

Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.
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Molecular dynamics of anhydrous glycolipid self-assembly in lamellar and hexagonal phases.

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Supporting Information

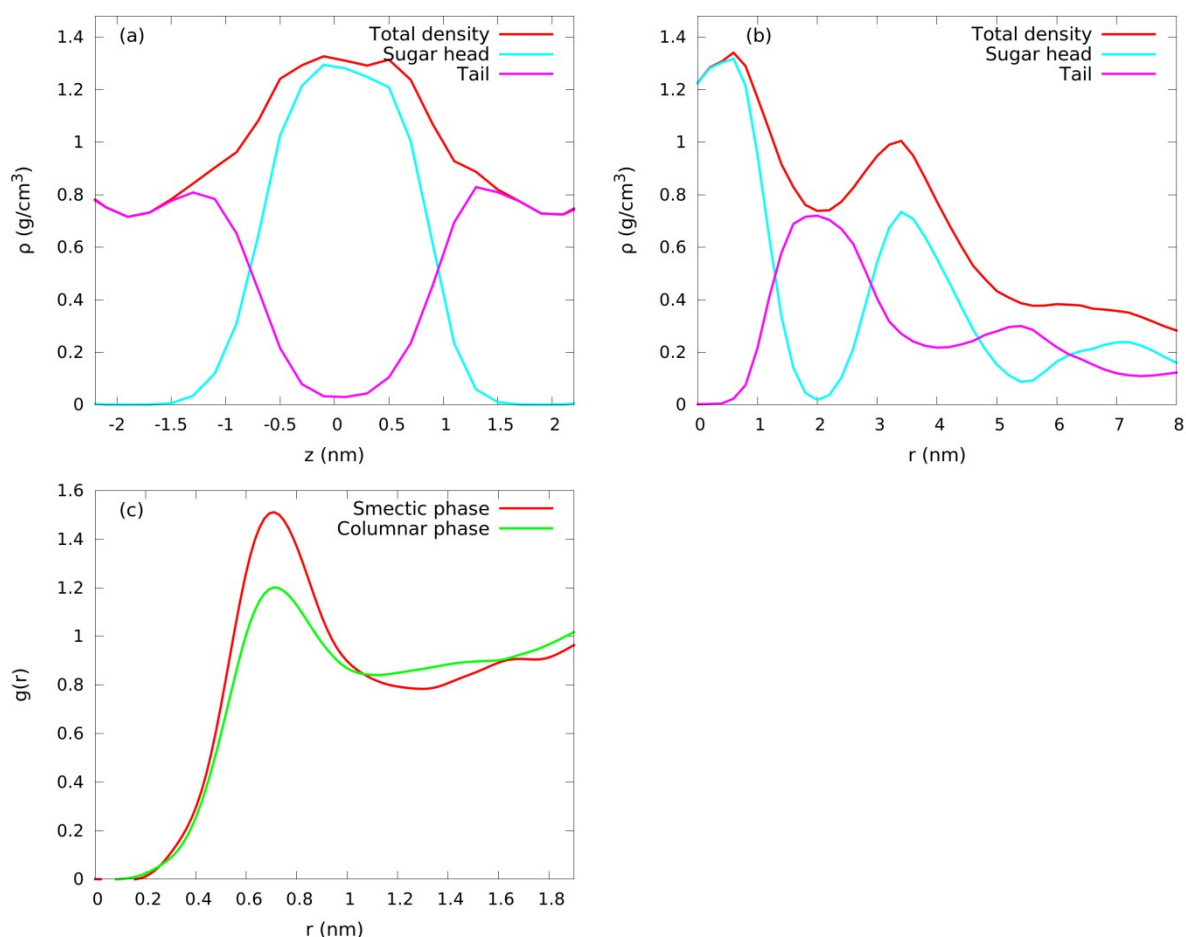


Fig. S1. Structural properties from MD simulation of 2-decyl-tetradecyl-β-D-maltoside (C₁₄₋₁₀G₂) in the smectic (T=348K) and columnar (T=433 K) phases (a) The local density profiles of headgroup (turquoise), tail (magenta) and total (red) in the smectic phase and z is distance along the normal to the smectic layer (b) The local density profiles of headgroup (turquoise), tail (magenta) and total (red) in the columnar phase, and r is the radial distance measured from the center of a selected column; (c) The radial distribution functions of the center of mass of the glycolipid molecules in smectic (red) and columnar (green) phases.

