Supporting Information

Binding Patterns and Dynamics of Double-stranded DNA on Phosphorene Surface

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Supplementary Simulation Methods

For the contact number between dsDNA and phosphorene, the GROMACS built-in utility *g_mindist* was used. It allows selecting two groups (dsDNA and phosphorene) and calculating the atom pairs from two groups and their distances within pre-defined distance value. Here, a contact is defined if the distance between an atom of dsDNA and an atom of phosphorene is less than 0.5 nm.

The interaction energy between phosphorene and dsDNA was calculated using *mdrun* program within GROMACS which allows (re)calculation of energies of designated groups (here are dsDNA and phosphorene) for the input trajectories. Then the *g_energy* program was used to compute the interaction energies between the phosphorene and dsDNA throughout the trajectory frames.

To describe the orientation of dsDNA upon binding to phosphorene, the contact angle profiles of dsDNA with phosphorene surface were calculated by employing the Tcl scripts running on the VMD TkConsole. Here, the contact angle between dsDNA

and the phosphorene is defined by the dsDNA axial direction and phosphorene plane.

The intramolecular hydrogen bond in dsDNA was calculated using the *g_hbond* program within GROMACS. The formation of a hydrogen bond is defined when the angle of "Hydrogen–Donor–Acceptor" is ≤ 30° and the distance of "Donor–Acceptor" is ≤ 0.35 nm.

Supplementary Figures

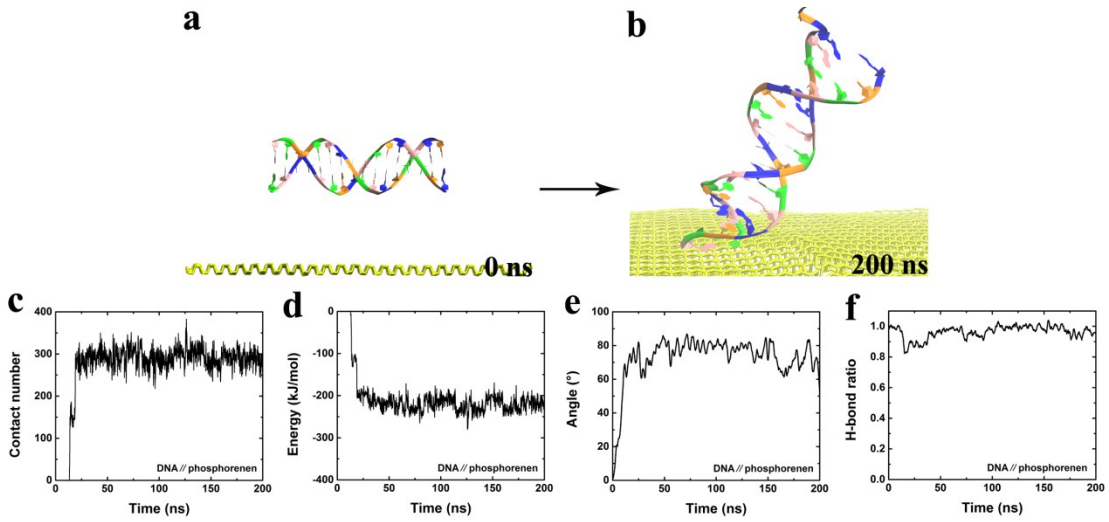

Figure S1. (a) The initial configuration for the DNA // phosphorene system where the phosphorene was not fixed. (b) The binding patterns of dsDNA on phosphorene at 200 ns. Time evolutions of (c) the contact number and (d) the interaction energy between dsDNA and phosphorene. (e) Time evolution of the defined contact angle between the axis of dsDNA and phosphorene surface. (f) The ratio of the intramolecular hydrogen bond in dsDNA as a function of simulation time.

