Electronic Supplementary Information for

Morphological Transition Difference of Linear and Cyclic Block Copolymer with Polymer Blending in Selective Solvent by Combining Dissipative Particle Dynamics and All-atom Molecular Dynamics Simulation Based on ABEEM Polarizable Force Field

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1 Methods and models

1.1 Dissipative particle dynamics simulation and all-atom molecular dynamics simulation based on ABEEM polarizable force field

The dissipative particle dynamics method is a mesoscopic simulation technique for complex fluids. It realizes the simulation of coarse-grained systems over long length and time scales, which may be beyond conventional molecular dynamics simulation methods. In dissipative particle dynamics simulation, several atoms or repeat units are grouped together and presented by a single bead according to their chemical identity and their environment. Therefore, the algorithm increases simulation scale by several orders of magnitude compared to atomistic simulation. The time evolution of the position and velocity of all beads is governed by Newton's equation of motion,

$$\frac{d\boldsymbol{r}_i}{dt} = \boldsymbol{v}_i , \ m_i \frac{d\boldsymbol{v}_i}{dt} = \boldsymbol{F}_i \tag{1}$$

where $\boldsymbol{r}_i$ and $\boldsymbol{v}_i$ are the position and velocity vectors of the ith particle, respectively,

and $\boldsymbol{F}_i$ is the total force vector acting on each particle. The total force acting on a

particle within a cutoff radius r_c is composed of five different components:

conservative force ($\vec{F}_{ij}^{C}$), dissipative force ($\vec{F}_{ij}^{D}$), random force ($\vec{F}_{ij}^{R}$), ， spring force

($\vec{F}_{i}^{S}$), and angle force ($\vec{F}_{i}^{A}$).

$$\boldsymbol{F}_i = \sum_{j \neq i} (\boldsymbol{F}_{ij}^{C} + \boldsymbol{F}_{ij}^{D} + \boldsymbol{F}_{ij}^{R}) + \boldsymbol{F}_{i}^{S} + \boldsymbol{F}_{i}^{A} \tag{2}$$

where $\boldsymbol{F}_{ij}^{C}$ is the conservative repulsive force representing excluded volume, $\boldsymbol{F}_{ij}^{D}$ is the

dissipative force representing the viscous drag between moving beads, and $\boldsymbol{F}_{ij}^{R}$ is the

random force representing stochastic impulse. Both $\boldsymbol{F}_{ij}^{D}$ and $\boldsymbol{F}_{ij}^{R}$ act together as a

thermostat for the beads. All forces are short-ranged and effective within a cutoff

radius. The remaining terms are bonded interactions: $\boldsymbol{F}_{i}^{S}$ controlling the bond

stretching and $\boldsymbol{F}_{i}^{A}$ representing the angle bending.

The conservative force F_{ij}^{C} is a purely soft repulsive force that acts along the line connecting two bead centers, and is given by:

$$F_{ij}^{C} = \begin{cases} a_{ij}(1 - r_{ij}/r_c)e_{ij} & (r_{ij} < r_c) \\ 0 & (r_{ij} \geq r_c) \end{cases} \tag{3}$$

where $r_{ij} = r_i - r_j$, $r_{ij} = |r_{ij}|$, $e_{ij} = r_{ij}/r_{ij}$, r_i and r_j are the position vectors of particle i and j, respectively. a_{ij} is the maximum repulsive interaction parameter between two interacting beads i and j and describes the interaction strength between the beads, and r_c is the cutoff radius, with $r_c = 1.0$. The soft repulsion force used here allows the simulation for a larger length-scale and longer time-scale. The interaction parameter a_{ij}, which is dependent on the characteristics of the mixture, plays a significant role in determining the nanostructure of the equilibrated polymer solution. In principle, the conservative force can include various kinds of forces such as electrostatic and van der Waals forces.

