Supporting Information

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

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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-2PS₅; (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\textsubscript{13} to a cylinder structure when it is heated up to 600 K.