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Supporting Material

On the role of acylation of transmembrane proteins

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On the role of acylation of transmembrane proteins – Supplement

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I. EQUILIBRATION TOWARDS STEADY STATE

Before monitoring the quantities of interest, all systems were equilibrated for 10^5 time steps. Within that time the thermostat quickly enforced a convergence of the system's temperature to the steady state value (Fig. S1) while the barostat enforced a tensionless membrane by leading the membrane edge length L towards its steady state value L_0 (Fig. S2). After the equilibration process the system length L was fixed and the barostat was switched off. For the remaining time series, the tilting angles ϕ of the transmembrane proteins did only show stationary fluctuations (Fig. S3).

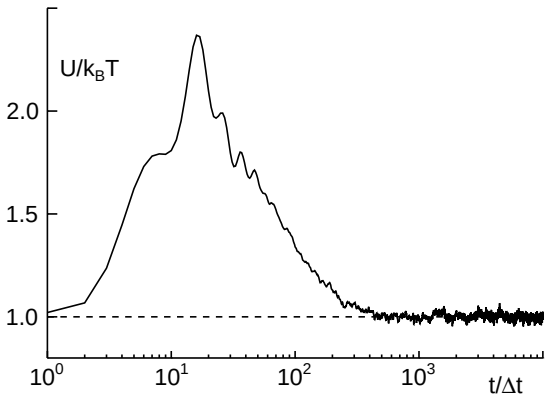

FIG. S1 The system temperature (shown as the ratio of the inner energy U per bead and thermal energy, k_BT) quickly converged towards unity during the equilibration process.

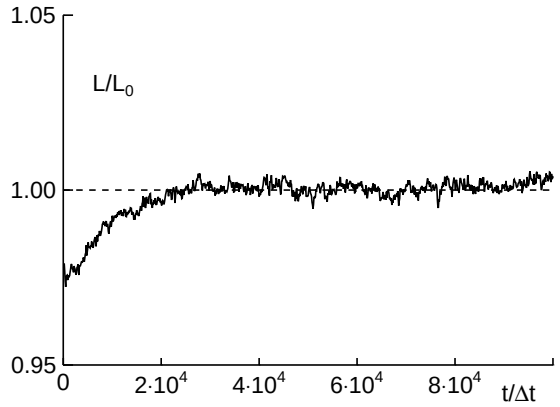

FIG. S2 The membrane edge length L quickly converged towards its steady state value L_0 (here: $L_0 \approx 12.6 r_0$) during the equilibration process.