The velocity-dependent dissipative force corresponding to a viscous drag force acts on the relative velocities of particles reducing velocity differences between the particles. It depends on both the position and relative velocities of the beads. The random force compensates for the loss of kinetic energy due to the dissipative force. The dissipative force and the random force are responsible for the thermostat and the conservation of total momentum in the simulation. They are given by the following expressions:

$$F_{ij}^{D} = -\gamma \omega^{D}(r_{ij})(v_{ij} \cdot e_{ij})e_{ij} \tag{4}$$

$$F_{ij}^{R} = \sigma \omega^{R}(r_{ij})\xi_{ij}\Delta t^{-1/2}e_{ij} \tag{5}$$

where $v_{ij} = v_i - v_j$, v_i and v_j are the velocity vectors of particle i and j, respectively. σ is the noise amplitude, γ is the friction coefficient, σ and γ define magnitude of the dissipative and random forces, respectively, $\omega^{D}(r_{ij})$ and $\omega^{R}(r_{ij})$ are weight functions vanishing for $r_{ij} > r_c$ that describe the r-dependent range of the dissipative and random forces, and ξ_{ij} is a randomly fluctuating variable with a Gaussian probability distribution, i.e., zero mean and unit variance chosen independently for each interacting pairs of beads at each time step Δt.

$$\langle \xi_{ij}(t) \rangle = 0, \langle \xi_{ij}(t)\xi_{kl}(t') \rangle = (\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})\delta(t - t') \tag{6}$$

In order to satisfy the fluctuation-dissipation theorem and for the system to evolve to an equilibrium state that corresponds to the Gibbs canonical ensemble, the following relation needs to be imposed:

$$\omega^D(r_{ij}) = \left[\omega^R(r_{ij})\right]^2 \tag{7}$$

either $\omega^D(r_{ij})$ or $\omega^R(r_{ij})$ can be chosen arbitrarily, and the other one is then fixed. In addition, the values of parameters γ and σ are coupled by the following relation

$$\sigma^2 = 2\gamma k_B T \tag{8}$$

where T is the absolute temperature and k_B is the Boltzmann constant. γ and σ are generally set to be 4.5 and 3.0 in the present simulations. The temperature $k_B T$ is chosen to be 1.0. Generally, according to Groot and Warren, the following weight function within the cutoff distance is optimized and chosen for soft chains in aqueous solution

$$\omega^D(r_{ij}) = \left[\omega^R(r_{ij})^2\right] = \begin{cases} (1-r_{ij}/r_c)^2 & (r_{ij} < r_c) \\ 0 & (r_{ij} \geq r_c) \end{cases} \tag{9}$$

The spring force has to be included to simulate the motion of adjacent beads on the polymer chains. The interaction force between bonded consecutive particles is given by

$$\boldsymbol{F}_i^S = \sum_j C\boldsymbol{r}_{ij} \tag{10}$$

where beads j are those that are connected to bead i. C is the spring constant between two adjacent beads in a Gaussian chain and is chosen to be 4.0 to properly account for the distance between connected beads. Due to the domination of repulsive forces between soft spheres in the mean segment length, the end point distribution of the polymers is not very sensitive to the value of constant C. The value results in a slightly smaller distance for bonded particles than for nonbonded ones, and the sum runs over all particles to which particle i is connected.

In some conditions, an angle force between every two consecutive bonds is introduced to characterize the rigidity of the rod blocks well.

$$\boldsymbol{F}_i^A = k_\theta (\theta - \theta_0) \tag{11}$$

where k_θ is the bending modulus and represents the flexible and rigid nature of polymer chain. $\theta_0 = \pi$ represents the equilibrium angle between consecutive bonds. $k_\theta = 0$ corresponds to a flexible block, such as the coil block in the present model. Since the rod block is not involved in the polymers studied here, the angle force $\boldsymbol{F}_i^A$

is not thus applied in this study.

