Supporting Information

Microstructure and Intercalation Dynamics of Polymer Chains in Layered Sheets

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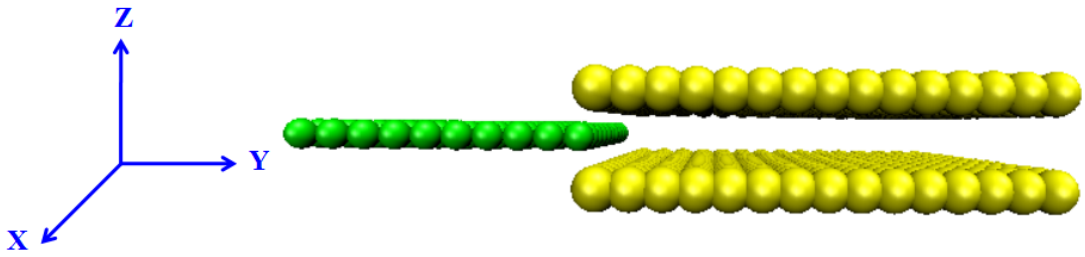

Figure S0. The snapshot for the intial state, where the yellow spheres denote the layered sheets and the polymer chain is represented by green spheres.

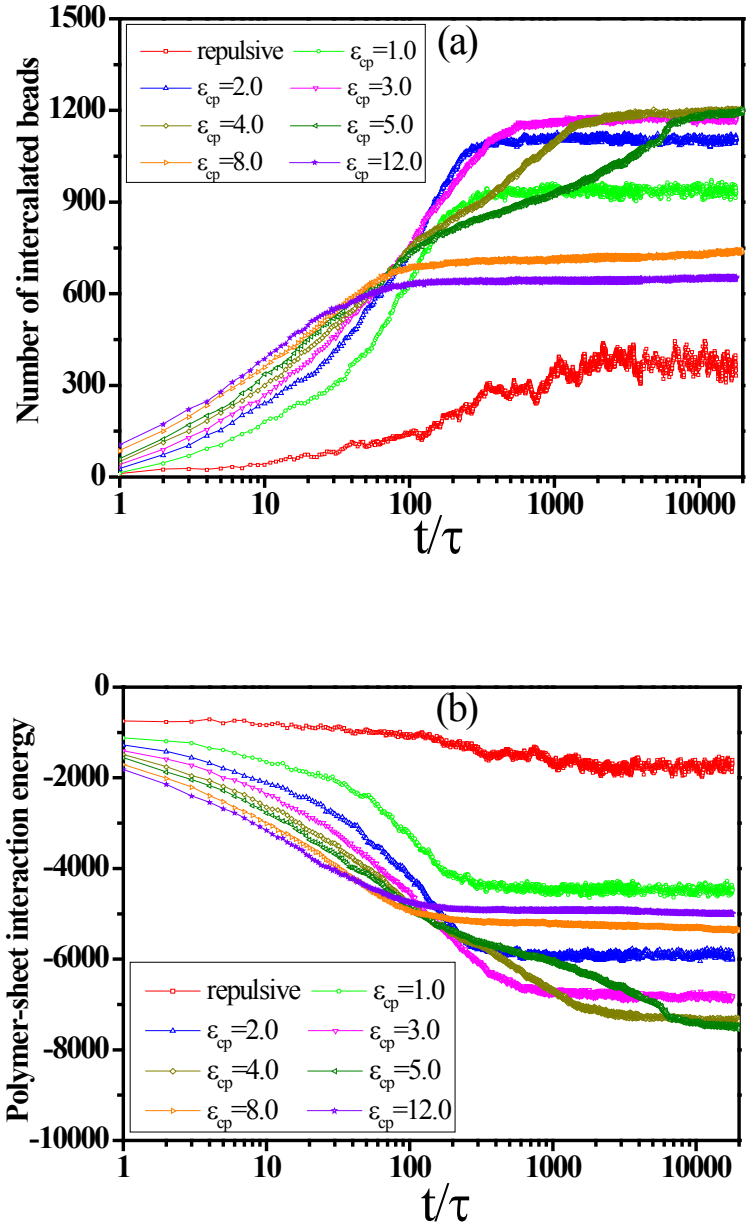

Figure S1. (a) The number of intercalated beads as a function of the simulation time for different polymer-sheet interaction ε_{cp}. (b) The polymer-sheet interaction energy as a function of the simulation time for different polymer-sheet interaction ε_{cp}.

