Short Talk B13

Understanding the Binding Mechanism of Various Chiral SWCNTs and ssDNA: A Computational Study

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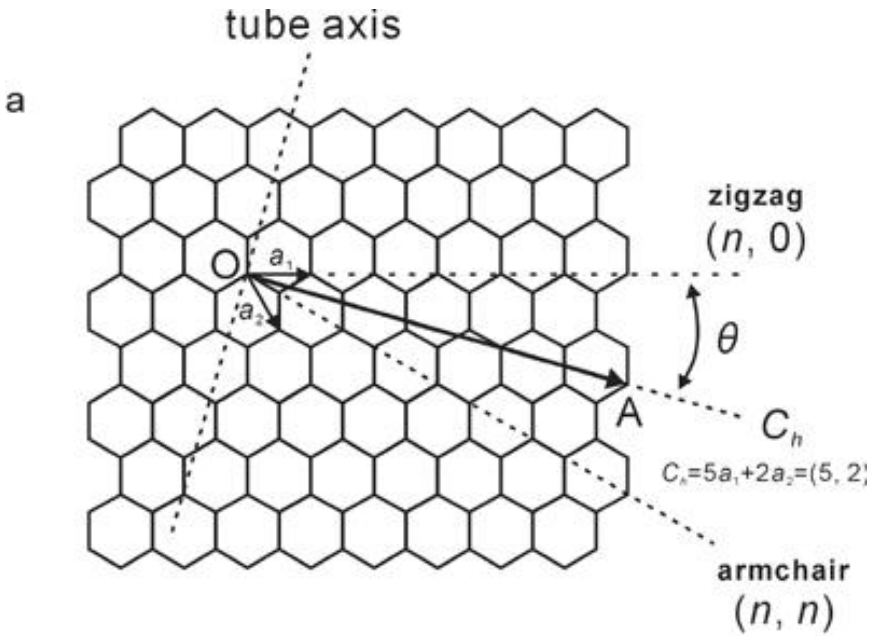
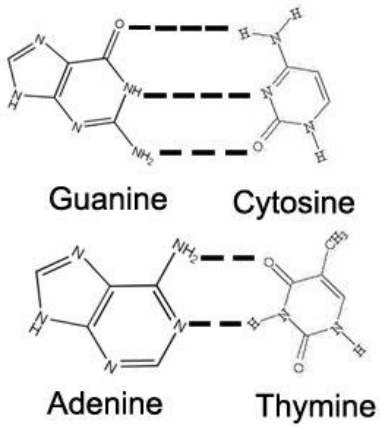
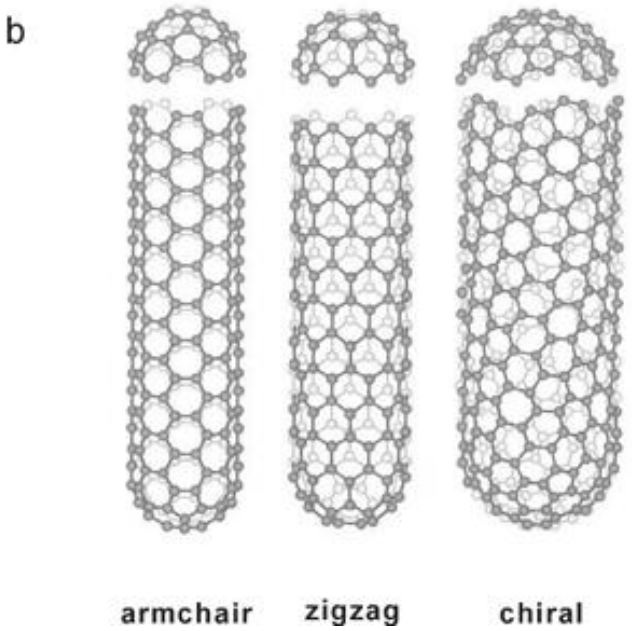
Outline of the talk