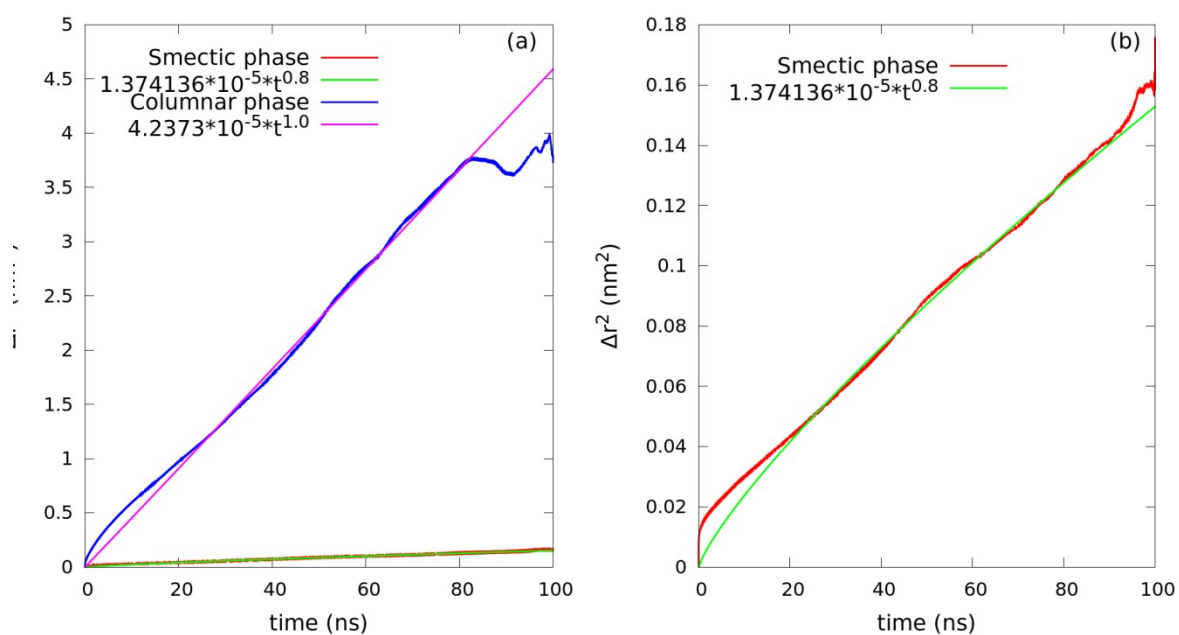


Fig. S2. (a) The average mean square displacement (Δr^2) versus time in smectic phase (red) and columnar phase (green) of 2-decyl-tetradecyl- β -D-maltoside ($C_{14-10}G_2$) at 348 K and 433 K respectively. (b) The average mean square displacement (Δr^2) versus time in smectic phase (extended y-axis).

