Supplement Materials

Characteristic structural knowledge for morphological identification and classification in meso-scale simulations using principal component analysis

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Table S1. Parameters used in DPD simulation in dimensionless unit.

Parameter	
Particle number, N	24,000
Simulation box volume	8000
Coarse-grained degree, N_m	5
Spring constant, C_{ij}	4
Thermal energy, k_BT	1
Repulsion parameter of the same beads, a_{ii}	131.50
Repulsion parameter of the different beads, a_{ij} at temperature of 393 K	142.18
Time step, Δt	0.01
Equilibrium step number	1×10^6
Production step number	$\geq 1 \times 10^7$

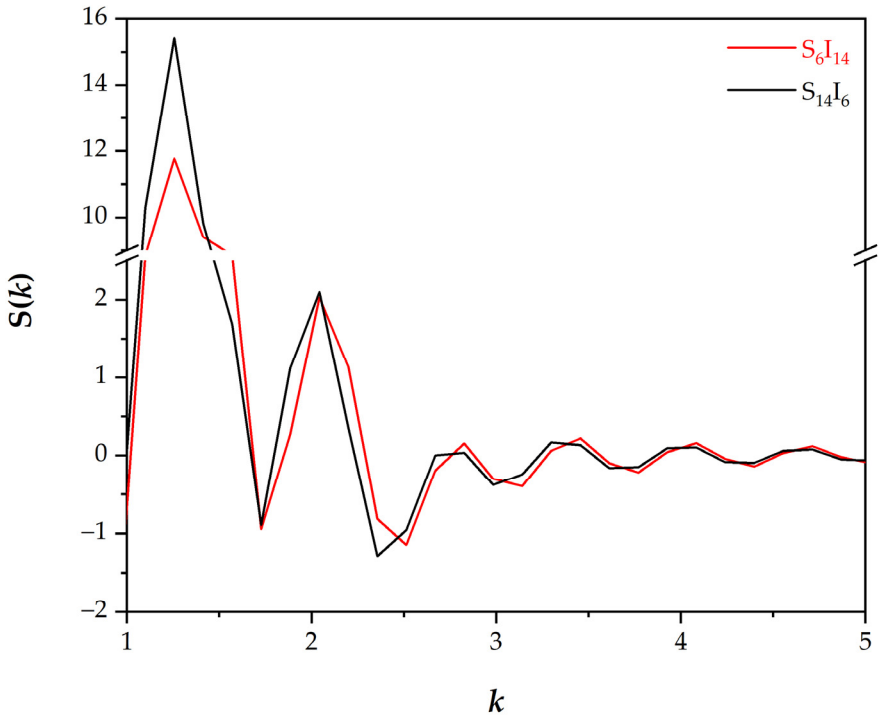

Figure S1. Structure factors S(*k*) between chain-chain types of the gyroidal morphologies of S_6I_{14} and $S_{14}I_6$ were represented as red and black lines, respectively.