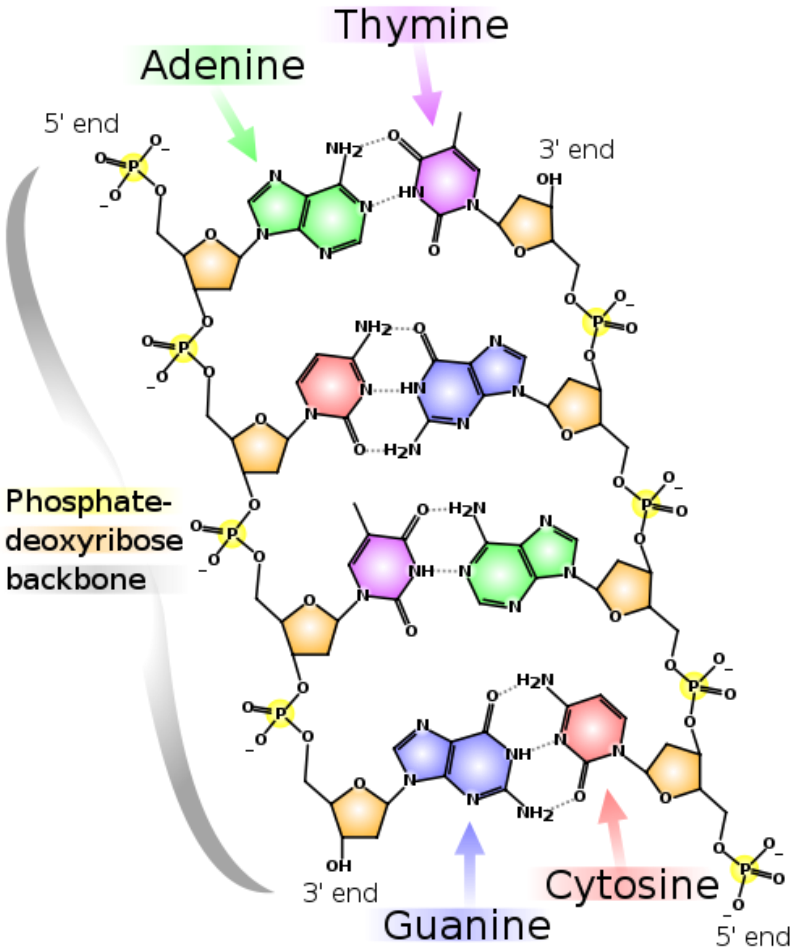
- Introduction to DNA & SWCNTs.
- Motivation & Aim of the work
- Molecular Dynamics Simulation of DNA & SWCNTS Hybrids.
- Results & Summary
- Acknowledgements

Introduction









Introduction & Motivation

- CNTs are stiff, hydrophobic, excellent thermal conductor, 100-fold-higher tensile strength than steel. DNA is a biomolecule which is flexible and amphiphillic.
- SWNTs possess a vast application such as in transistors, chemical sensing, photovoltaic devices and detection of DNA hybridization.
- However, the there is a difficulty of getting pure and homogeneity of SWNTs with respect to their chirality.
- Atomic Force Microscopy(AFM) strongly suggested that DNA converts bundled CNTs to individual tubes.

Huajian Gao, Yongkong, *Annu. Rev. Mater. Res*. **2001**, 34, 123

Aim of the work

To understand the interactions between various SWCNTs and various ssDNA sequences