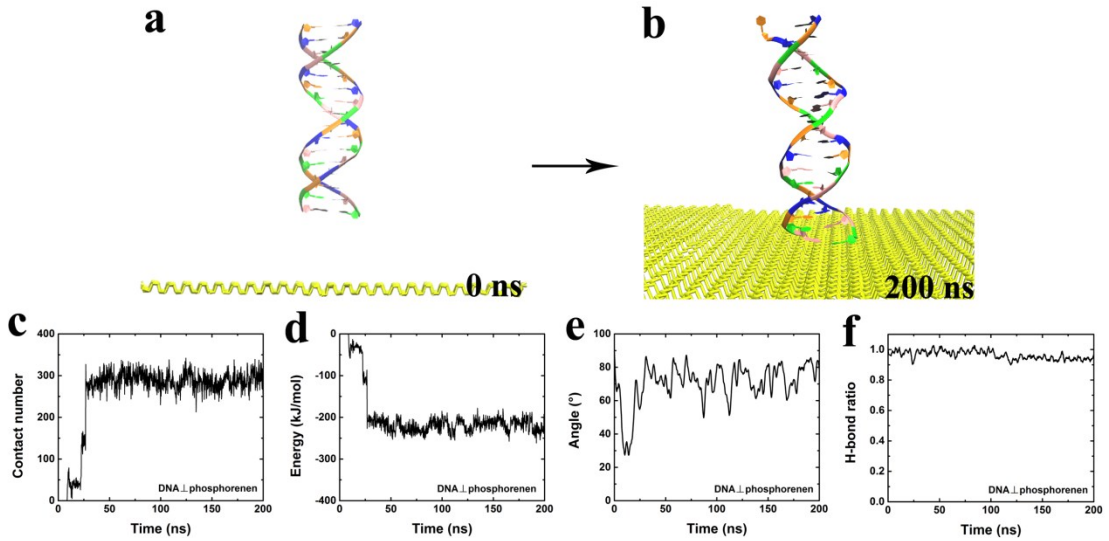

Figure S2. (a) The initial configuration for the DNA⊥phosphorene system where the phosphorene was not fixed. (b) The binding patterns of dsDNA on phosphorene at 200 ns. Time evolutions of (c) the contact number and (d) the interaction energy between dsDNA and phosphorene. (e) Time evolution of the defined contact angle between the axis of dsDNA and phosphorene surface. (f) The ratio of the intramolecular hydrogen bond in dsDNA as a function of simulation time.

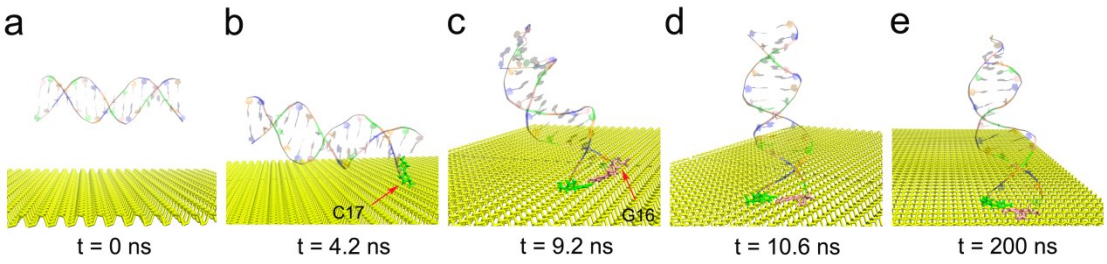

Figure S3. Some representative snapshots obtained from traj-2 of the DNA∥phosphorene system to show the binding process of dsDNA to phosphorene.

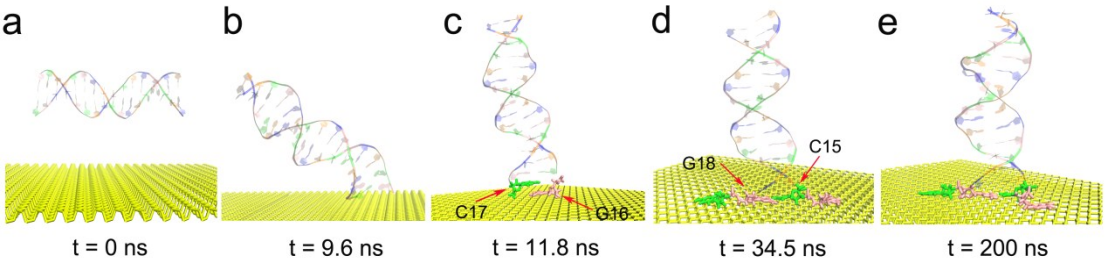

Figure S4. Some representative snapshots obtained from traj-3 of the DNA∥phosphorene system to show the binding process of dsDNA to phosphorene.

