Electronic Supplementary Material (ESI) for Soft Matter.

Supplementary Information

A simulation study of self-assembly of ABC star terpolymers confined between two parallel surfaces

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Table S1 The estimated characteristic length L_1 values as functions of x ($x = N_C/N_A$, $N_A = N_B$) and λ ($\lambda = \varepsilon_{AC}/\varepsilon_{AB}$, $\varepsilon_{AC} = \varepsilon_{BC}$) for phases listed in Fig. 1.

λ \ x (L_1)	2/6	3/6	4/6	5/6	6/6	7/6	8/6	9/6	10/6	11/6	12/6	13/6	14/6	15/6
2.0	13.1	17.5	17.6	18.6	19.6	—	—	—	11.5	12.3	12.5	12.5	12.6	13.2
1.0	10.5	11.2	12.6	18.8	19	19.4	21.4	—	—	—	—	12.6	13.3	13.5
0.5	10.4	13.9	12.3	12.1	12.2	20.6	20.2	20	20.4	—	—	—	—	—

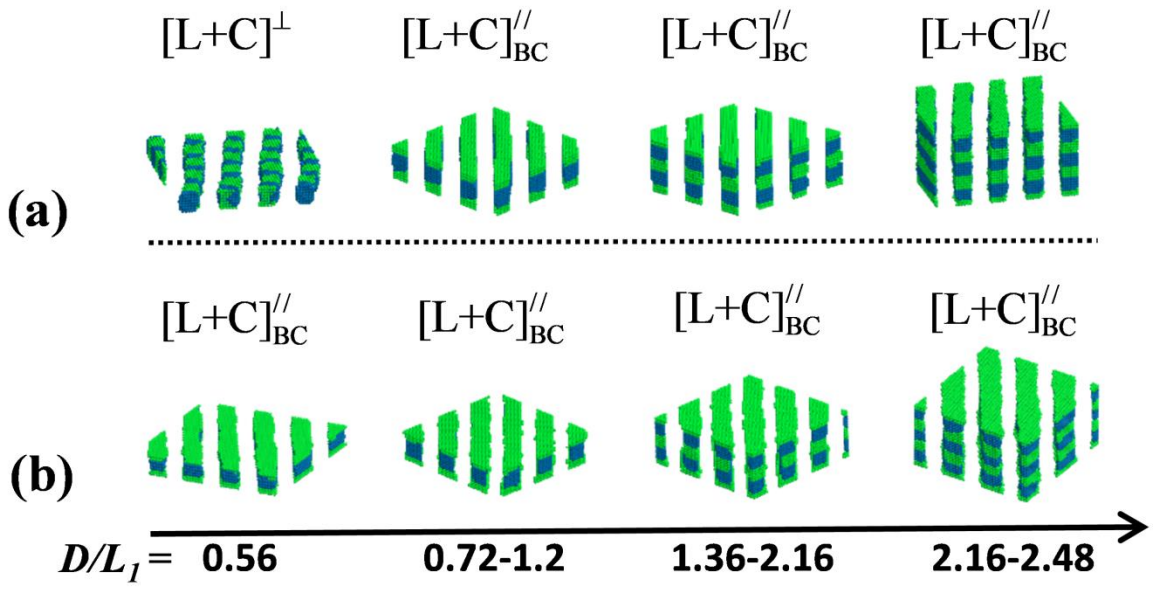

Fig. S1 Phase sequences as a function of D/L_1 for the bulk [L+C]-forming star terpolymers $A_6B_6C_{12}$ with λ=2 in the thin films at different surface filed: (a) ε_{AS}=1.0, ε_{BS}=0.3, ε_{CS}=0.2; (b) ε_{AS}=1.0, ε_{BS} = 0, ε_{CS}=0.5. Oblique views of A- and B- domains are shown. Color scheme: A (blue), B (green).