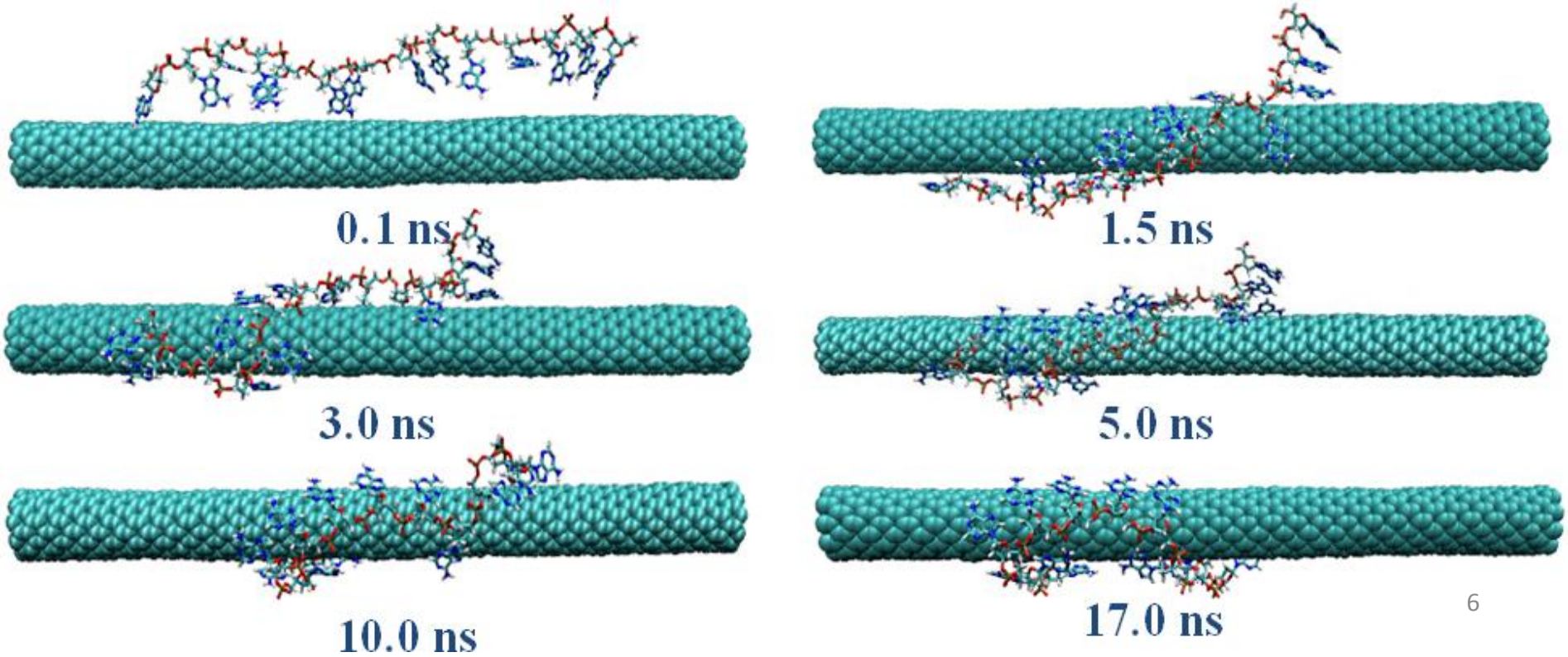
Xiaomin Tu, Suresh Manohar, Anand Jagota, Ming Zheng, *Nature*, **2009**, 460, 250

Robert R. Johnson, A. T. Charlie Johnson, Michael L. Klein, *Nano Letters*, **2008**, 8, 69

Sang N. Kim, Zhifeng Kuang, James G. Grote, Barry L. Farmer, Rajesh R. Naik, *Nano Letters*, **2008**, 8, 4415

Results & Discussions

The DNA is placed at ~13 A from the SWCNT. It is found that at 1.5 ns the DNA bases start to wrap around the SWCNT. At 10 ns, 50 % of the DNA bases are already in contact with the graphitic wall of the SWCNT. The simulation is continued for 17ns and for few systems to 40ns.



