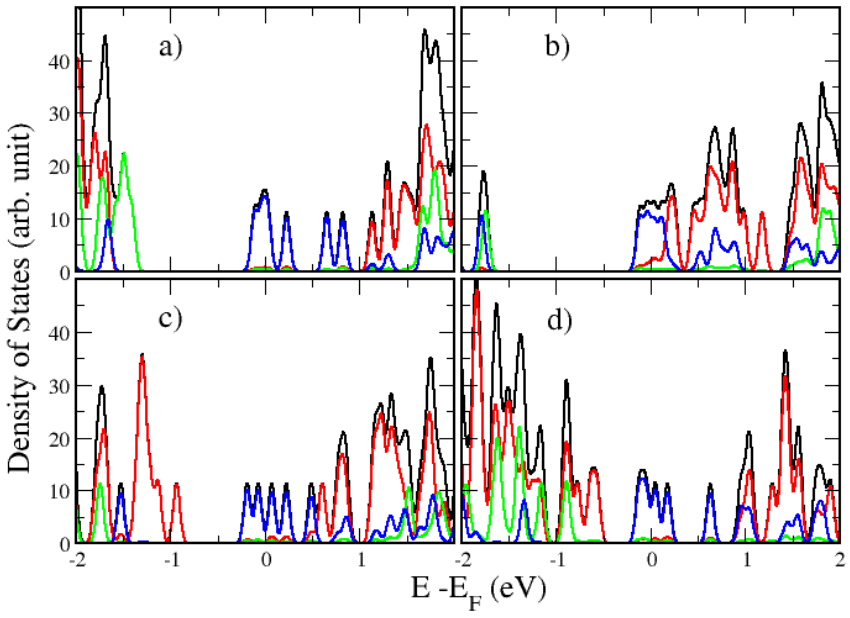

Figure S5. Electronic total density of states (DOS) and projected density of states (pDOS) of (a) Ag_{12}-ssdA_{12}, (b) Ag_{12}-ssdT_{12}, (c) Ag_{12}-ssdG_{12} and (d) Ag_{12}-ssdC_{12} (black, red, green and blue lines denote total DOS, pDOS of base, backbone and metal respectively). The energy (E) is scaled with respect to the Fermi energy (E_F).

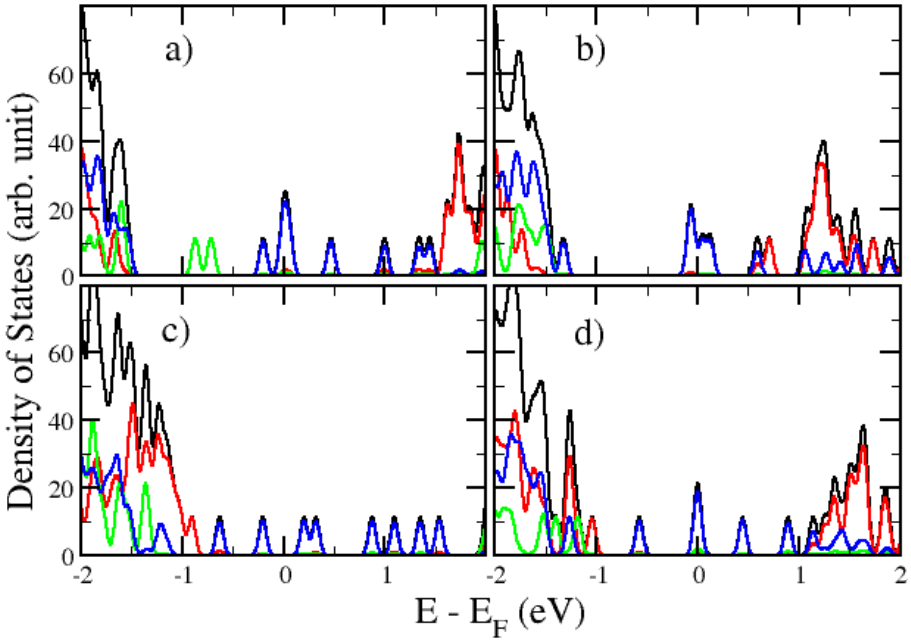

Figure S6. Electronic total density of states (DOS) and projected density of states (pDOS) of (a) Au_{12}-ssdA_{12}, (b) Au_{12}-ssdT_{12}, (c) Au_{12}-ssdG_{12} and (d) Au_{12}-ssdC_{12} (black, red, green and blue lines denote total DOS, pDOS of base, backbone and metal respectively). The energy (E) is scaled with respect to the Fermi energy (E_F).