Monte Carlo Study of Degenerate Behavior of AB Diblock Copolymer/Nanoparticle under Cylindrical Confinement

Yingying Wang[†,‡,§], Yuanyuan Han*[,†], Jie Cui*[,†], Wei Jiang[†], Yingchun Sun[‡]

[†]*State Key Laboratory of Polymer Physics and Chemistry, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, Changchun 130022, Jilin, China*

[‡]*Northeast Normal University, School of Physics, Changchun 130024, Jilin, China*

[§]*University of Chinese Academy of Sciences, Beijing 100049, People's Republic of China*

*Corresponding authors: *E-mail: yyhan@ciac.ac.cn (Yuanyuan Han); jcui@ciac.ac.cn (Jie Cui). Telephone: 86-431-85262642. Fax: 86-431-85262126.

ASSOCIATED CONTENT

Supporting Information

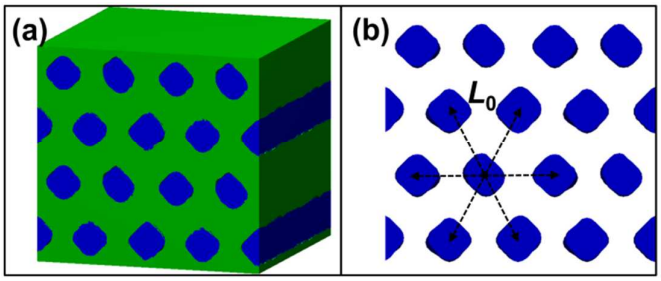

Figure S1. Typical hexagonally packed cylindrical phase formed by A_5B_{15} diblock copolymers in bulk (a). For the purpose of clarity, only minor component A is drawn in blue (b). The minority block A and majority block B are represented by blue and green, respectively.

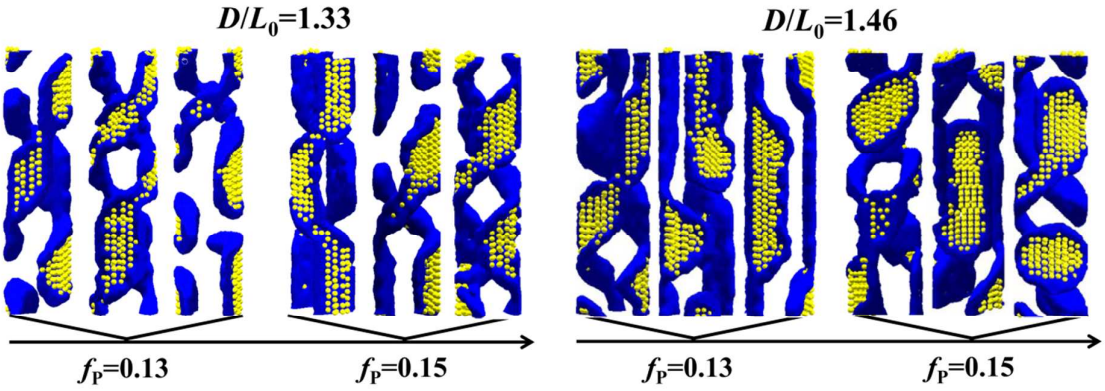

Figure S2. Typical disordered structures formed by A_5B_{15} diblock copolymer/NP mixture in cylindrical pores with different pore sizes (D/L_0) and NP contents (f_P). For the purpose of clarity, only minor component A and NPs are drawn. The minority block A and NPs are represented by blue and yellow, respectively.