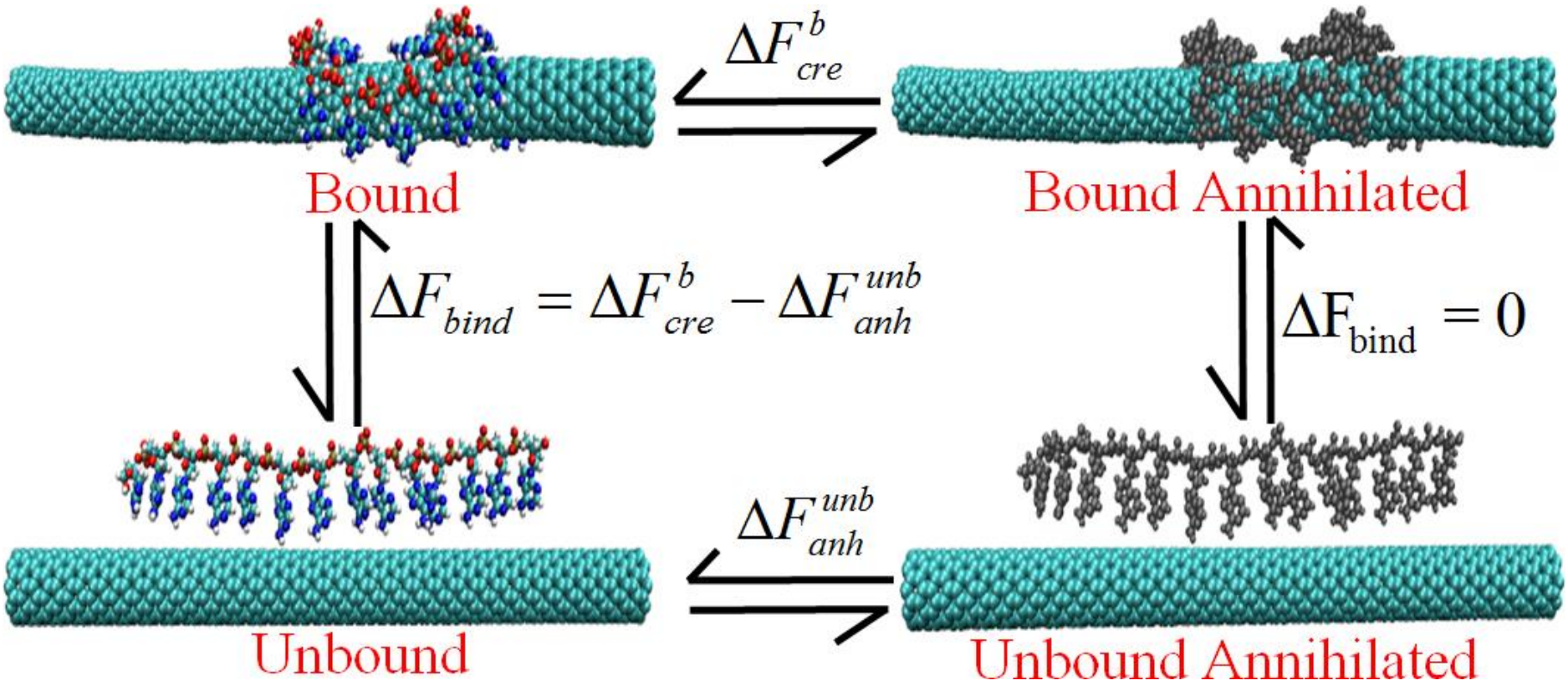


Figure 1. Schematic representation of thermodynamic cycle used for free energy computations.