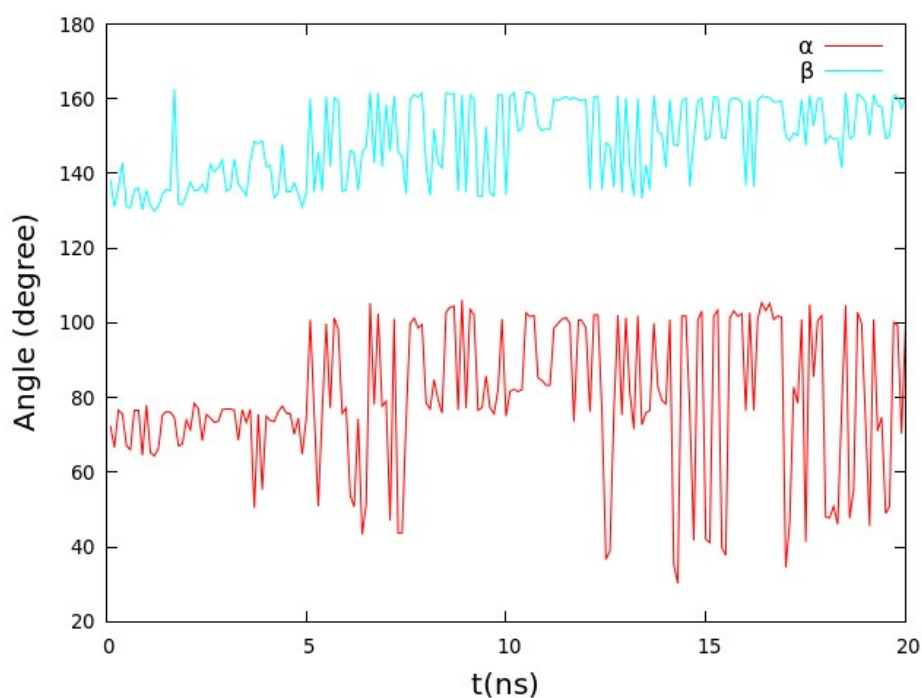


Fig. S3. The distribution of tilt angles α and β versus time obtained during the REMD simulation of 2-decyl-tetradecyl- β -D-maltoside ($C_{14-10}G_2$) in the smectic phase at 348 K.