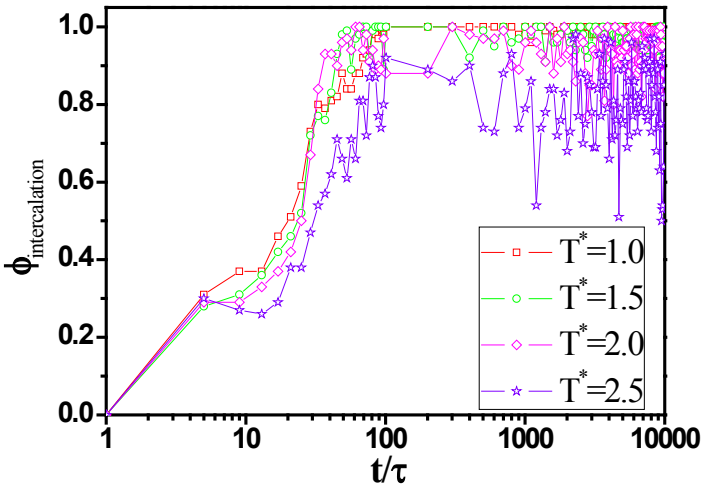

Figure S2. The percentage of the polymer intercalation beads $\phi_{intercalation}$ as a function of the simulation time for different temperature. $T^* = 1.0, 1.5, 2.0, 2.5.$

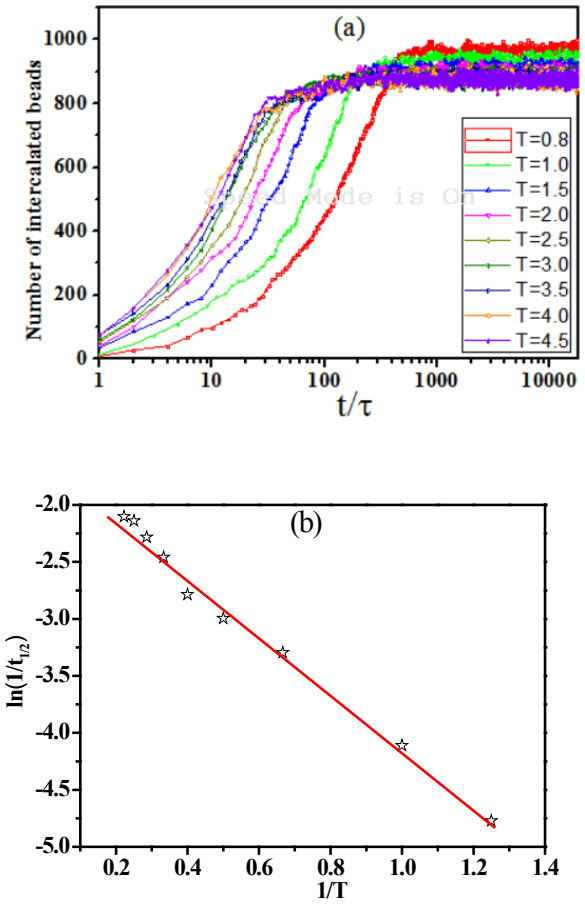

Figure S3. (a) The number of intercalated beads as a function of the simulation time for different simulation temperature. (b) Logarithm of the intercalation rate (the inverse of the intercalation time $t_{1/2}$) as a function of the inverse of the temperature

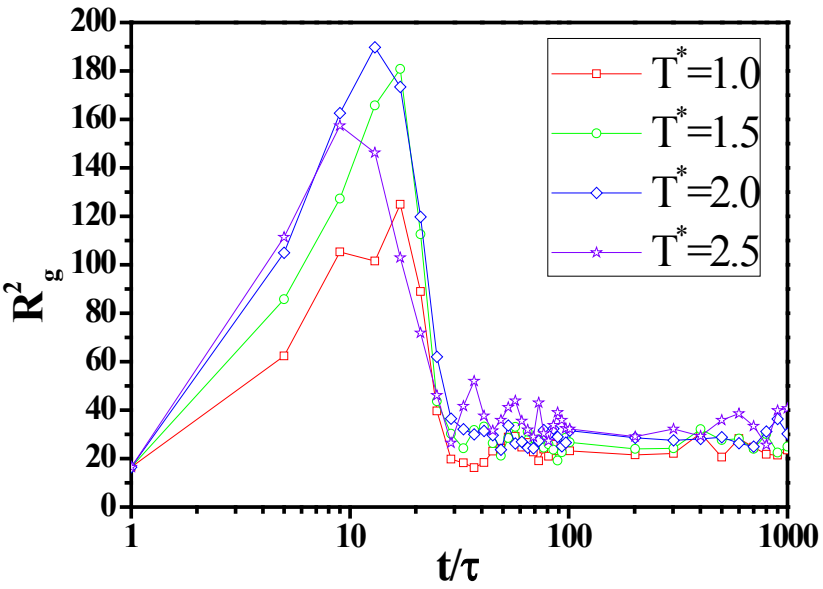

Figure S4. The mean-square radius of gyration R_g as a function of the simulation time for different temperature.