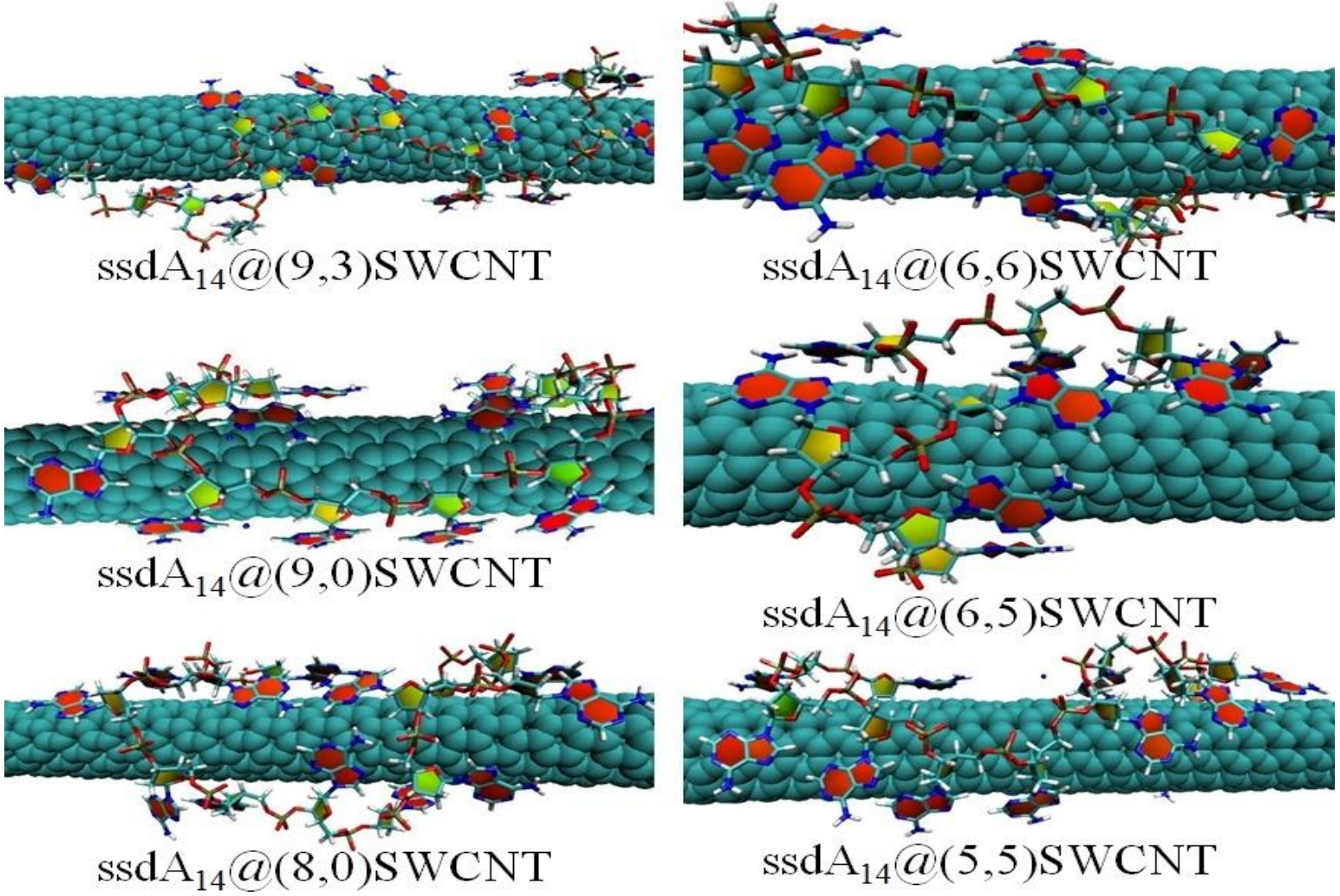


Figure 2. The MD simulated structure of $ssdA_{14}$@ (n, m) SWCNT composite. Note that the hybrid zones are enlarged to show the orientation of DNA scaffolds (sugar, phosphate and nuclobases) in order to form perfect π-stacking

Table 1. The average total number of H- bonds (within 3.5 Å) within ssDNA and between the water and ssDNA throughout the 17 ns MD simulation. Diameters (nm) of the SWCNTs are also given.

Systems		Average number of intra-locked H-bonding interaction with in ssDNA	Average number of H-bonds between ssDNA and water
Chirality of SWCNT	ssDNA		
without SWCNT	ssdA14	-	157
	ssdG14	-	172
	ssdC14	-	162
	ssdT14	-	146
(8,0)	ssdA14	2	157
0.63	ssdG14	10	161
	ssdC14	6	145
	ssdT14	2	141

(5,5)	$ssdA_{14}$	2	152
0.68	$ssdG_{14}$	9	162
	$ssdC_{14}$	6	147
	$ssdT_{14}$	2	141
(9, 0)	$ssdA_{14}$	2	150
0.70	$ssdG_{14}$	6	161
	$ssdC_{14}$	5	155
	$ssdT_{14}$	2	139
(6, 5)	$ssdA_{14}$	2	151
0.77	$ssdG_{14}$	6	163
	$ssdC_{14}$	5	153
	$ssdT_{14}$	2	139
(6, 6)	$ssdA_{14}$	1	150
0.81	$ssdG_{14}$	5	163
	$ssdC_{14}$	3	148
	$ssdT_{14}$	1	139
(9,3)	$ssdA_{14}$	0	153
0.84	$ssdG_{14}$	5	164
	$ssdC_{14}$	3	150
	$ssdT_{14}$	1	139