As anticipated, particles represent groups of real atoms or polymer monomers in dissipative particle dynamics; thus, atomic level details are lost while interactions between different bead types become the main parameters governing the mesoscopic system behavior. The parameter a_{ij} is the main dissipative particle dynamics interaction parameter with the dimension of a force. As a consequence of the purely repulsive nature of the conservative force defining a_{ij}, only liquid-liquid or solid-liquid interfaces can be simulated in constant volume dissipative particle dynamics ensembles. In this respect, the dissipative particle dynamics theory is similar to the Flory-Huggins theory of lattice polymers, and indeed the interaction parameter a_{ij} of the dissipative particle dynamics conservative force can be mapped onto the Flory-Huggins parameter χ_{ij} by assuming that, for a polymer, the beads are connected in a chain by springs. In order to calculate a_{ij}, both a_{ii} and χ_{ij} should be determined. When i equals to j, the repulsion parameter between two identical type beads is given by

$$a_{ii} = \frac{75k_BT}{\rho} \tag{12}$$

where ρ is the bead number density usually chosen as 3, and the conservative interaction potential, k_BT, is chosen as 1. In principle, the density chosen in dissipative particle dynamics simulation is a free parameter, but the system with a larger ρ requires a longer computational time. Groot and Warren suggested that $\rho = 3$ and hence $a = 25k_BT$ are reasonable parameters for liquids.

For $\rho = 3$, the repulsive parameter between different types of beads a_{ij} is the key to the simulation and is calculated according to the linear relation with Flory-Huggins χ_{ij} parameters proposed by Groot and Warren[1]:

$$a_{ij} = a_{ii} + 3.27\chi_{ij} \tag{13}$$

where χ_{ij} is calculated from the solubility parameters, which depend on the chemical character of beads and can be obtained by all-atom molecular dynamics simulation based on ABEEM polarizable force field.

The more critical factor is to choose a force field with better performance. The parameterization of the force field is a very important and tough task. When a new

force field or a parameter beyond original force field is introduced to compute new property, there needs substantial work to fit the parameter in order to arrive at an agreement. The force field is very sensitive to a few parameters, which is usually used to compute the nonbonded interaction and torsional interaction. It could take a lot of time in fitting and testing the nonbonded and torsional interaction parameters. Actually the quality of the nonbonded interaction presents the advantage of a force field. The explicit inclusion of electronic polarization will represent the next significant development in the treatment of nonbonded interactions in biomolecular force fields.[2] Based on ABEEM, a polarizable force field with multiple fluctuating partial charges per atom, ABEEM PFF, has shown its prominent performance.[3] ABEEM PFF can present well the nonbonded interaction in the system, especially to the electrostatic interactions. In fact, the intermolecular interaction not only comes from van der Waals interaction and electrostatic interaction, but also the change in the bond length and angle, whose contribution is not dominant. The major contribution to the nonbonded interaction is van der Waals interaction and electrostatic interaction. The intermolecular nonbonded interaction in ABEEM PFF is summed up for all sites including atoms, bonds, and lone pair electrons.

The nonbonded part of the energy of a system is generally computed as a sum of the Coulomb and Lennard-Jones contributions for pairwise intra- and intermolecular interaction. E_{vdW} describes the van der Waals nonbonded atom-atom interaction:

$$E_{vdW} = \sum_{i<j} 4 f_{ij} \varepsilon_{ij} (\sigma_{ij}^{12} / r_{ij}^{12} - \sigma_{ij}^{6} / r_{ij}^{6}) \tag{14}$$

Geometric combining rules for the Lennard-Jones coefficients are employed: $\sigma_{ij} = (\sigma_{ii}\sigma_{jj})^{1/2}$ and $\varepsilon_{ij} = (\varepsilon_{ii}\varepsilon_{jj})^{1/2}$. The summation runs over all of the pairs of nonbonded atoms i and j, If i and j are intramolecular, the coefficient $f_{ij} = 0.0$ for any i-j pair connected by a valence bond (1-2 pairs) or a valence bond angle (1-3 pairs), $f_{ij} = 0.5$ for 1-4 pairs connected by a torsional angle and $f_{ij} = 1.0$ for all other intramolecular and intermolecular cases. Compared to other force fields, the key difference of ABEEM PFF is the treatment of the electrostatic interaction energy. The electrostatic interaction energy is actually expressed as