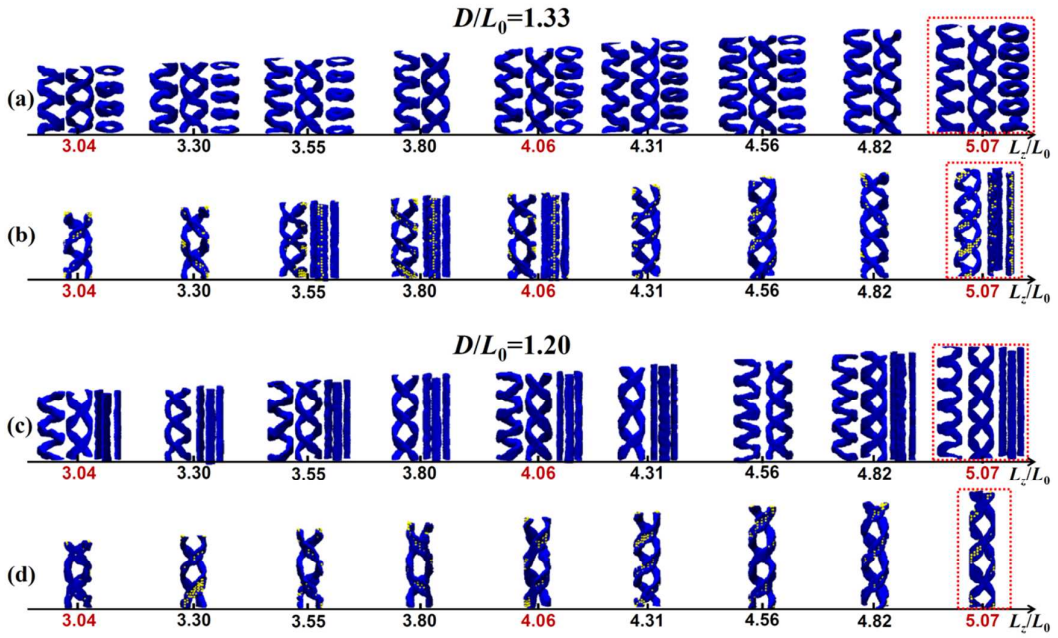

Figure S3. Nanostructures self-assembled by BCP/NP mixture in cylindrical pores as a function of the pore length (L_z/L_0). The pore diameters and NP contents are (a) $D/L_0=1.33$, $f_P=0$; (b) $D/L_0=1.33$, $f_P=0.05$; (c) $D/L_0=1.20$, $f_P=0$;(d) $D/L_0=1.20$, $f_P=0.05$. The nanostructures obtained at $L_z=80$ ($L_z/L_0=5.07$) (Figure 2 in the manuscript) are also given for the purpose of comparison, which are marked with red boxes. Only the minority blocks A and NPs are drawn for clarity.

Table S1. Average interactive enthalpy densities of double helices under different pore lengths (L_z/L_0) and NP contents (f_P). The pore size is fixed at $D/L_0=1.20$.

NP content (f_P)	Pore length (L_z/L_0)								
	3.04	**3.33**	**3.55**	**3.80**	**4.06**	**4.31**	**4.56**	**4.82**	**5.07**
0.00	1.029	1.032	1.031	1.032	1.031	1.030	1.034	1.030	1.030
0.05	1.024	1.024	1.025	1.030	1.028	1.027	1.035	1.026	1.026

Table S2. Average interactive enthalpy densities of double helices under different pore lengths (L_z/L_0) and NP contents (f_P). The pore size is fixed at $D/L_0 = 1.33$.

NP content (f_P)	Pore length (L_z/L_0)								
	3.04	**3.33**	**3.55**	**3.80**	**4.06**	**4.31**	**4.56**	**4.82**	**5.07**
0.00	1.037	1.026	1.026	1.015	1.021	1.023	1.029	1.026	1.032
0.05	1.025	1.020	1.028	1.022	1.027	1.025	1.020	1.021	1.025

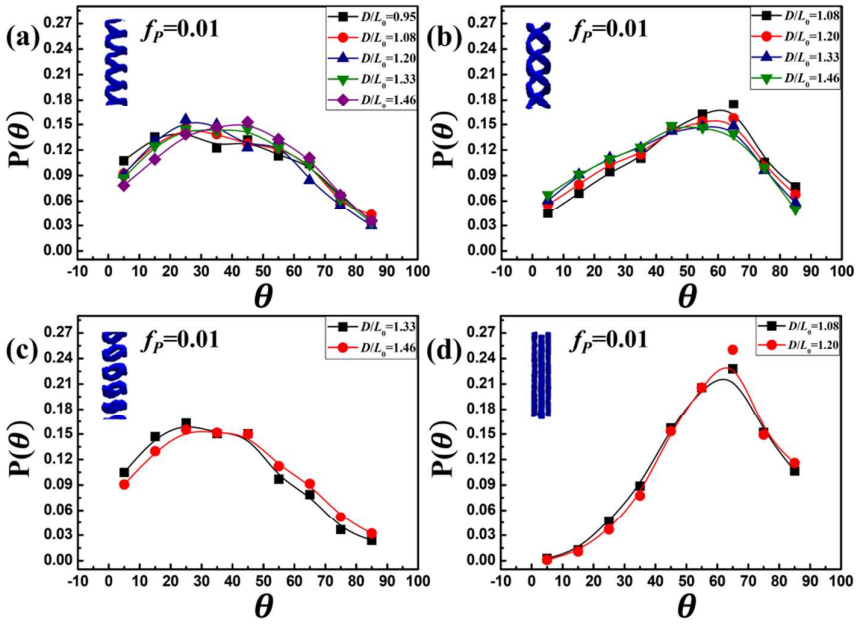

Figure S4. Distribution curves of the orientation angle θ for different degenerate structures obtained under different pore sizes in the case of $f_P = 0.01$.