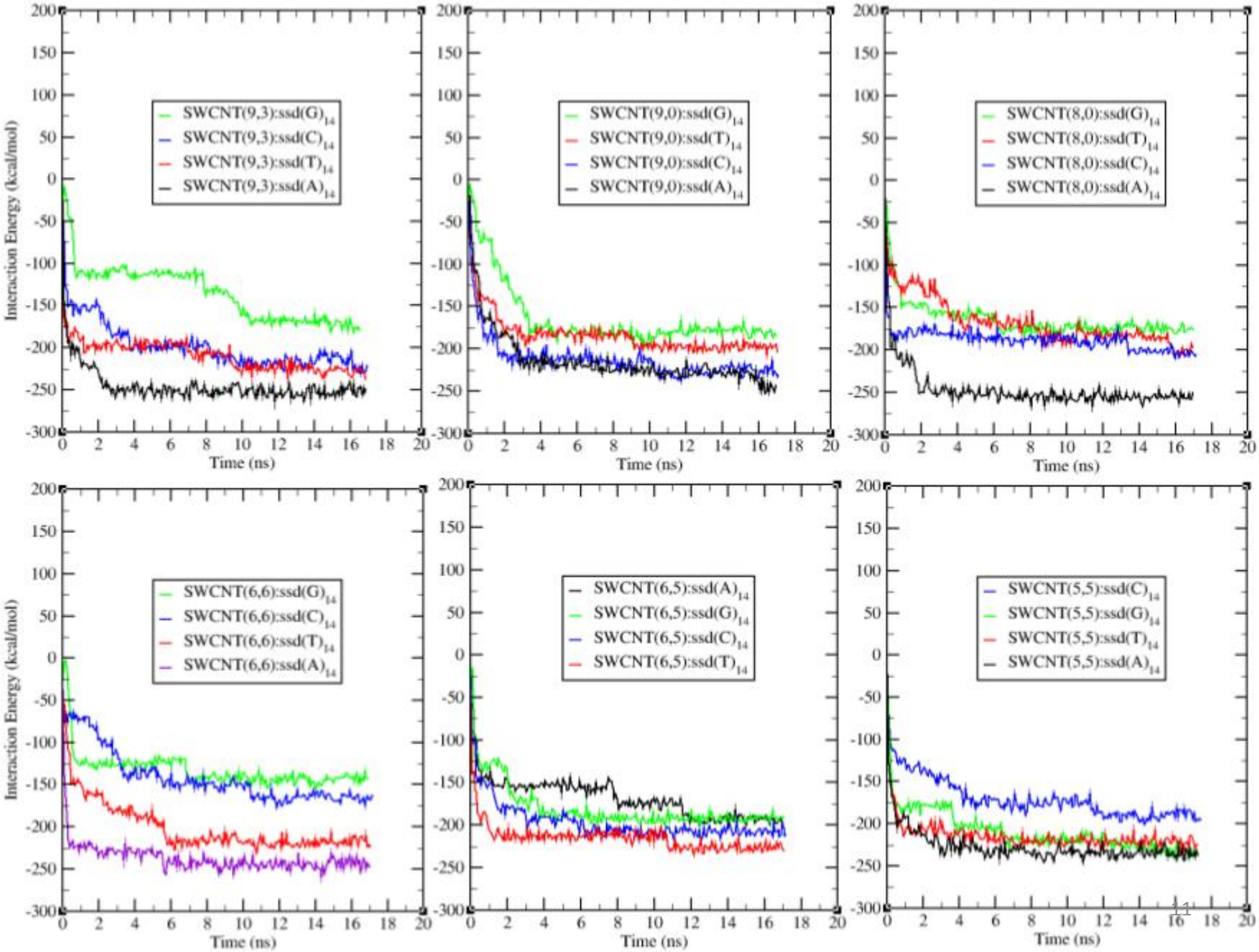

Interaction Energy (kcal/mol)
Time (ns)
SWCNT(9,3):ssd(G)14
SWCNT(9,3):ssd(C)14
SWCNT(9,3):ssd(T)14
SWCNT(9,3):ssd(A)14
SWCNT(9,0):ssd(G)14
SWCNT(9,0):ssd(T)14
SWCNT(9,0):ssd(C)14
SWCNT(9,0):ssd(A)14
SWCNT(8,0):ssd(G)14
SWCNT(8,0):ssd(T)14
SWCNT(8,0):ssd(C)14
SWCNT(8,0):ssd(A)14
SWCNT(6,6):ssd(G)14
SWCNT(6,6):ssd(C)14
SWCNT(6,6):ssd(T)14
SWCNT(6,6):ssd(A)14
SWCNT(6,5):ssd(A)14
SWCNT(6,5):ssd(G)14
SWCNT(6,5):ssd(C)14
SWCNT(6,5):ssd(T)14
SWCNT(5,5):ssd(C)14
SWCNT(5,5):ssd(G)14
SWCNT(5,5):ssd(T)14
SWCNT(5,5):ssd(A)14

Figure S1. Interaction energies between various SWCNTs and $ssdA_{14,}$ $ssdT_{14,}$ $ssdG_{14}$ and $ssdC_{14}$ as a function of time for the period of 17 ns.

