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Supporting Information

Crystallographic models of ribbons and ribbon-based J-aggregate nanotubes from geometry of tube ends

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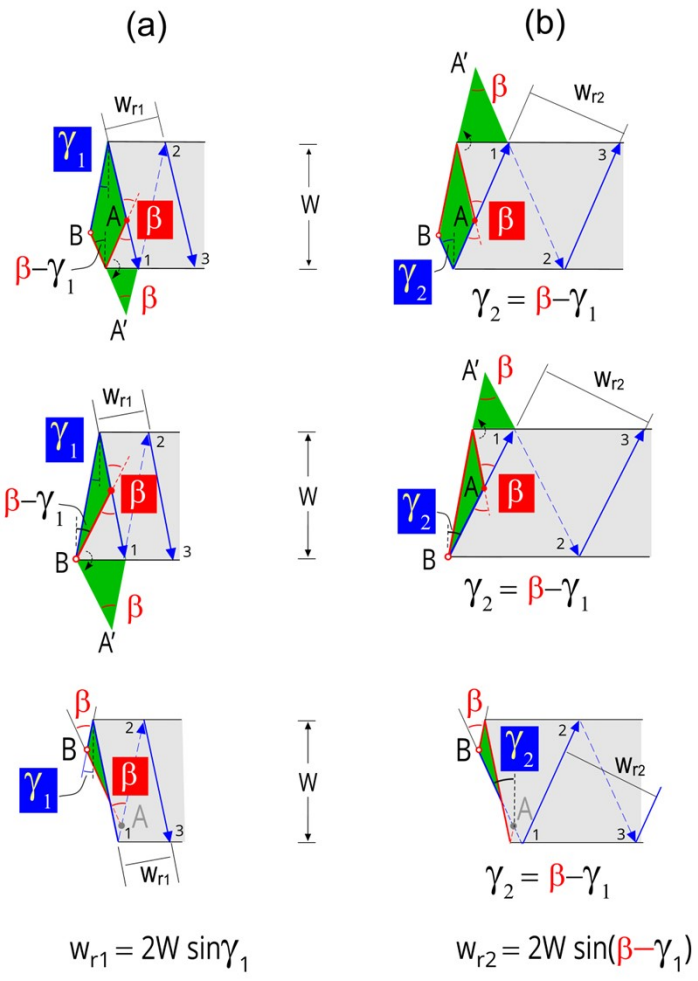

Fig. S1 Two ways of reconstructing the ribbon shape and the winding geometry of ribbon-based tubes. The inner side of tubes is shown in green, β is the ribbon vertex angle, γ is the ribbon pitch angle. The sides of green monolayer polygons belonging to the (either folded or non-folded) long and short ribbon sides are shown in blue and red, respectively.

The contour of the helically wrapped ribbon can be found by tracing to the right along the route 1-->2-->3 of any of two sides of the green polygon that enters at the inner vertex A. Blue and red colors are swapped in columns (a) and (b), causing the substitution $\gamma_2=\beta-\gamma_1$ and the change in the ribbon width w_r and tube helicity (opposite in (a) and (b)).

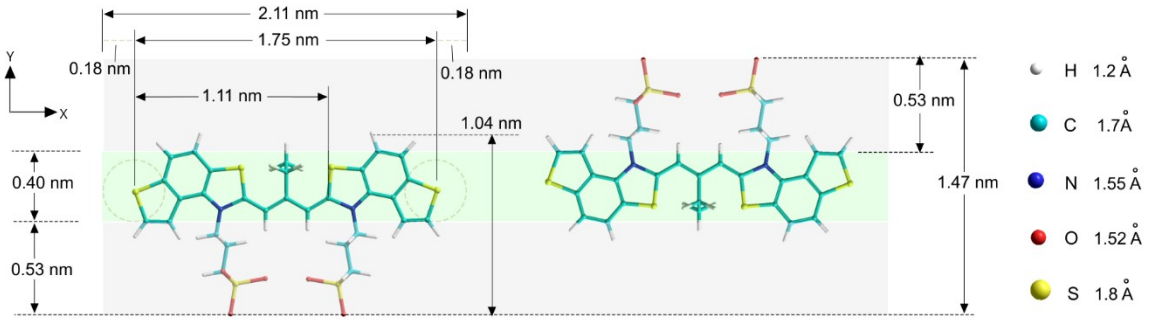

Fig. S2 TMC molecular structure and estimation of the monolayer thickness. van-der-Waals' radii of the constituent atoms are shown to the right.

The distance between terminal left and right sulphur atoms is 1.75 nm. The **a** size of the unit cell shown in Fig. 3c1 of the main text additionally includes two van-der-Waals' radii of sulphur (1.8 Å) and equal 1.75nm+2*0.18nm=2.11 nm.

For estimates of the molecular size in Y-direction, the extended/stretched conformation of aliphatic sulfopropyl tails was chosen for simplicity as a first approximation shown in Fig. S2. The Y-dimension of this conformation is 1.04 nm + 0.152 nm + 0.12 nm = 1.32 nm (1.04 nm is the distance between Y-projections of the terminal oxygen and hydrogen atoms plus van-der-Waals' radii of oxygen and hydrogen).

The Y-size 1.32 nm is lesser than the monolayer thickness measured by AFM which is about 1.5 nm (see the topography profile in Fig. 2a). This observation suggests that sulfopropyl tails of dye molecules occupy both monolayer sides, leading to a larger effective monolayer layer thickness, as shown schematically in Fig. S2 by the opposite Y-orientation of two TMC molecules placed somewhere in the monolayer. Assuming additionally that the heterocycles (marked in light green here) occupy the same Y-position in both Y-orientations, the thickness of such a monolayer is estimated at ~1.77 nm (1.47 nm shown in Fig. S2 plus two van-der-Waals radii of oxygen atoms on the opposite monolayer sides). This value is larger than the monolayer thickness measured by AFM. The main overestimation very probably comes from the simplification of the aliphatic tails stretched conformation (shown in Fig. S2) whereas in reality, this conformation is expected to be kinked.[1] The second source of the uncertainty is the difference in the Y-disposition of the oppositely oriented dye molecules in comparison with that shown in Fig. S2.

1. I. Patmanidis, A. H. De Vries, T. A. Wassenaar, W.Wang, G. Portale, S. J. Marrink, Structural Characterization of Supramolecular Hollow Nanotubes with Atomistic Simulations and SAXS. *Phys. Chem. Chem. Phys*., 2020, **22 (37)**, 21083-21093. https://doi.org/10.1039/d0cp03282d