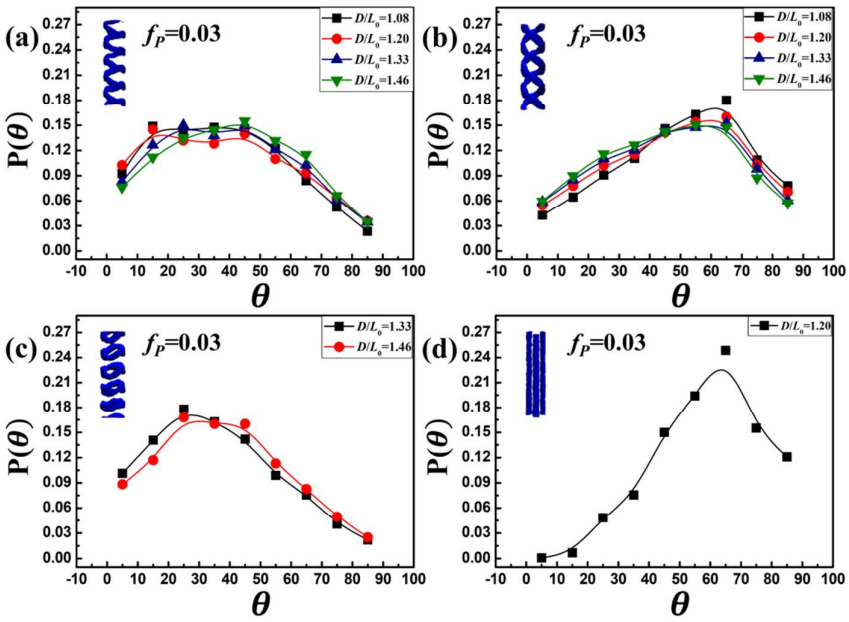

Figure S5. Distribution curves of the orientation angle θ for different degenerate structures obtained under different pore sizes in the case of $f_P = 0.03$.

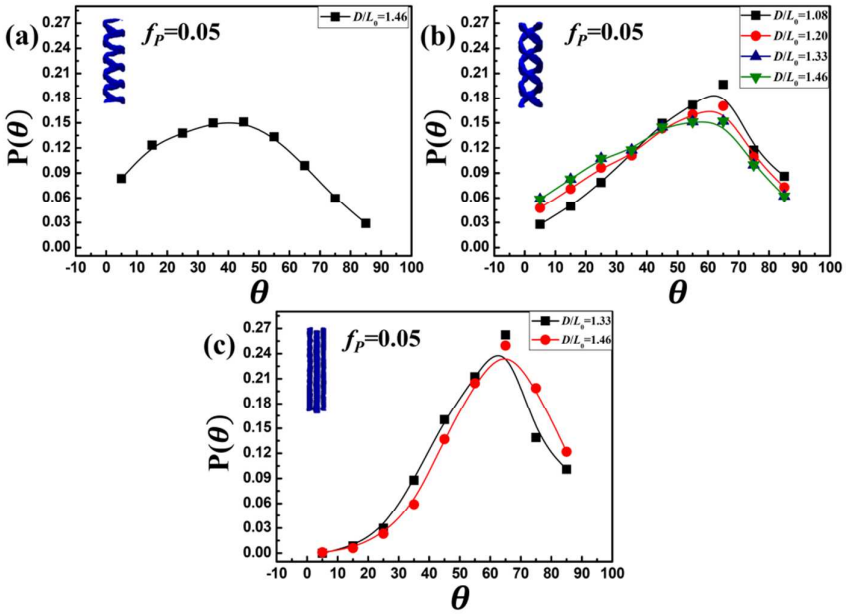

Figure S6. Distribution curves of the orientation angle θ for different degenerate structures obtained under different pore sizes in the case of $f_P = 0.05$.

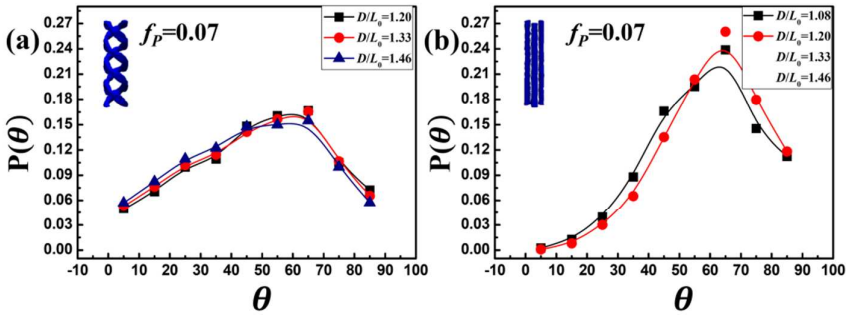

Figure S7. Distribution curves of the orientation angle θ for different degenerate structures obtained under different pore sizes in the case of $f_P = 0.07$.

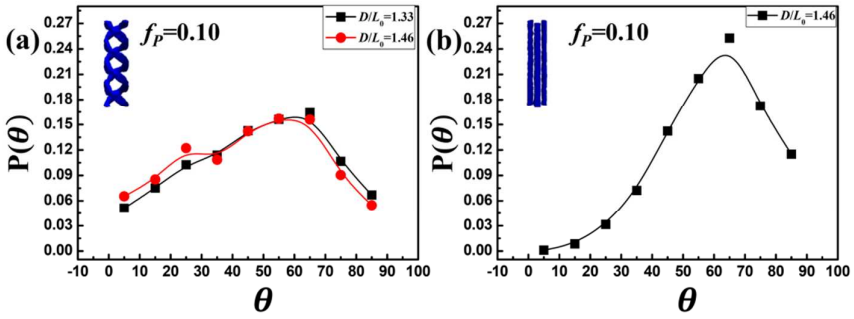

Figure S8. Distribution curves of the orientation angle θ for different degenerate structures obtained under different pore sizes in the case of $f_P = 0.10$.