Electronic Supplementary Material (ESI) for Journal of Materials Chemistry B

Supporting Information

Theoretical Understanding of Single-stranded DNA Assisted Dispersion of Graphene

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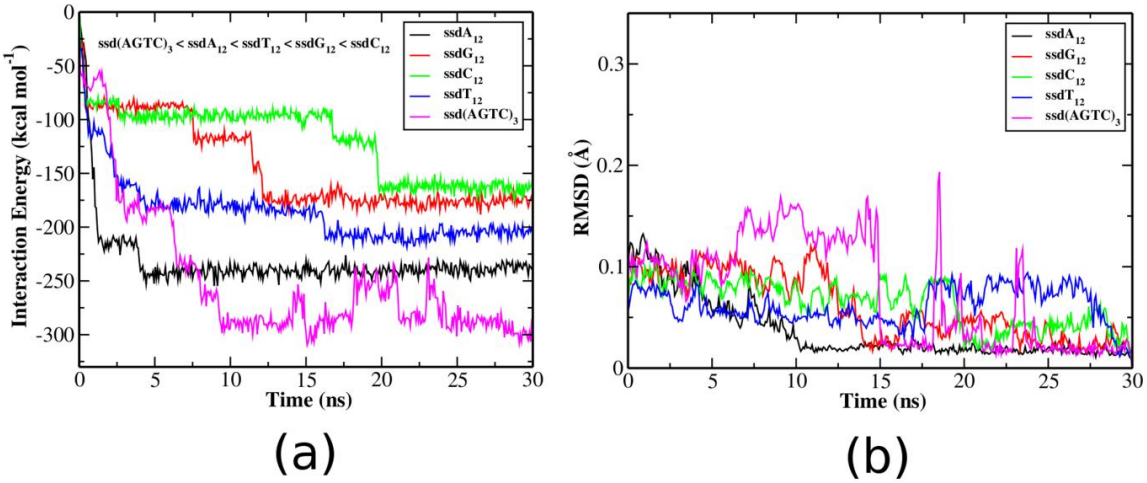

Figure S1: Interaction energy between different ssDNA and graphene, and the root mean square deviation (RMSD) of various interacting ssDNA with respect to their final energy minimized structure as a function of simulation time.

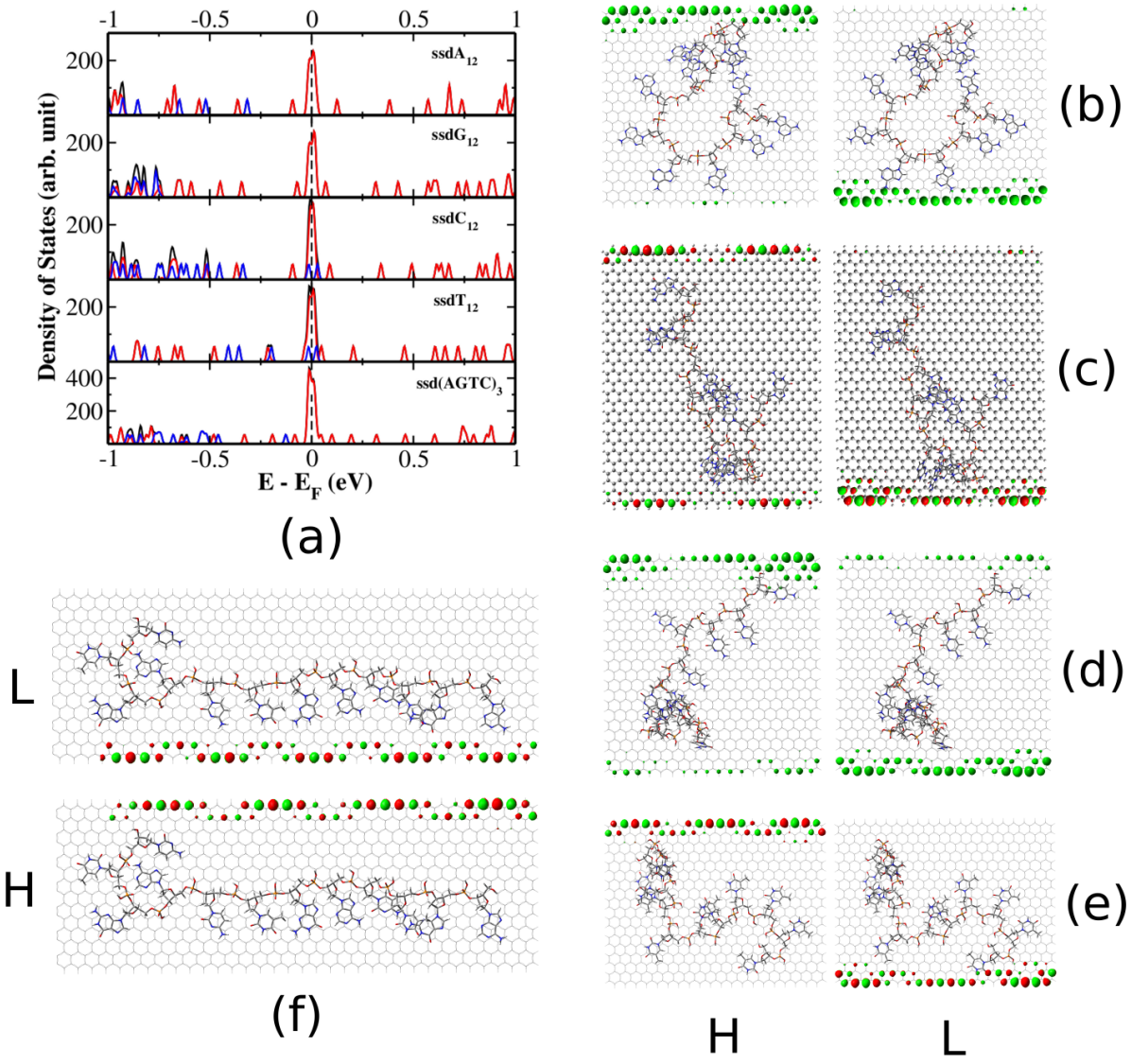

Figure S2: (a) shows electronic density of states (DOS) and projected density of states (pDOS) for various ssDNA adsorbed graphene complexes. In panel (a), the black, red and blue colours indicate the total DOS andpDOS of graphene and ssDNA, respectively. (b), (c), (d), (e), and (f) represent the frontier molecular orbitals of $ssdA_{12}$, $ssdG_{12}$, $ssdC_{12}$, $ssdT_{12}$, and $ssd(AGTC)_3$ adsorbed graphene complexes, respectively. H and L denote the highest occupied and lowest unoccupied molecular orbitals, respectively.