$$E_{elec} = \sum_{i<j} k_{ij} q_i q_j / r_{ij} \tag{15}$$

where r_{ij} is the distance between sites i and j. q_i and q_j are the partial charges of regions or sites i and j, which are calculated by the ABEEM. The introduced parameter k_{ij} may be said to be a result of considering the exchange, penetration, and shielding effect in the interaction between the two pieces of electron clouds i and j. k_{ij} is optimized and set to be 0.57 empirically, except for hydrogen-bond regions. In

molecular simulations, ABEEM is applied to calculate partial charges of all regions, namely, atoms, lone pairs, σ bonds, and π bonds, and then compute the total energy of the system. If there is a geometrical change, for instance, a change of bond length, angle, dihedral angle, or relative position between molecules, we will recalculate the partial charges using ABEEM, and then the total energy. In this manner, a systematic partial charge fluctuation in accordance with molecular environment variation is provided by ABEEM.[3]

The calculation of electrostatic interaction energies is often determined by "fixed" atom-centered monopoles. The invariant nature of this representation prevents the response to an external electrostatic field, i.e. electronic polarization. Polarization effects are known to yield an additional attractive intermolecular force. The error in the intermolecular interactions due to the absence of polarization effects can be compensated with an overestimate of the dispersion interaction and atomic partial charges. This compensation of errors is one of the reasons why nonbonded parameters for nonpolarizable force fields obtained from high-level ab initio calculations on dimers in the gas phase are not simply transferable to condensed phase systems. An explicit treatment of polarization is indispensable for the transferability of force field parameters from the ab initio gas-phase reference data to large-scale biochemical simulations.

In this study, ABEEM PFF is adopted to compute cohesive energy and further the solubility parameter. The solubility parameter is calculated from the molar cohesive energy, which is obtained from the difference between the total nonbonded energy of the system in isolated chains and that of the amorphous cell in the period boundary condition. The cohesive energy of a material is the increase in the internal energy per mole of the material if all of the intermolecular forces are eliminated. In all-atom molecular dynamics simulations, we can obtain the cohesive energy E_{coh} by[4]

$$E_{coh} = \left(\sum_{i=1}^{n} E_{nb}^{isolated}(i) - E_{nb}^{n} \right) \bigg/ n \tag{16}$$

where $E_{nb}^{isolated}(i)$ is the nonbonded energy for the ith isolated chain in vacuum, and

E_{nb}^{n} is the nonbonded energy of the model with n chains in periodic boundary conditions.

The key to the dissipative particle dynamics simulation is to obtain the interaction parameter between beads. The interaction parameter is closely related to the miscibility between beads. According to the polymer theory, the miscibility between polymers could be related to the solubility parameter. The solubility parameter δ is a temperature dependent property, and is widely used to give a rough and ready approximation of solubility behavior. The solubility parameter δ is the square root of the cohesive energy density. The cohesive density is the energy needed to remove unit volume of molecule from the neighbor to the infinite place. This is a measure of the strength of its intermolecular forces.

$$\delta = \sqrt{\frac{E_{coh}}{V}} \tag{17}$$

where V is the volume of the box at equilibrium. The Flory-Huggins parameter χ can be calculated from the solubility parameters by the equation

$$\chi_{12} = \frac{V_{bead}}{k_B T}(\delta_1 - \delta_2)^2 \tag{18}$$

where V_{bead} is the volume of the polymer segment corresponding to the particle size in the dissipative particle dynamics.

For a dilute solution, the volume fractions of polymer and solvent are very different. In this case, we have to adopt the following equations, and the χ parameter is defined as

$$\chi = V_{bead}\left(\frac{\Delta E_{mix}}{k_B T}\right) \tag{19}$$

The mixing energy ΔE_{mix} is the total energy of mixing per unit volume for pure components and their blends as in following equation:

$$\Delta E_{mix} = \phi_A\left(\frac{E_{coh}}{V}\right)_A + \phi_B\left(\frac{E_{coh}}{V}\right)_B - \left(\frac{E_{coh}}{V}\right)_{AB} \tag{20}$$

Here, ϕ_A and ϕ_B are the volume fractions of the two components in the dilute solution. In this work, $\phi_{solvent} \approx 1.0$ and $\phi_{polymer} \approx 0.0$ are used.