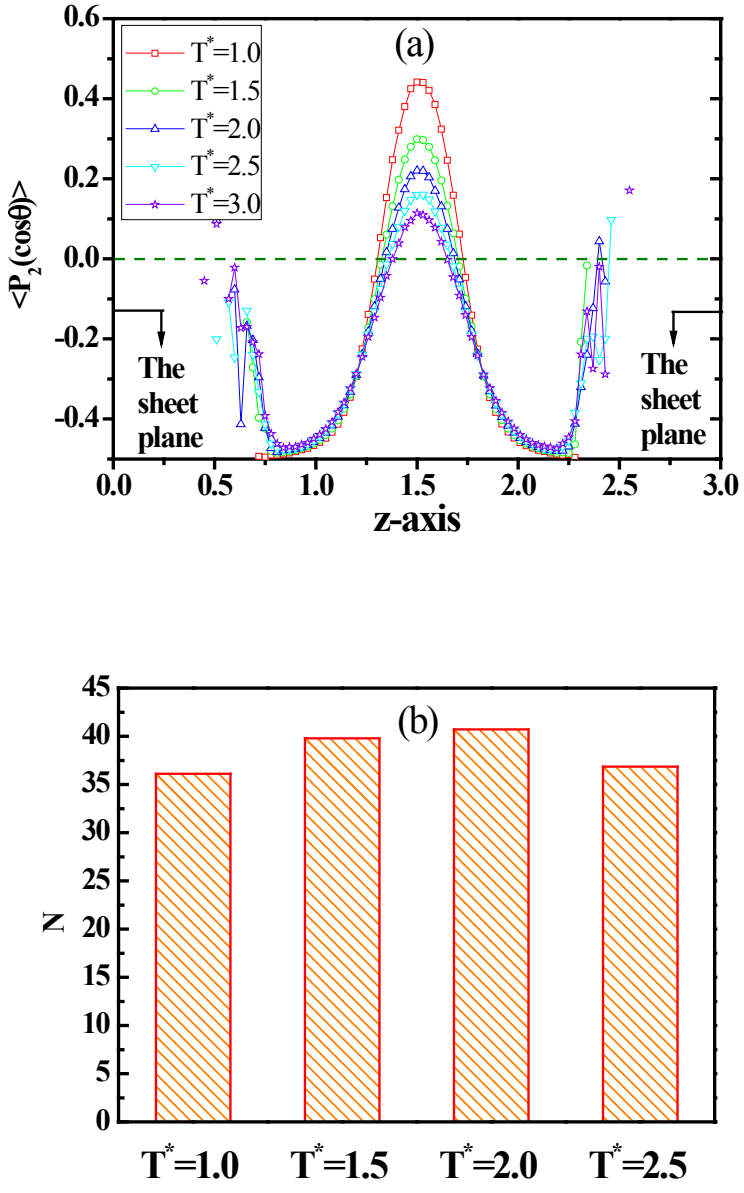

Figure S5. (a) The orientation order parameter $< P_2(\cos\theta) >$ versus the relative position Z for different temperature; (b) The number of bridged chain N is plotted versus different temperature.