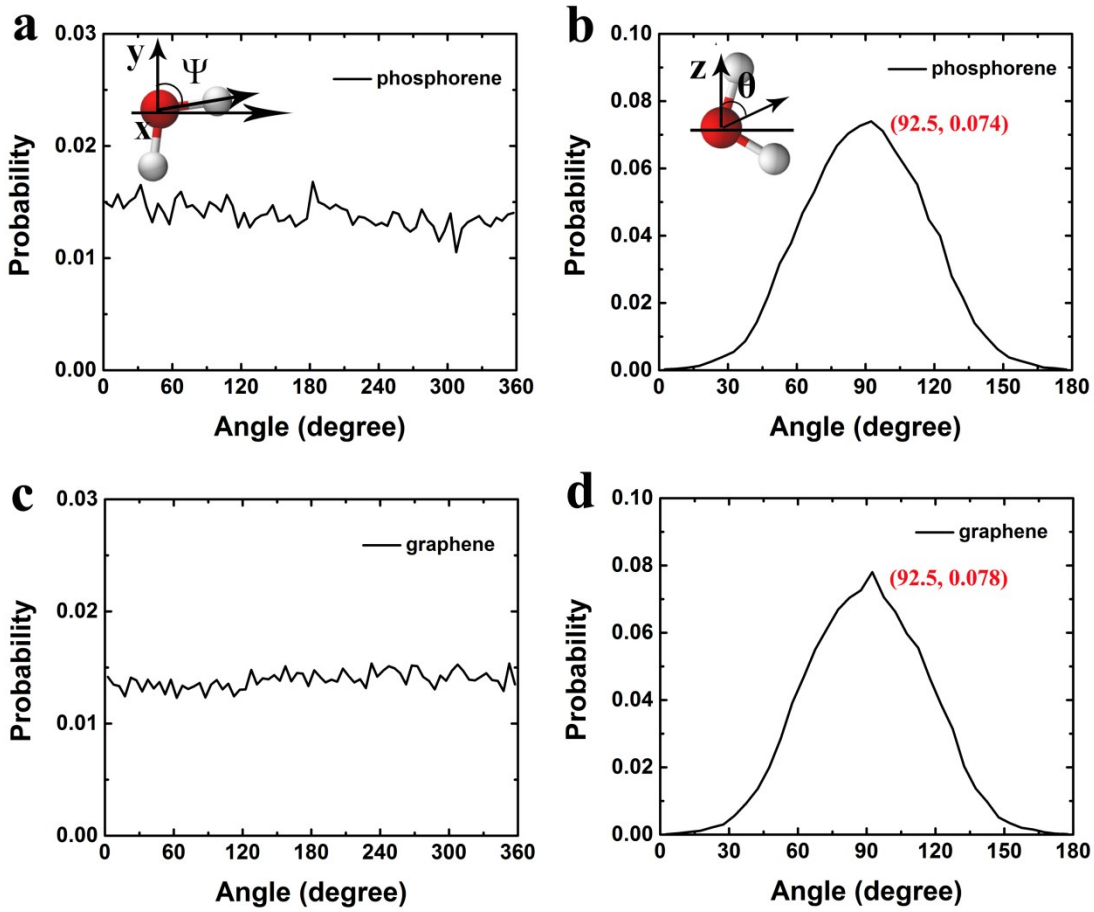

Figure S5. (a) The average probability distribution of the angle Ψ between the OH bonds of the first solvation shell (FSS) waters and the y-axis of the simulation box for the phosphorene system. (b) The average probability distribution of the angle θ between the x–y plane projection of the dipole moment of the FSS waters and the normal of the phosphorene surface. (c) The average probability distribution of the angle Ψ between the OH bonds of the first solvation shell (FSS) waters and the y-axis of the simulation box for the graphene system. (d) The average probability distribution of the angle θ between the x–y plane projection of the dipole moment of the FSS waters and the normal of the graphene surface. Here, the normal of the phosphorene and graphene surface is parallel to the z-axis of the simulation box.