1.2 Dissipative particle dynamics simulation model of PS$_{290}$-PI$_{110}$ block copolymer

In the first stage, we first need to determine the coarse-grained model. According to the computation of volume in previous study,[5] the volume of one PS (or PI) is considered to be almost the same as that of five molecules of water. Dissipative particle dynamics assumes that all beads are of the same equilibrium volume so as to conform to Flory-Huggins theory. The number of beads in each model is determined using the molar mass of diblock copolymer, molar mass of a repeat unit, degree of polymerization and characteristic ratio of each system. Consistent with current most setups, the volume of each chain of PS and PI is roughly the same volume of 1500 Å^3 as one bead in dissipative particle dynamics simulation, where the PI and PS polymers

consisted of 10 monomers per chain, respectively. This mapping in turn resulted in the following mesoscopic copolymer architecture PS_{29}-PI_{11} for the PS_{290}-PI_{110} copolymer. The chemical structure and corresponding coarse-grained model of linear PS-PI diblock copolymers as an illustrative example is shown in Fig.S1.
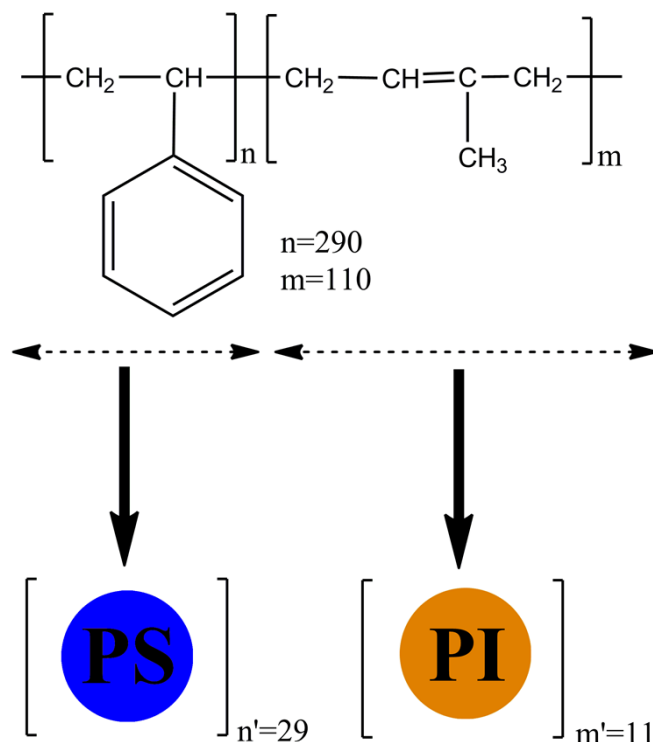

Fig. S1. Illustration of the coarse-grained mapping of PS-b-PI diblock copolymer from atomistic to DPD model. Every S and I particle represents 10 PS and PI monomers, respectively.

2 Simulation details

2.1 All-atom molecular dynamic simulation based on ABEEM polarizable force field

The all-atom molecular dynamics simulations were first carried out to obtain the interaction parameters in the dissipative particle dynamics simulations. The first concern to all-atom molecular dynamics is the setup of the initial system. Concerning the polymeric studies, the number of the repeating unit and the chains in the polymers needs to be set reasonably. Unnecessarily long chains will become a great load for the systems studied. It is usable to choose a system that could represent the system in a reasonable way. The shortest length of the chain that presents interaction strength similar to the polymer with high molecular mass is chosen. Through the trial studies carried out many times, the numbers of the monomers in PS and PI polymer chain in

all-atom molecular dynamics simulations were finally set as 10 and 10, respectively. This setup can reasonably describe the interactions with less computational cost.

In all-atom molecular dynamics simulations, the systems of PS, PI, n-heptane, PS/n-heptane and PI/n-heptane were firstly constructed in a simulation box of the side length L=22Å with three dimensional periodic boundary conditions at experimental densities, respectively. Amorphous cells (either pure or binary mixture) with highly efficient packing were built up by the packmol package.[6] To eliminate unfavorable contacts and relax totally unfavorable structures of the chains, the initial configurations were subjected to energy minimization using a limited memory L-BFGS algorithm with preliminary minimization of trial structures to an rms gradient of 0.01 kcal/mol/Å.