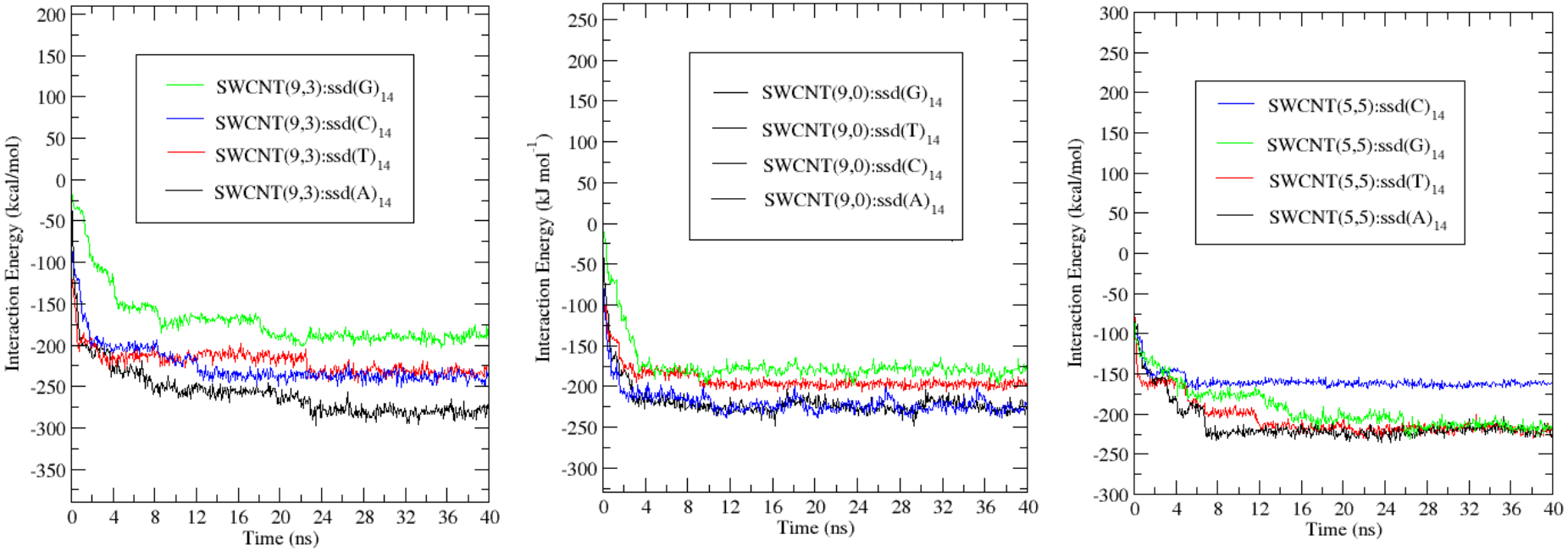


Figure S1. Interaction energies between various SWCNTs and $ssdA_{14,}$ $ssdT_{14,}$ $ssdG_{14}$ and $ssdC_{14}$ as a function of time for the period of 40 ns.

Table 2. The Binding Free Energies (ΔF_{bind}, in kcal mol^{-1}) between various ssDNA and SWCNTs.

Systems	$ssdA_{14}$ (A)	$ssdT_{14}$ (T)	$ssdG_{14}$ (G)	$ssdC_{14}$ (C)	Order
(9, 3) SWCNT	-19.21 (1.06)	-19.84 (1.10)	-20.90 (1.22)	-25.54 (1.32)	C>G>T>A
(9, 0) SWCNT	-43.45 (0.55)	-25.87 (0.30)	-54.46 (1.22)	-67.39 (1.33)	C>G>A>T
(8, 0) SWCNT	-24.77 (1.59)	-16.67 (1.10)	-12.66 (0.28)	-13.55 (0.41)	A>T>C>G
(6, 6) SWCNT	-34.98 (1.45)	-16.57 (1.41)	-28.05 (1.46)	-17.03 (1.42)	G>A>C>T
(6, 5) SWCNT	-58.00 (2.69)	-23.41 (2.49)	-18.01 (2.31)	-29.70 (2.57)	A>C>T>G
(5, 5) SWCNT	-19.50 (1.66)	-15.37 (1.53)	-30.72 (1.75)	-12.94 (1.55)	G>A>T>C