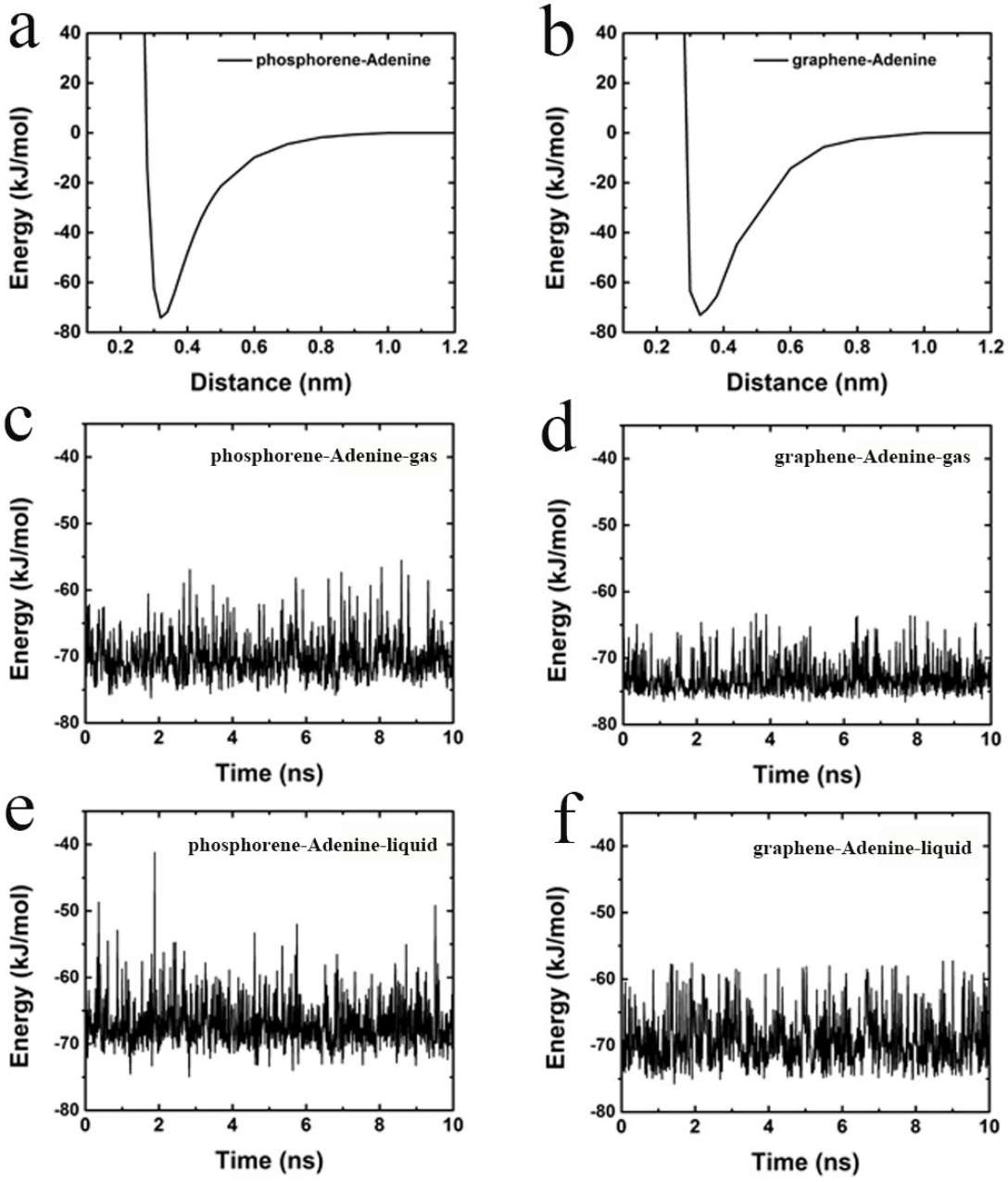

Figure S6. (a) Adsorption energy profiles between phosphorene and an adenine molecule in the gas phase as a function of vertical separation distance. (b) Adsorption energy profiles between graphene and an adenine molecule in the gas phase as a function of vertical separation distance. The interaction energy of adenine with phosphorene (c) and graphene (d) as a function of simulation time in the gas phase at the temperature of 300 K. The interaction energy of adenine with phosphorene (e) and graphene (f) as a function of simulation time in the liquid phase at the temperature of 300 K.