

## Supporting Information

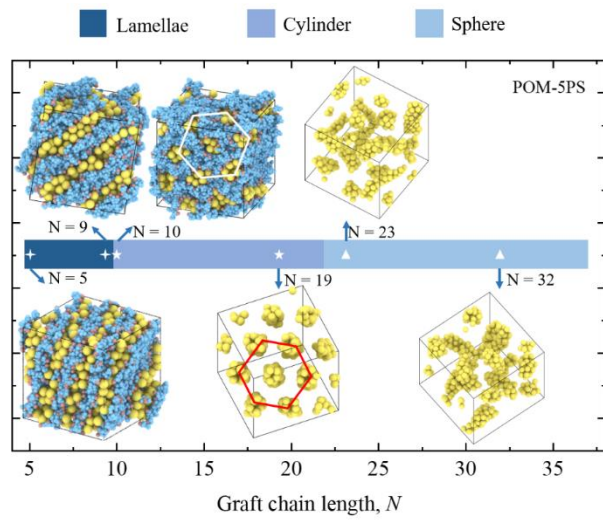
# Block-copolymer-like self-assembly behavior of mobile-ligand grafted ultra-small nanoparticles

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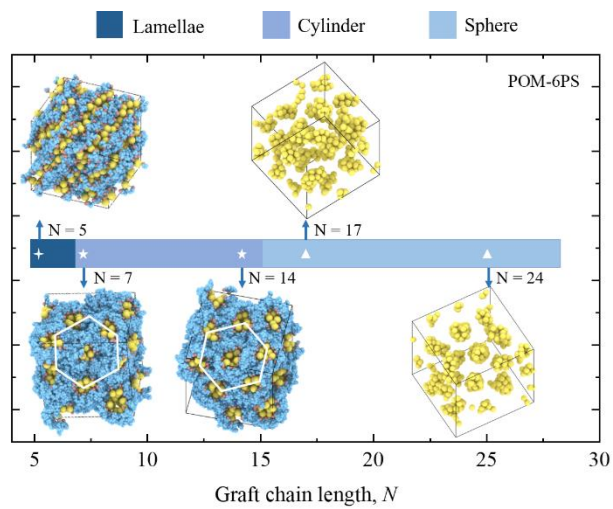
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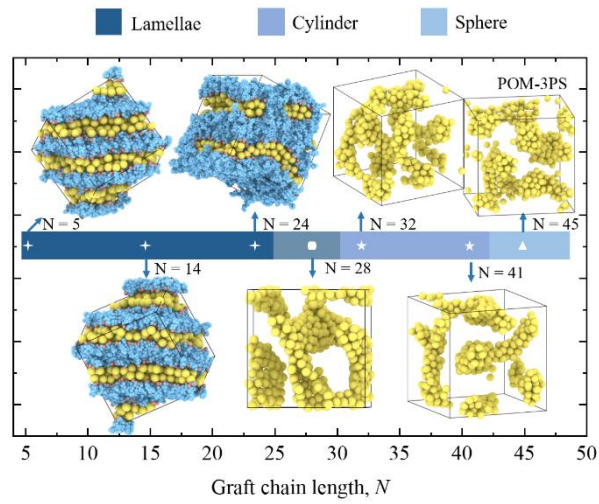
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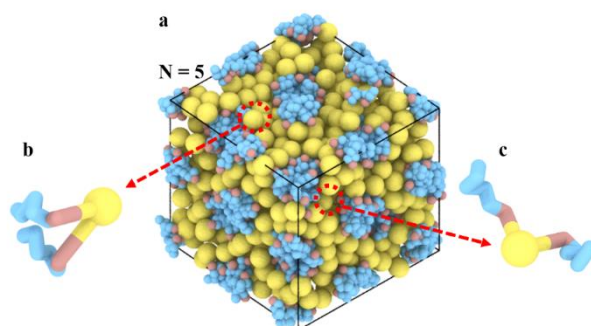
**Figure S1.** Phase boundary diagrams of POM-5PS with different graft chain length. Regions for different phases are shown in different colors as indicated by the legends.



