Electronic Supplementary Information

Cross-sectional structures of a molecular monolayer nanotube explored with SAXS: An evidence for the parallel orientation of the headgroups in asymmetric bolaiphilic

Kenta Yoshida, a Rintaro Takahashi, a Shota Fujii, a Naohiro Kameta, b Toshimi Shimizu, c Kazuo Sakurai * a

a Department of Chemistry and Biochemistry, University of Kitakyushu, 1-1 Hibikino, Wakamatsu-ku, Kitakyushu, Fukuoka 808-0135, Japan
b Nanomaterials Research Institute, Department of Materials and Chemistry, National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba Central 5, 1-1-1 Higashi, Tsukuba, Ibaraki 305-8565, Japan
c AIST Fellow, AIST, Tsukuba Central 5, 1-1-1 Higashi, Tsukuba, Ibaraki 305-8565, Japan
TEM image.

Fig. S1 TEM image of the nanotubes formed from NKNT2-C18 stained by sodium phosphotungstate.

**Scattering function.** Excess scattering intensity $I(q)$ from the long three-layer tubular structure can be expressed as follows:

$$I(q) \propto \left( \rho_{in} - \rho_{a} \right) R_{1}^{2} \left[ \frac{J_{1}(qR_{1})}{qR_{1}} \right] + \left( \rho_{a} - \rho_{b} \right) R_{2}^{2} \left[ \frac{J_{1}(qR_{2})}{qR_{2}} \right] + \left( \rho_{b} - \rho_{c} \right) R_{3}^{2} \left[ \frac{J_{1}(qR_{3})}{qR_{3}} \right] + \left( \rho_{c} - \rho_{out} \right) R_{4}^{2} \left[ \frac{J_{1}(qR_{4})}{qR_{4}} \right]$$ (S1)

where $J_{1}(x)$ is the first order Bessel function of the first kind. $R_{1}$ denotes the cross-sectional radius of the inside surface, and $R_{2}, R_{3},$ and $R_{4}$ are defined by $R_{2} = R_{1} + D_{A}, R_{3} = R_{2} + D_{B},$ and $R_{4} = R_{3} + D_{C},$ respectively. This is an extension of the form factor for a core-shell cylinder under the assumption that the cylinder height is much larger than its radius.$^{1,2}$

Model curves calculated by the different values.
**Fig. S2** (a) SAXS profile of NKNT2-C18 in aqueous solution (the same as Fig. 1). (b) Electron density distributions to calculate the scattering intensity of the solid curves in the panel a. The red and green curves in the panel b correspond to the red and green curves in the panel a, respectively.
Fig. S3 SAXS profiles of NKNT2-C18 in aqueous solution (the same as Fig. 1). The red solid curves in each panel represent the fitted model curves by the electron density distribution shown in Fig. 2. The blue and dark yellow solid curves represent the model curves by using the values increased and decreased from the best-fit by 10 % (×1.1 and
×0.9) about all the radial distance (i.e., \( R_1, R_2, R_3, \) and \( R_4 \)) (a), only \( R_1 \) (b), only \( R_2 \) (c), only \( R_3 \) (d), and only \( R_4 \) (e). In the panel f, the blue and dark yellow solid curves represent the model curves by using the values increased by 100 % (×2) and decreased by 50 % (×1/2) from the best-fit about the radial distance of only \( R_4 \). When the parameter was changed, the other parameters were fixed to the values listed in Table 1.

References
