Electronic Supplementary Information

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

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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:

$$I(q) \propto \left\{ (\rho_{\rm in} - \rho_{\rm A}) R_1^2 \left[\frac{J_1(qR_1)}{qR_1} \right] + (\rho_{\rm A} - \rho_{\rm B}) R_2^2 \left[\frac{J_1(qR_2)}{qR_2} \right] + (\rho_{\rm B} - \rho_{\rm C}) R_3^2 \left[\frac{J_1(qR_3)}{qR_3} \right] + (\rho_{\rm C} - \rho_{\rm out}) R_4^2 \left[\frac{J_1(qR_4)}{qR_4} \right] \right\}^2 q^{-1}$$
(S1)

where $J_1(x)$ is the first order Bessel function of the first kind. R_1 denotes the crosssectional 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 coreshell 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 % (\times 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

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- G. V. Jensen, R. Lund, J. Gummel, T. Narayanan, J. S. Pedersen, *Angew. Chem. Int. Ed.* 2014, 53, 11524.