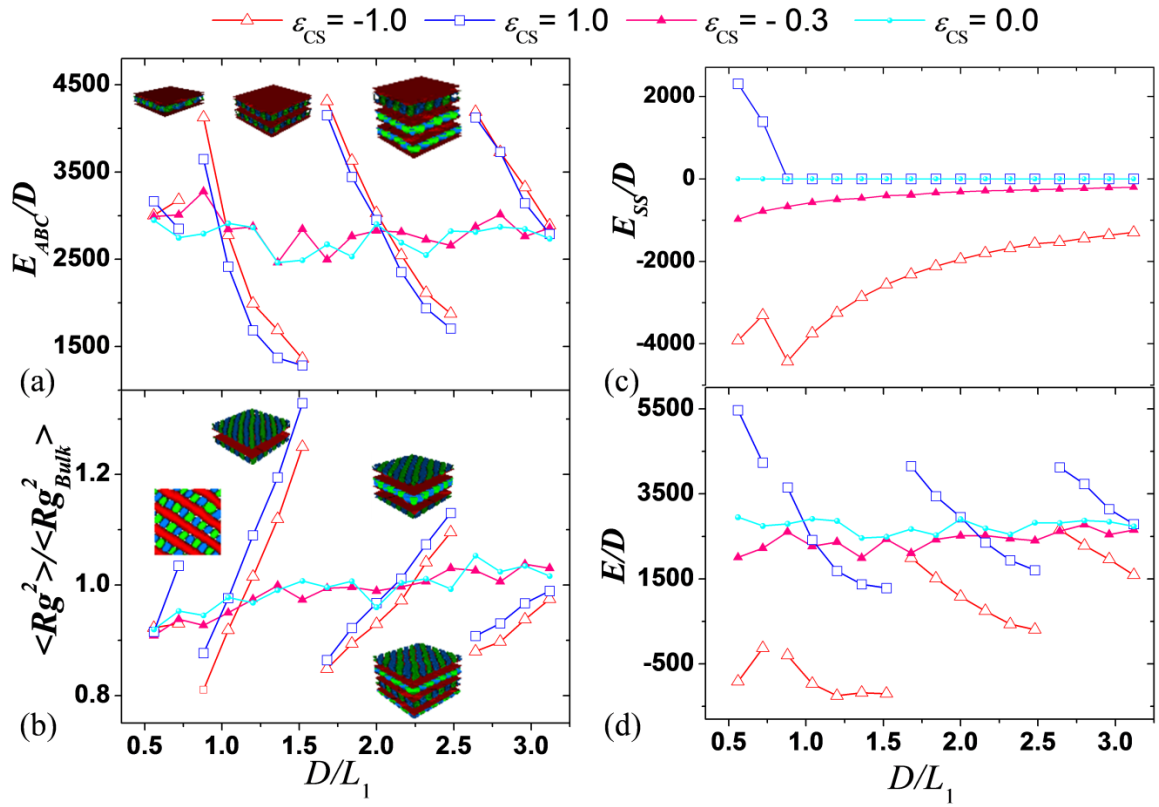

Fig. S2 Variations of normalized (a) interface energy, (b) mean-square radius of gyration, (c) surface energy and (d) total energy with D/L_1 for terpolymers $A_6B_6C_{12}$ with λ =2 (ε_{AB}=1.0, ε_{AC}=ε_{BC}=2.0). $< Rg^2_{Bulk} >$ is the mean-square radius of gyration for the corresponding bulk phase. $E_{ABC} / D = (\varepsilon_{AB} \times n_{AB} + \varepsilon_{AC} \times n_{AC} + \varepsilon_{BC} \times n_{BC}) / D$, $E_{SS} / D = (\varepsilon_{CS} \times n_{CS}) / D$, n_{AB}, n_{AC}, n_{BC} and n_{CS} are the average of the contact number between segments A and B, A and C, B and C, and surfaces and C, respectively. $E = E_{SS} + E_{ABC}$. Some snapshots obtained at ε_{CS} = -1.0 and ε_{CS} = 1.0 are also shown in (a) and (b), respectively.