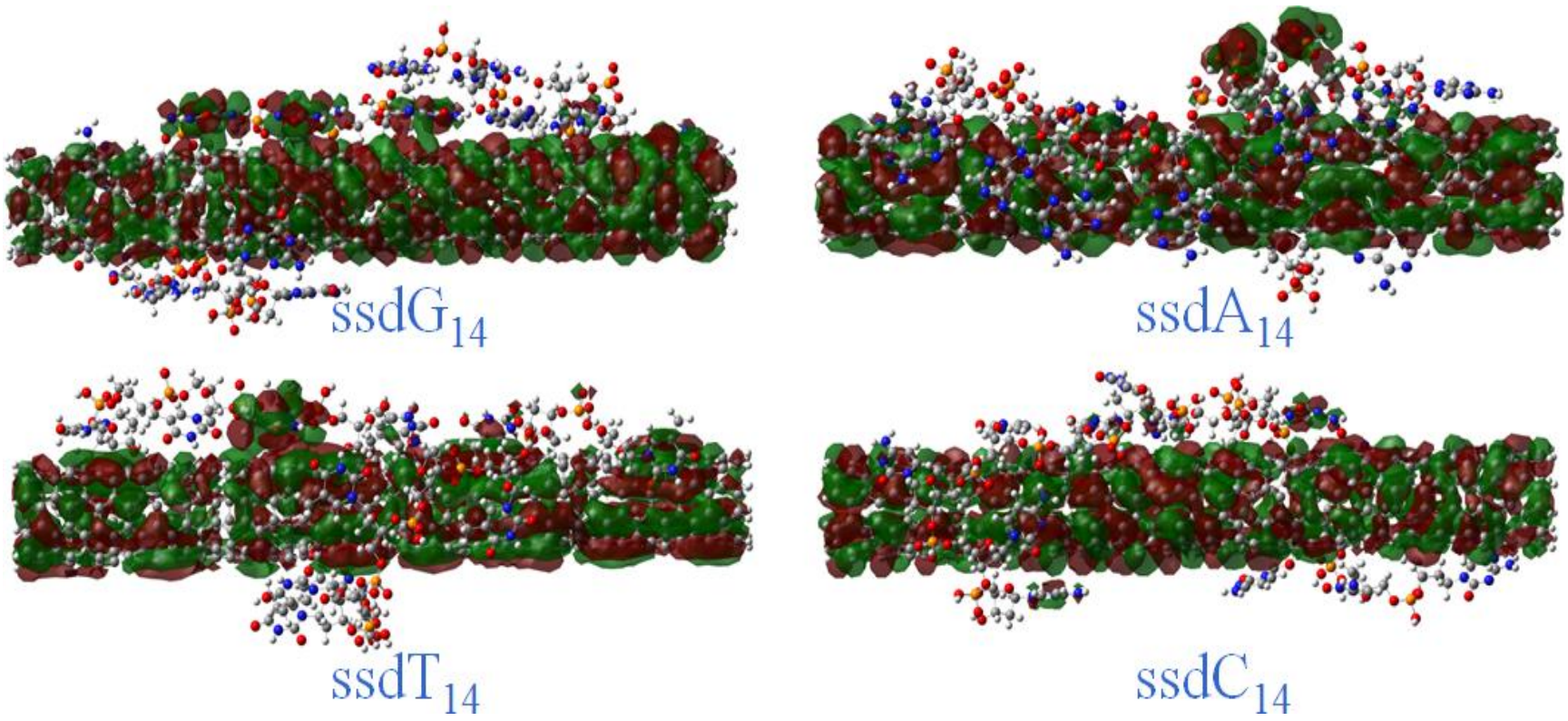


Figure 3. The computed highest energy delocalized frontier MOs (where the ssDNA start to contribute) of various sDNA@(5,5)SWCNT hybrids. The isocontour value of 0.002 is used for plotting.

Summary

- MD simulations studies reveal that ssDNA undergoes rapid structural changes and wrapped around the SWNTs via the pi-pi bonding between ssDNA bases and the graphitic SWNTs wall. The phopsphates interacts through weak van der Waals force

- The ssDNA wrap around the wall of CNT within 1 ns and than the interaction energy becomes stable around 5-10ns

- The order of the Interaction energy is consistent with the number of the residue in the bonding and non-bonding around SWCNT.

- Except for SWCNT(11,0) and SWCNT(6,5) , all others CNT interacts more with Adenine

- our results provide evidence that the electronic factors of the hybrid determine the sequence selectivity. The quantum mechanical studies at HF level show that the wrapping makes the system chemically more stable with larger HOMO-LUMO gap. This occurs due to larger delocalization of MO's over ssDNA and SWCNT in the ssDNA@SWCNT hybrid.

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Thank You for your kind attention !