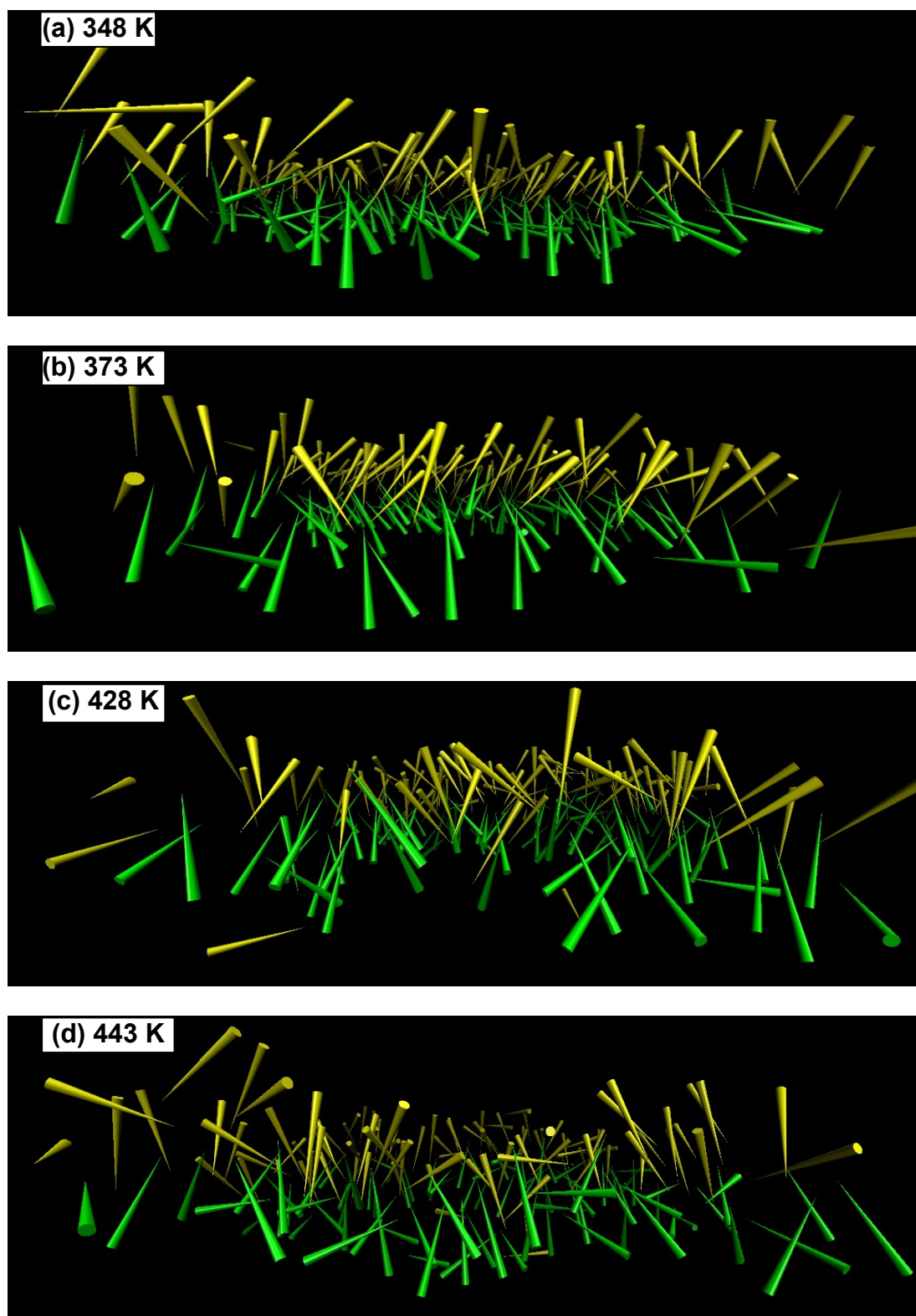


Fig. S4. The graphical representations of 2-decyl-tetradecyl-β-D-maltoside ($C_{14-10}G_2$) in the sugar head region of smectic phase from the final REMD configurations at temperatures (a) 348 K, (b) 373 K, (c) 428 K and (d) 443 K.

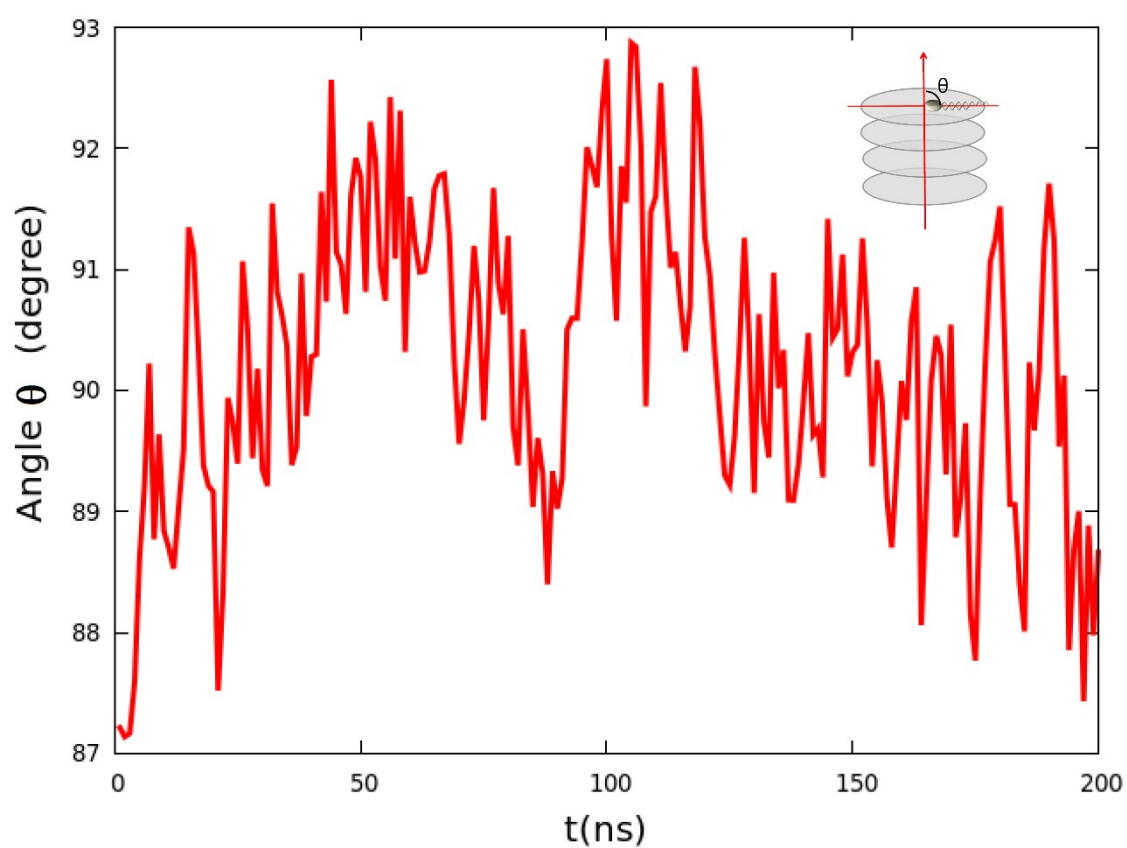


Fig. S5. The fluctuation of the average tilt angle θ (which is the angle made by the sugar head vector with the column axis) over time of 2-decyl-tetradecyl- β -D-maltoside ($C_{14-10}G_2$).