Electronic Supplementary Material (ESI) for Soft Matter.

Supplementary information

Self-Assembly of Rod-Coil-Rod Block Copolymers in a Coil-Selective Solvent: Coarse-Grained Simulation Results

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Results and discussion

Morphology diagrams

All simulation results are comprehensively documented in the figures displayed below, presented in the form of a morphology diagram that includes snapshots of all simulations performed in this work. The scaling of the x and y axes has deliberately not been adjusted for quality considerations. Fig. S1 illustrates the morphology diagram associated to triblocks with flexible ending blocks, while Fig. S2 portrays the morphology diagram corresponding to triblocks with rigid blocks.

To helpin the construction of the morphology diagram on the main text, the shape anisotropy parameter was computed. It has a value that ranges between 0 and 1, where a value close to 0 suggests a shape akin to a sphere, and proximity to 1 indicates an elongated shape. By employing cluster analysis with Ovito, we computed the gyration tensor for each cluster defined as:

$$S_{ij} = \frac{1}{N}\sum_{k=1}^{N}(r_i^{(k)} - r_{i_{CM}})(r_j^{(k)} - r_{j_{CM}})$$

where N is the total number of particles in the cluster, $r^{(k)}$ is the position vector of the k^{th} particle, i and j represent the coordinates and $r_{i_{CM}}$ is the i^{th} coordinates of the position of the centre of mass of the cluster (*Handan Arkın et al. J. Chem. Phys. 7 February 2013; 138 (5): 054904*). Subsequently, the anisotropy parameter was derived for individual clusters, which were then averaged:

$$A_3 = 1 - 3\frac{\lambda_1\lambda_2 + \lambda_2\lambda_3 + \lambda_3\lambda_1}{(\lambda_1 + \lambda_2 + \lambda_3)^2}$$

where λ_1, λ_2 and λ_3 are the eigenvalues of the gyration tensor and $\lambda_1 > \lambda_2 > \lambda_3$. The resulting colormap of the average anisotropy parameter (as depicted in Fig. S3) closely aligns with the established morphology diagrams. It is noteworthy, however, that certain scenarios warrant additional consideration. For instance, when a mixture of spheres (low A_3) and tactoids (medium A_3) coexists, the average asphericity may not yield precise results, necessitating reliance on direct morphological observations. Similarly, in the case of vesicles with an A_3 close to that of a sphere, distinguishing between them becomes challenging in the colormap, emphasizing the importance of

morphology-based observations in such instances.