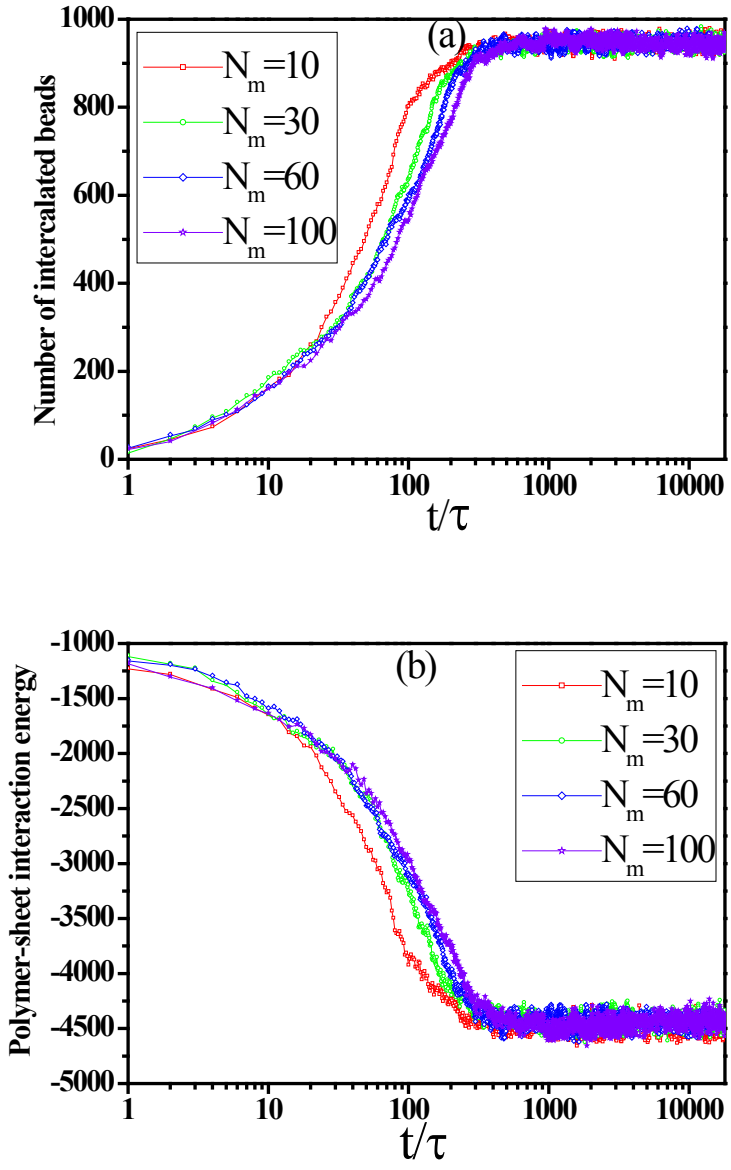

Figure S6. (a) The number of intercalated beads as a function of the simulation time for different polymer chain length; (b) The polymer-sheet interaction energy as a function of the simulation time for different polymer chain length.

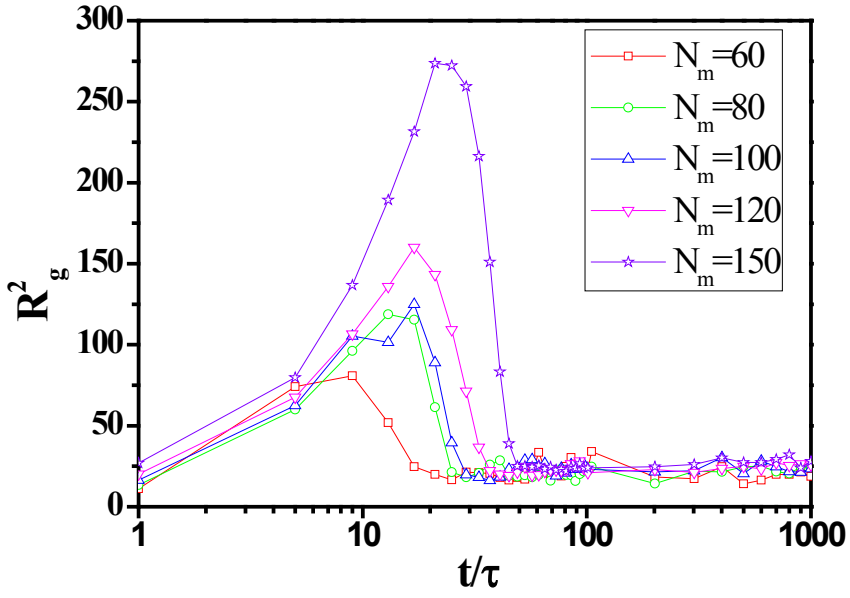

Figure S7. The mean-square radius of gyration R_g^2 as a function of the simulation time for different polymer chain length;