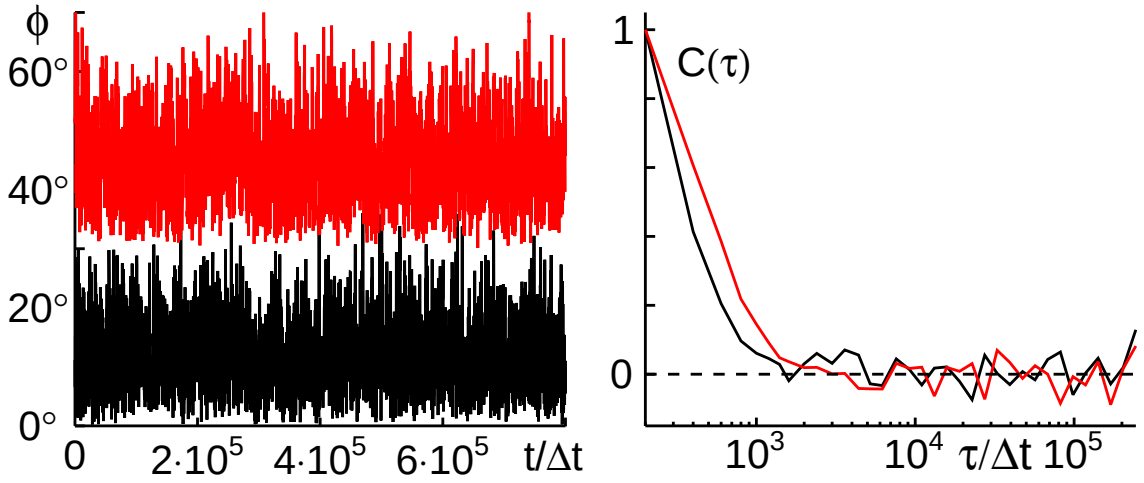

FIG. S3 Left: The tilt angle $\phi(t)$ (here shown for HT_5H and HT_5H^A in black and red) only show stationary fluctuations after the equilibration process. Data for HT_5H^A have been shifted by 30° for better visibility. Right: The associated autocorrelation curves $C(\tau) = \langle(\phi(t) - \langle\phi\rangle)(\phi(t+\tau) - \langle\phi\rangle)\rangle_t$ show a rapid decay within much less than 10^4 time steps and an asymptotic fluctuation around zero, hence supporting the notion that the system is equilibrated.

II. SUPPLEMENTAL RESULTS

A positive hydrophobic mismatch ($n > 5$) leads to an increase of $\langle\phi\rangle$ for both, the acylated and nonacylated constructs (Fig. S4). The ratio between acylated and nonacylated angles has been shown in Fig. 2b in the main text while Fig. S4 shows the underlying angles for each of the considered constructs. When changing the preferred angle θ_0 between the TMD and the acyl chain for the $(HT_nH)_7^A$ construct, an enhanced tilting due to the acylation is observed (Fig. S5) that is similar, yet somewhat weaker, than the data for $\theta_0 = 90°$ (cf. Fig. 2b, main text).

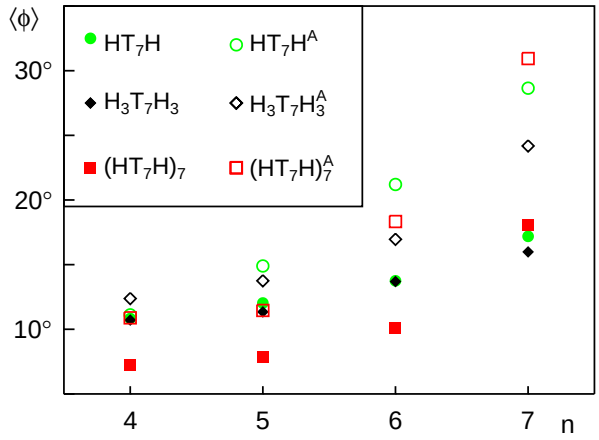

FIG. S4: Tilt angles $\langle\phi\rangle$ for the indicated constructs as a function of the TMD length n. An increased tilting for growing hydrophobic mismatches is seen that is even enhanced upon acylation (cf. also Fig. 2b of the main text).

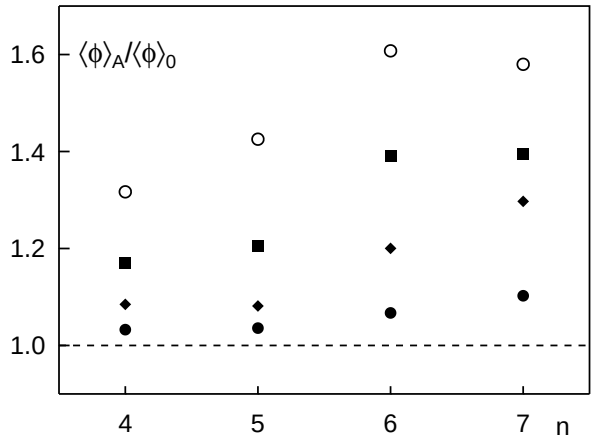

FIG. S5: The ratio of average tilt angles with and without acylation, $\langle\phi\rangle_A$ and $\langle\phi\rangle_0$, highlights an increased tilting of $(HT_nH)_7$ when the preferred angle between the TMD and the acyl chain ($m = 4$) is varied. Shown are data for $\theta_0 = 20°, 40°, 60°, 80°$ (filled circles, diamonds, squares, open circles).