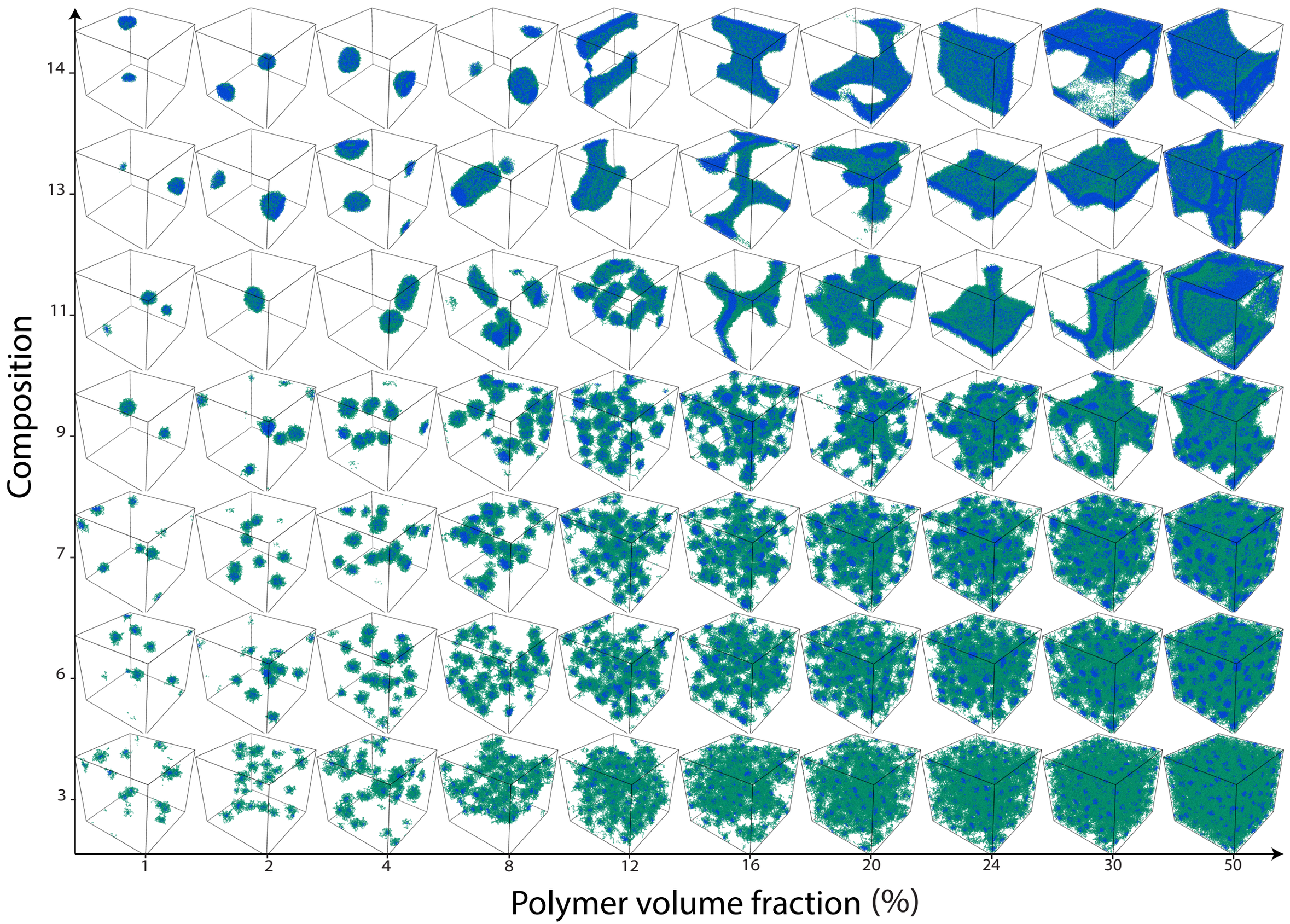

Fig. S1: Morphology diagram for triblock copolymer where the A blocks are flexible