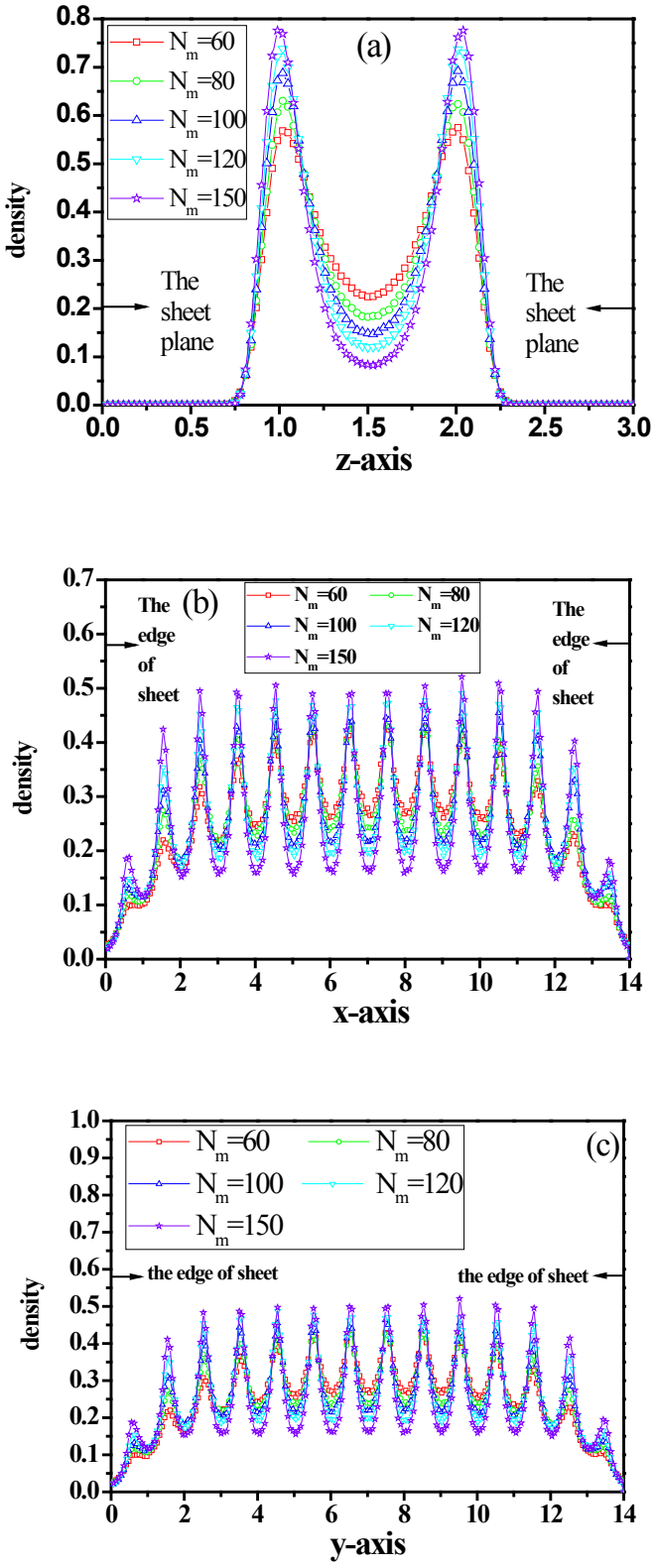

Figure S8. (a) The atomic density profiles in the direction normal to the layered sheets surface versus the relative position Z; (b) The atomic density profiles in the direction parallel to the layered sheets surface versus the relative position X; (c) The atomic density profiles in the direction parallel to the layered sheets surface versus the relative position Y.