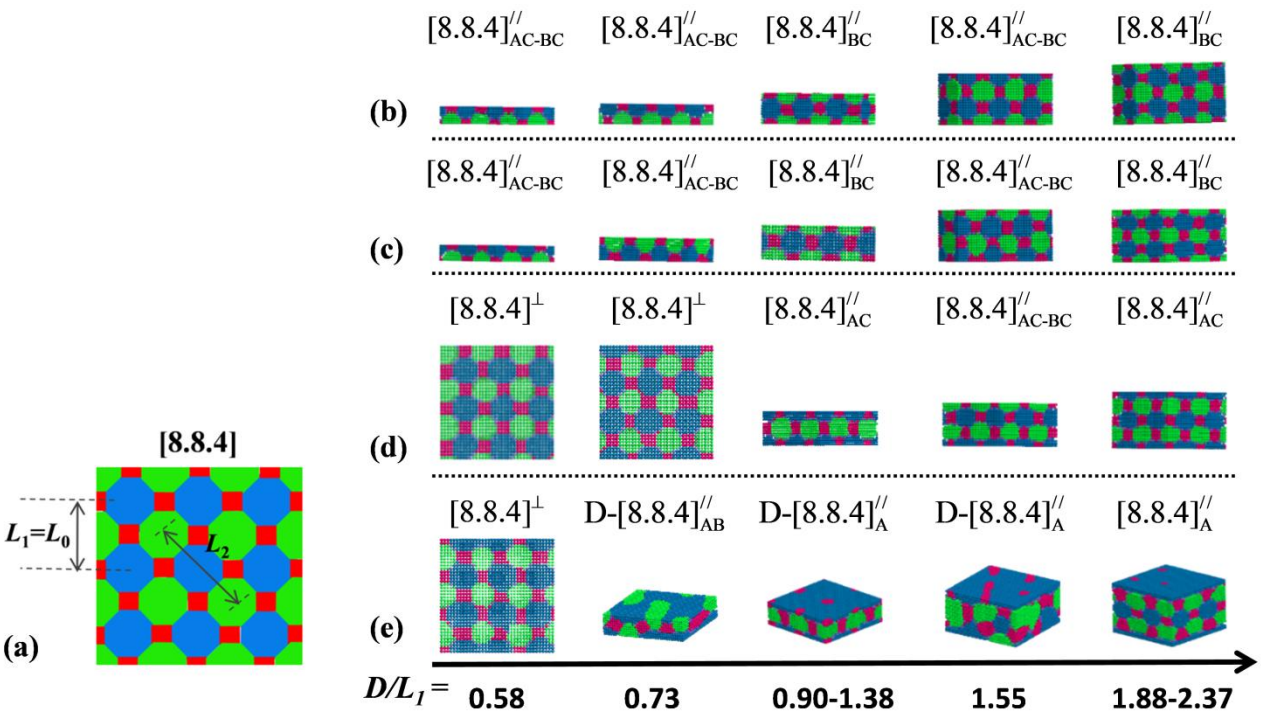

Fig. S3 (a) A schematic illustration of the characteristic lengths L_1 and L_2 in a [8.8.4] phase. Phase sequences as a function of D/L_1 for the bulk [8.8.4]-forming star terpolymers $A_6B_6C_4$ with λ=0.5 in the thin films at different ε_{AS} values. (b) ε_{AS} = 0.2, (c) ε_{AS} = 0.5, (d) ε_{AS} = -0.2, (e) ε_{AS} = -0.5. Top view is given for phase $[8.8.4]^{\perp}$, side view is given for parallel phases $^{/}$and oblique view is given for phases with A-wetting layers.

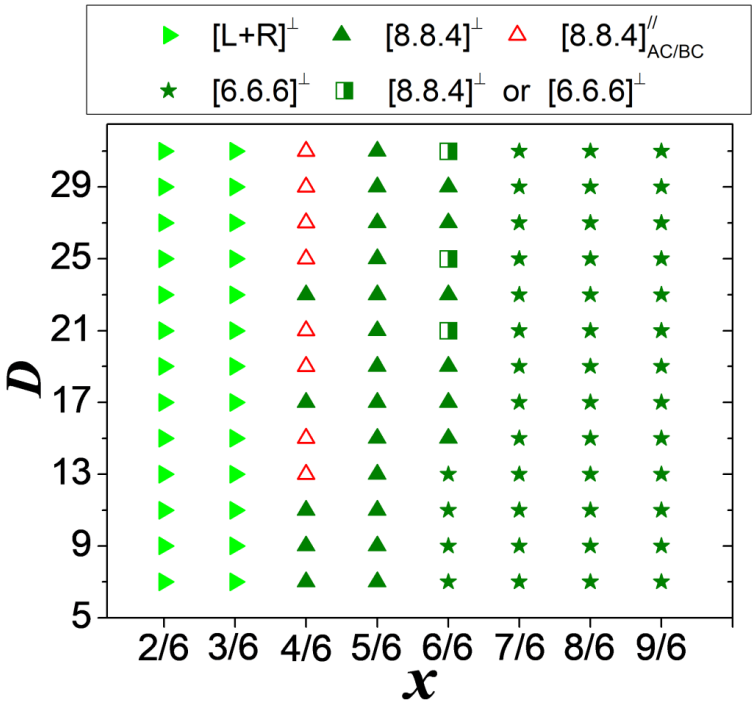

Fig. S4 Phase diagrams in space of arm length ratio $x = N_C/N_A(N_A=N_B)$ and film thickness D for ABC star terpolymers with λ=0.5 ($\varepsilon_{AC}=\varepsilon_{BC}$=1.0, ε_{AB}=2.0) confined between neutral surfaces.