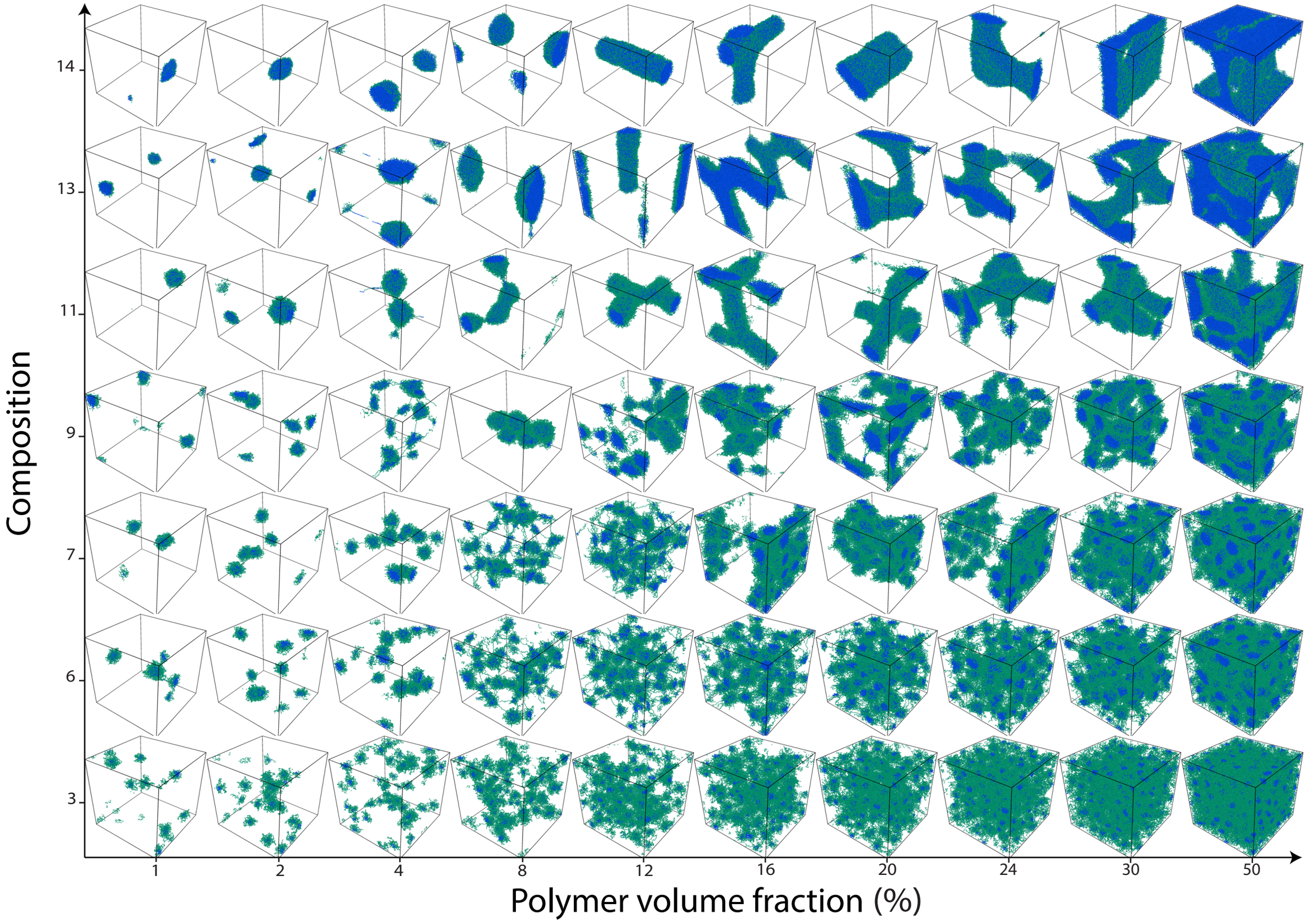

Fig. S2: Morphology diagram of the triblock copolymer where A blocks are rigid.

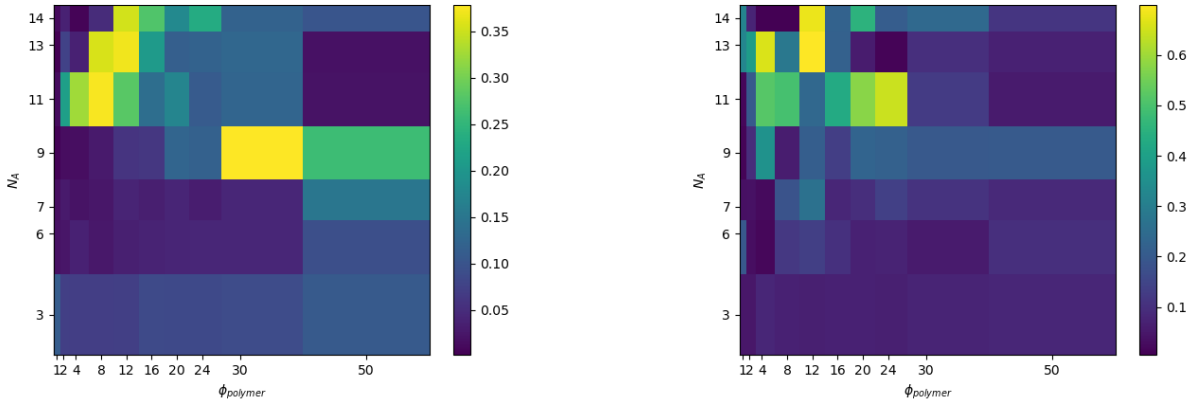

Fig. S3: Colormap of asphericity parameter for the case where the ending blocks are flexible (left) and rigid (right)