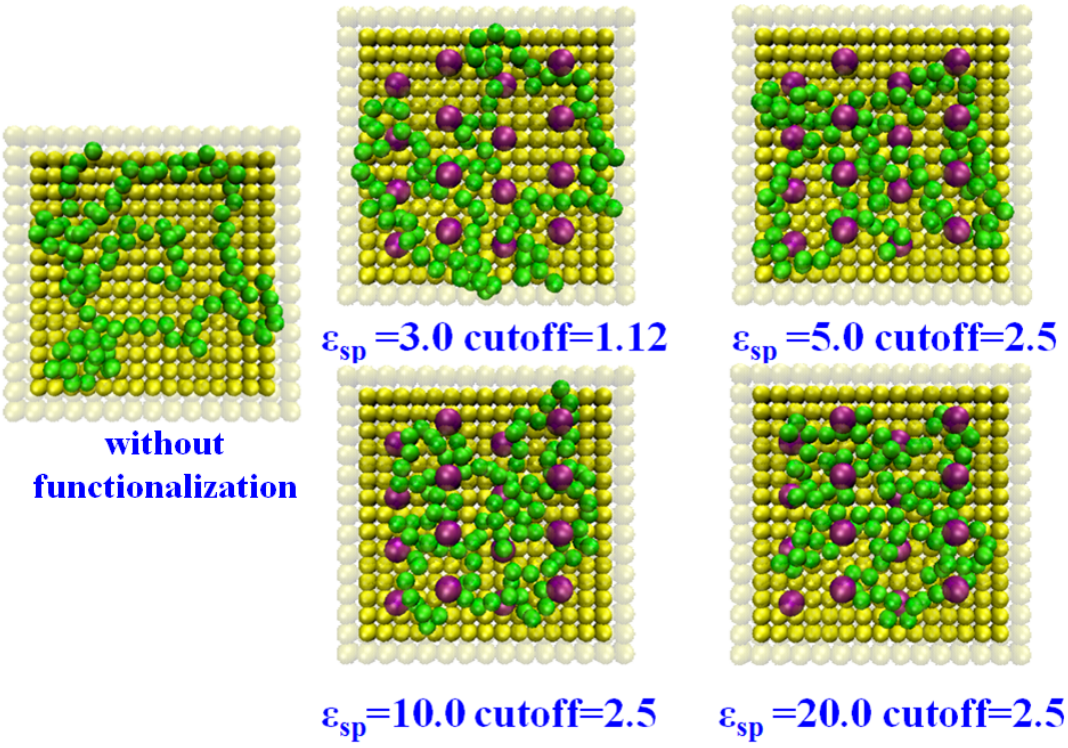

Figure S9. The snapshot for different polymer-surfactant interaction; The yellow and glass yellow spheres denote the layered sheets, a purple sphere denotes a surfactant and the polymer chain is represented by green spheres.

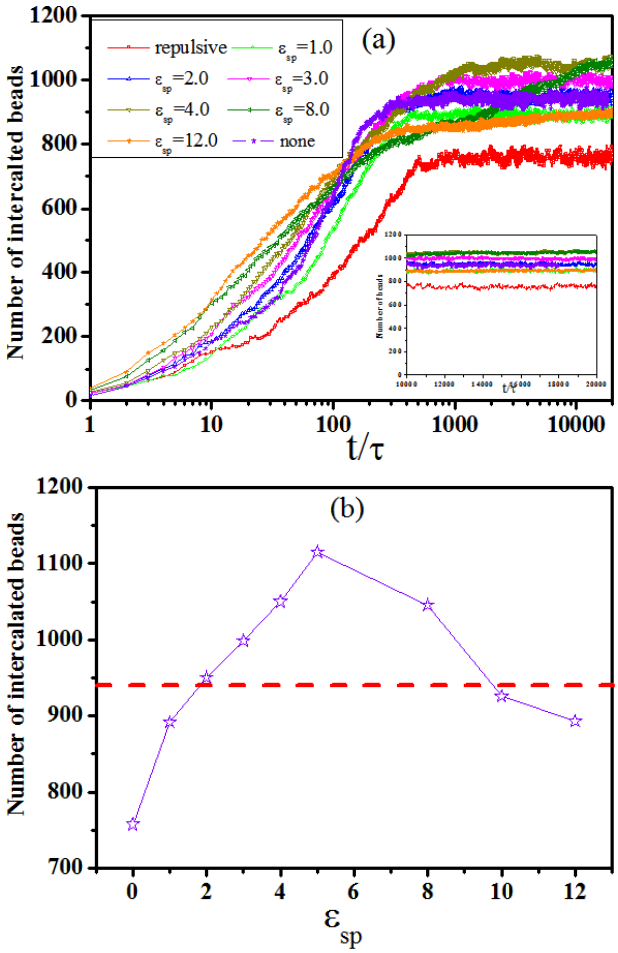

Figure S10. (a) The number of intercalated beads as a function of the simulation time for different polymer-surfactant interaction. (b) The number of intercalated beads as a function of polymer-surfactant interaction ε_{sp}. The red line denotes the system without modification.