All-atom simulations were carried at constant temperature 298K using modified Tinker program. All the simulations were conducted in the NVT ensemble for 1 ns with integration time step 1 fs. The ABEEM PFF was adopted in our simulation, which was known to accurately reproduce experimental structures, and heat of vaporization, and so on.[7] Berendsen thermostat was applied to control the temperature of the simulation system. The equation of motion was integrated using velocity-Verlet method. Period boundary condition and the nearest image were applied. The distance-based cutoffs were used for electrostatic and van der Waals interaction. Considering that the solvents have been simulated explicitly, the dielectric constants are not needed. In order to reflect the charge distribution varying with molecular conformation, the charge distribution was recomputed per 0.1 ps. The charge transfer was allowed to occur intramolecular, while not allowed intermolecular. Trajectory was saved every 1ps and the final 10 ps were used to calculate the equilibrium potential and intermolecular interaction energies. In order to test the reliability of our simulated solubility parameters, we checked our results and compared them with known experimental data.

2.2 Dissipative particle dynamics simulation

All simulations were performed in a cubic simulation box of $40r_c \times 40r_c \times 40r_c$

containing 1.92×10^5 dissipative particle dynamics beads by using HOOMD package[8] on a NVIDIA Tesla C2050 GPU processor. The same density of the beads for all the species was restricted to 3 in order to make a stronger link with experiments.[9] The dissipative particle dynamics simulations started from the random distribution of coarse-grained polymers and n-heptane beads inside the simulation box with three-dimensional periodic boundary conditions. The velocity-Verlet algorithm was used here to integrate the equations of motion. A total of 1.0×10^6 time steps simulation with a step size of 0.02 was performed for each system considered in this study. The computing time is long enough for the system to achieve an equilibrium state and

form stable morphology.

3 Flory-Huggins parameters χ_{ij} and the repulsion parameters α_{ij}

Table S1. The Flory-Huggins parameters χ_{ij} obtained from all-atom molecular dynamics simulations.

χ_{ij}	PS	PI	Heptane
PS	0.00		
PI	3.79	0.00	
heptane	5.00	0.53	0.00

Table S2. The repulsion parameters α_{ij} resulted from Flory-Huggins parameters χ_{ij}.

α_{ij}	PS	PI	Heptane
PS	25.00		
PI	37.40	25.00	
heptane	41.35	26.73	25.00

4 ABEEM PFF parameters for n-heptane

Table S3. ABEEM PFF parameter set for n-heptane

atom type	description
CT	RCH_3 Alkane
CM	R_2CH_2 Alkane
HC	HR Alkane

The ABEEM$\sigma\pi$ nonbonded parameters χ^*,2η^*,σ(in Å) and ε (in kcal/mol)				
type	χ^*	$2\eta^*$	σ	ε
CT	2.5500	20.5630	3.5850	0.0660
CM	2.5000	7.8000	3.5850	0.0660
HC	2.2000	13.0380	2.5900	0.0300
CT-HC bond	6.0100	42.3500	—	—
CM-HC bond	6.0100	42.3500	—	—
CT-CM bond	6.7100	47.3400	—	—

Bond parameters (k_r in kcal/mol/Å^2 and r_{eq} in Å)		
type	k_r	r_{eq}
CT-HC	340.0	1.0900

CM-HC	340.0	1.0900
CT-CM	268.0	1.5290

Angle parameters (k_θ in kcal/mol/rad² and θ_{eq} in º)

type	k_θ	θ_{eq}
HC-CT-HC	33.00	107.80
HC-CT-CM	37.50	110.70
CT-CM-HC	37.50	110.70
CT-CM-CM	58.35	112.70
type	k_θ	θ_{eq}
HC-CM-HC	33.00	107.80
HC-CM-CM	37.50	110.70
CM-CM-CM	58.35	112.70