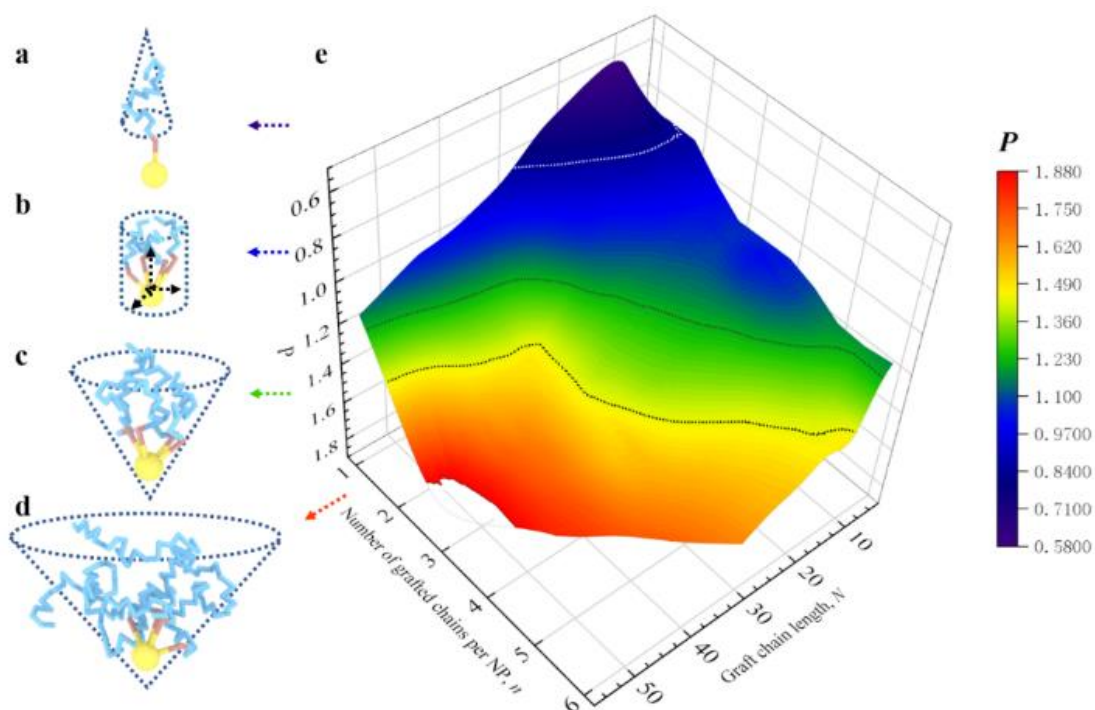
**Figure S2.** Phase boundary diagrams of POM-6PS with different graft chain length. Regions for different phases are shown in different colors as indicated by the legends.



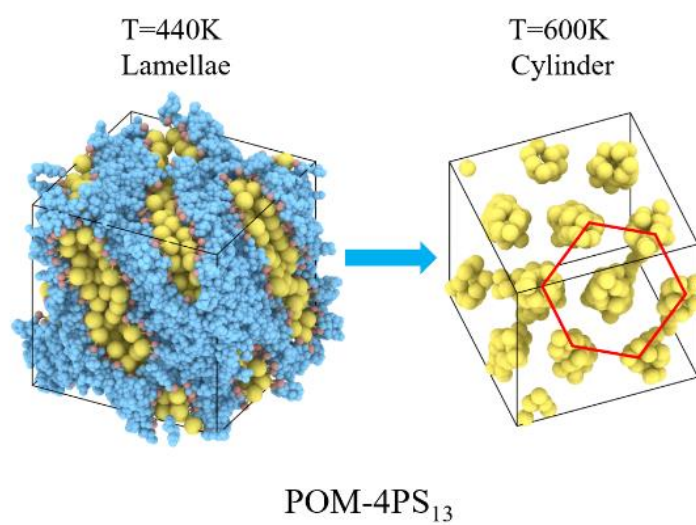
**Figure S3.** Phase boundary diagrams of POM-3PS with different graft chain length. Regions for different phases are shown in different colors as indicated by the legends.



**Figure S4.** (a) Inverse cylinder structure formed by POM-2PS<sub>5</sub>; (b) and (c) two typical configurations of grafted polymers: (b) two PS chains are in the same cylinder, and (c) two PS chains are in two distinct cylinders.



**Figure S5.** 3D plot of the calculated packing parameter  $P$  for systems with varied graft chain length  $N$  and graft density  $n$ . The pictures on the left show typical molecular conformation of PS grafted POM NP. The  $P$  value is shown in different colors as indicated by the color bars on the right.



**Figure S6.** Transformation of a lamellae structure formed at 440 K for system POSS-4PS<sub>13</sub> to a cylinder structure when it is heated up to 600 K.