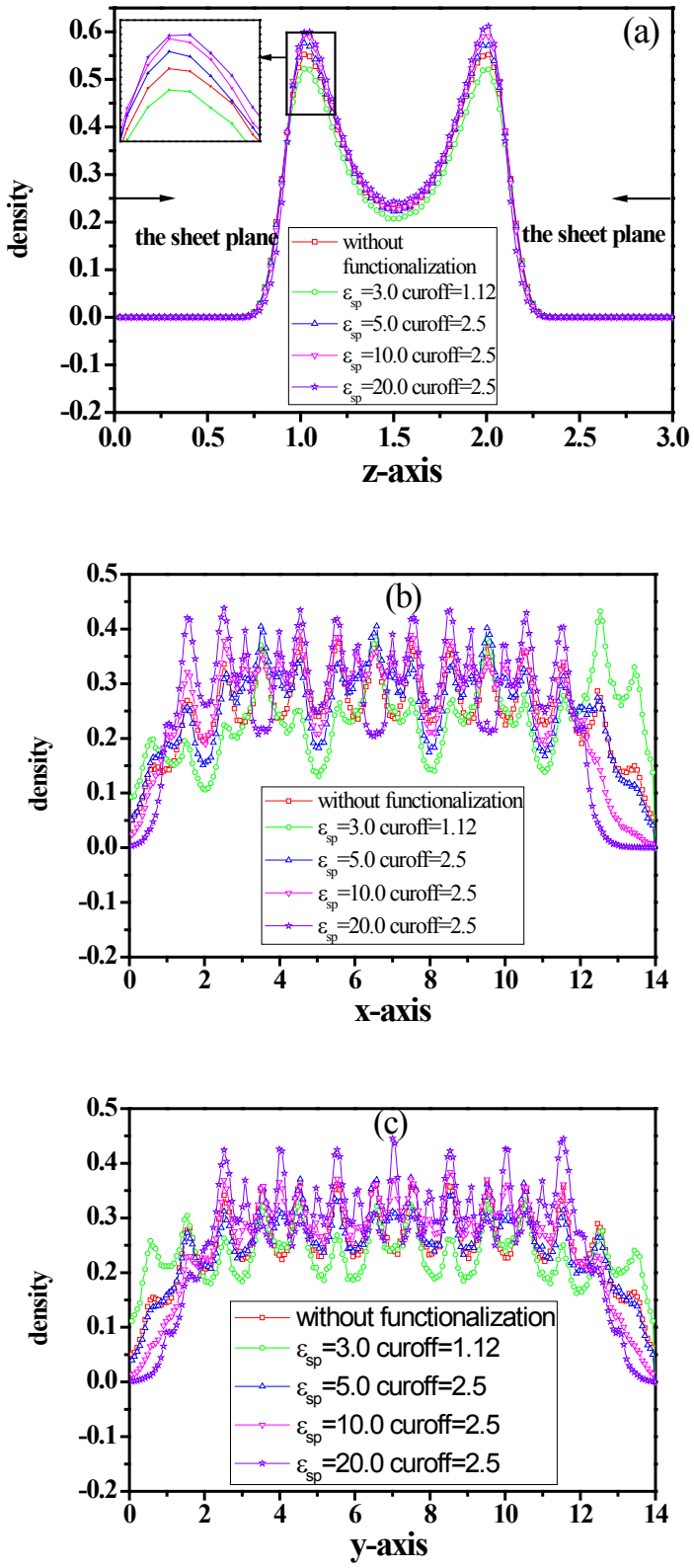

Figure S11. (a) The atomic density profiles in the direction normal to the layered sheets surface versus the relative position Z;(b) The atomic density profiles in the direction parallel to the layered sheets surface versus the relative position X;(c) The atomic density profiles in the direction parallel to the layered sheets surface versus the relative position Y.