Dihedral angle torsional Fourier coefficients (V_1, V_2 and V_3 in kcal/mol)

type	V_1	V_2	V_3
HC-CT-CM-HC	0.000	0.000	0.318
HC-CT-CM-CM	0.000	0.000	0.366
CT-CM-CM-HC	0.000	0.000	0.366
CT-CM-CM-CM	-0.585	-0.320	0.500
HC-CM-CM-HC	0.000	0.000	0.318
HC-CM-CM-CM	1.285	0.000	0.366
CM-CM-CM-CM	1.300	-0.050	0.200

5 Video Clips

1. Video clip S1 illustrates the dynamic pathway in the formation of spherical micelle from linear PS_{290}-PI_{110} diblock copolymer in heptane.
2. Video clip S2 illustrates the dynamic pathway in the formation of cylindrical micelle from cyclic PS_{290}-PI_{110} diblock copolymer in heptane.
3. Video clip S3 illustrates the dynamic pathway in the formation of cylindrical micelle from linear PS_{290}-PI_{110} diblock copolymer blended with PS homopolymers in heptane.
4. Video clip S4 illustrates the dynamic pathway in the formation of vesicle from cyclic PS_{290}-PI_{110} diblock copolymer blended with PS homopolymers in heptane.
5. Video clip S5 illustrates the dynamic pathway in the formation of spherical micelle from cyclic PS_{290}-PI_{110} diblock copolymer blended with linear PS_{290}-PI_{110} diblock copolymer in heptane.

References

1. Groot, R. D.; Warren, P. B., Dissipative particle dynamics: bridging the gap between atomistic and mesoscopic simulation. *J. Chem. Phys.* **1997,** *107* (11), 4423.

2. Mackerell, A. D., Empirical force fields for biological macromolecules: overview and issues. *J. Comput. Chem.* **2004,** *25* (13), 1584-1604.

3. Zhao, D.-X.; Liu, C.; Wang, F.-F.; Yu, C.-Y.; Gong, L.-D.; Liu, S.-B.; Yang, Z.-Z., Development of a Polarizable Force Field Using Multiple Fluctuating Charges per Atom. *J. Chem. Theory. Comput.* **2010,** *6* (3), 795-804.

4. Zhao, Y.; You, L.-Y.; Lu, Z.-Y.; Sun, C.-C., Dissipative particle dynamics study on the multicompartment micelles self-assembled from the mixture of diblock copolymer poly(ethyl ethylene)-block-poly(ethylene oxide) and homopolymer poly(propylene oxide) in aqueous solution. *Polymer* **2009,** *50* (22), 5333-5340.

5. Li, X.; Guo, J.; Liu, Y.; Liang, H., Microphase separation of diblock copolymer poly (styrene-b-isoprene): A dissipative particle dynamics simulation study. *J. Chem. Phys.* **2009,** *130* (7), 074908.

6. Martínez, L.; Andrade, R.; Birgin, E. G.; Martínez, J. M., Packmol: A package for building initial configurations for molecular dynamics simulations. *J. Comput. Chem.* **2009,** *30* (13), 2157-2164.

7. Yu, C.-Y.; Yang, Z.-Z., A Systemic Investigation of Hydrogen Peroxide Clusters (H_2O_2) $_n$(n=1-6) and Liquid-State Hydrogen Peroxide: Based on Atom-Bond Electronegativity Equalization Method Fused into Molecular Mechanics and Molecular Dynamics. *J. Phys. Chem. A* **2011,** *115* (12), 2615-2626.

8. Phillips, C. L.; Anderson, J. A.; Glotzer, S. C., Pseudo-random number generation for Brownian Dynamics and Dissipative Particle Dynamics simulations on GPU devices. *J. Chem. Phys.* **2011,** *230* (19), 7191.

9. Ortiz, V.; Nielsen, S. O.; Discher, D. E.; Klein, M. L.; Lipowsky, R.; Shillcock, J., Dissipative particle dynamics simulations of polymersomes. *J. Phys. Chem. B* **2005,** *109* (37), 17708-17714.