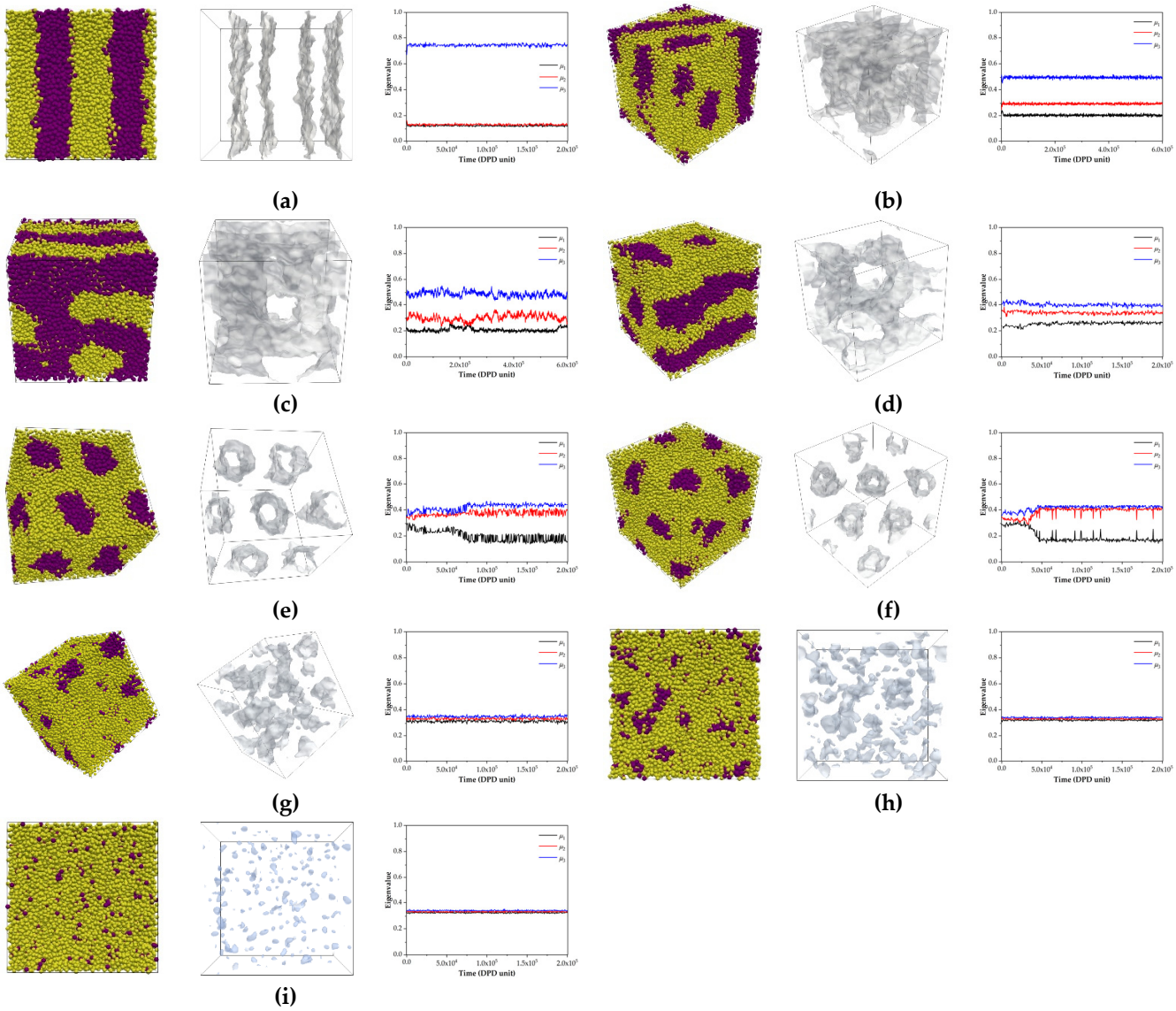

Figure S2. Panels in the composite figures illustrate apparent bead-arrangement, isosurface between distinct bead types and order parameter sorting from the left to right of (a) $S_{11}I_9$, (b) $S_{12}I_8$, (c) $S_{13}I_7$, (d) $S_{14}I_6$, (e) $S_{15}I_5$, (f) $S_{16}I_4$, (g) $S_{17}I_3$, (h) $S_{18}I_2$, and (i) $S_{19}I_1$, respectively. The order parameters were calculated using an executable, namely isosueface.exe, that is an implemented tool in DL_MESO software. Yellow and violet beads represent coarse-grained beads of styrene and isoprene, respectively.

Script S1: Structural knowledge analysis and PCA visualization
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Libraries

```
library(tidyverse)
library(ggforce)
library(factoextra)
library(ggrepel)
library(corrplot)
```

Data

```
data <- <name_of_excel_file>[<range_of_row>,<range_of_column>]
data
data.frame <- as.matrix.data.frame(data)
data.frame
```

Run the PCA

```
pca <- prcomp(data.frame,scale = TRUE)
pca

summary(pca)


eig.val <- get_eigenvalue(pca)
eig.val


options(ggrepel.max.overlaps = Inf)
fviz_eig(pca)
fviz_pca_ind(pca,title = " ",geom = "point",col.ind = "cos2", gradient.cols = c("#00AFBB", "#E7B800", "#FC4E07"))

fviz_pca_var(pca,title = " ",label = "none",col.var = "cos2",gradient.cols = c("#00AFBB", "#E7B800", "#FC4E07"))

res.var <- get_pca_var(pca)
res.var$coord
res.var$contrib
res.var$cos2


corrplot(res.var$cos2, is.corr = TRUE,)
```

#