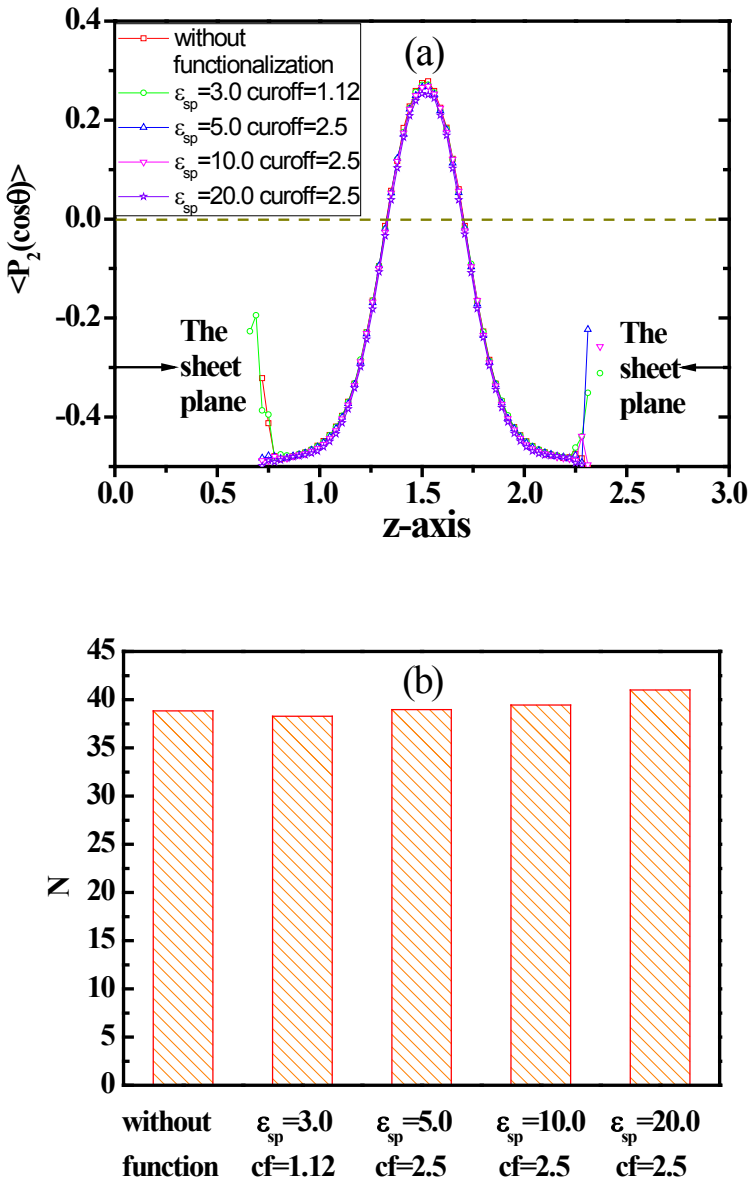

Figure S12. (a) The orientation order parameter $< P_2(\cos\theta) >$ versus the relative position Z for different polymer-surfactant interaction; (b) The number of bridged chain N is plotted versus different polymer-surfactant interaction.

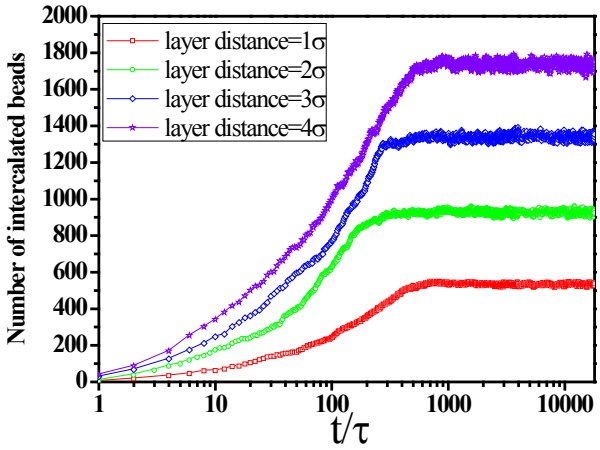

Figure S13. The number of intercalated beads as a function of the simulation time for different interlayer distances.

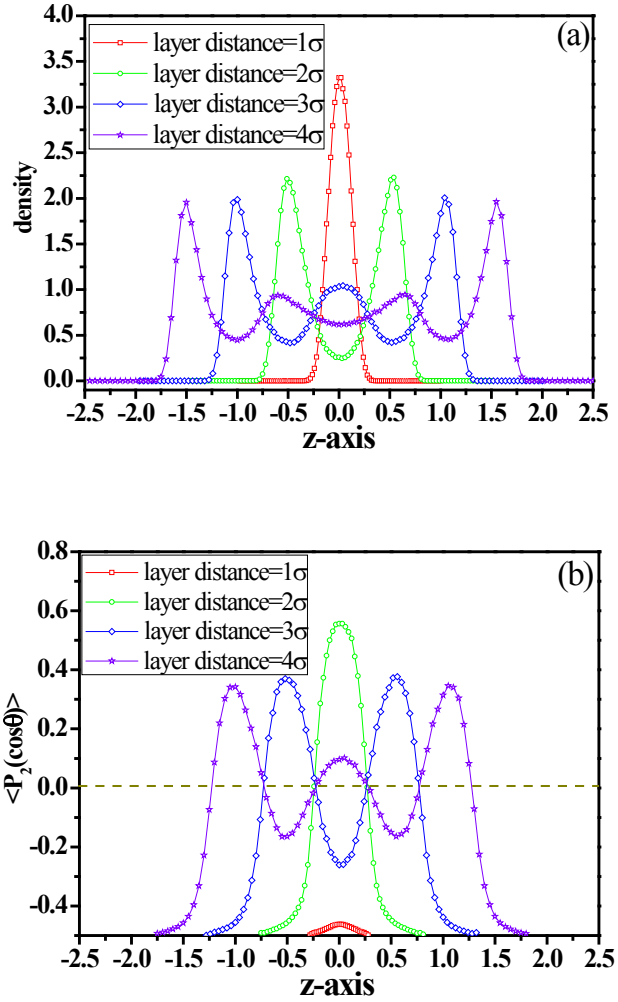

Figure S14. (a) The atomic density profiles in the direction normal to the sheet surface versus the relative position Z; (b) The orientation order parameter versus the relative position Z for different interlayer distance.