Supplemental: An equilibrium double-twist model for the radial structure of collagen fibrils

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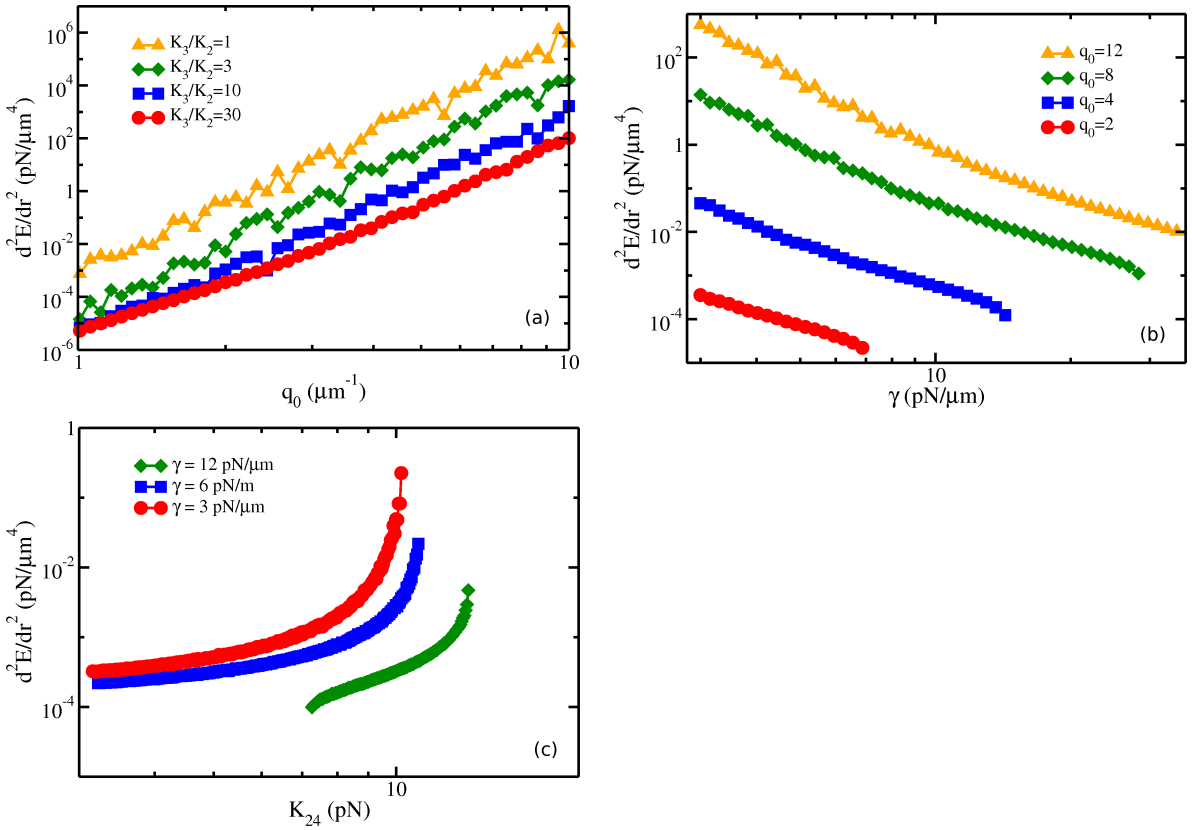

Figure S1 Second derivative of total energy with respect to radius at the extrema shown in (a) Fig. 3, (b) Fig. 4, and (c) Fig. 5. Parameters not indicated by the legends and x-axis are described in the captions of those figures. The second derivative is determined from the discrete radius-energy pairs from the modified midpoint method: if $i = i^*$ defines the discrete radius at which the derivative dE/dr changes sign, then the second derivative $d^2E/dr^2 = (E_{i^*+1} + E_{i^*-1} - 2E_{i^*})/(\Delta r)^2$. All second derivatives are positive, indicating the corresponding extrema are all minima.

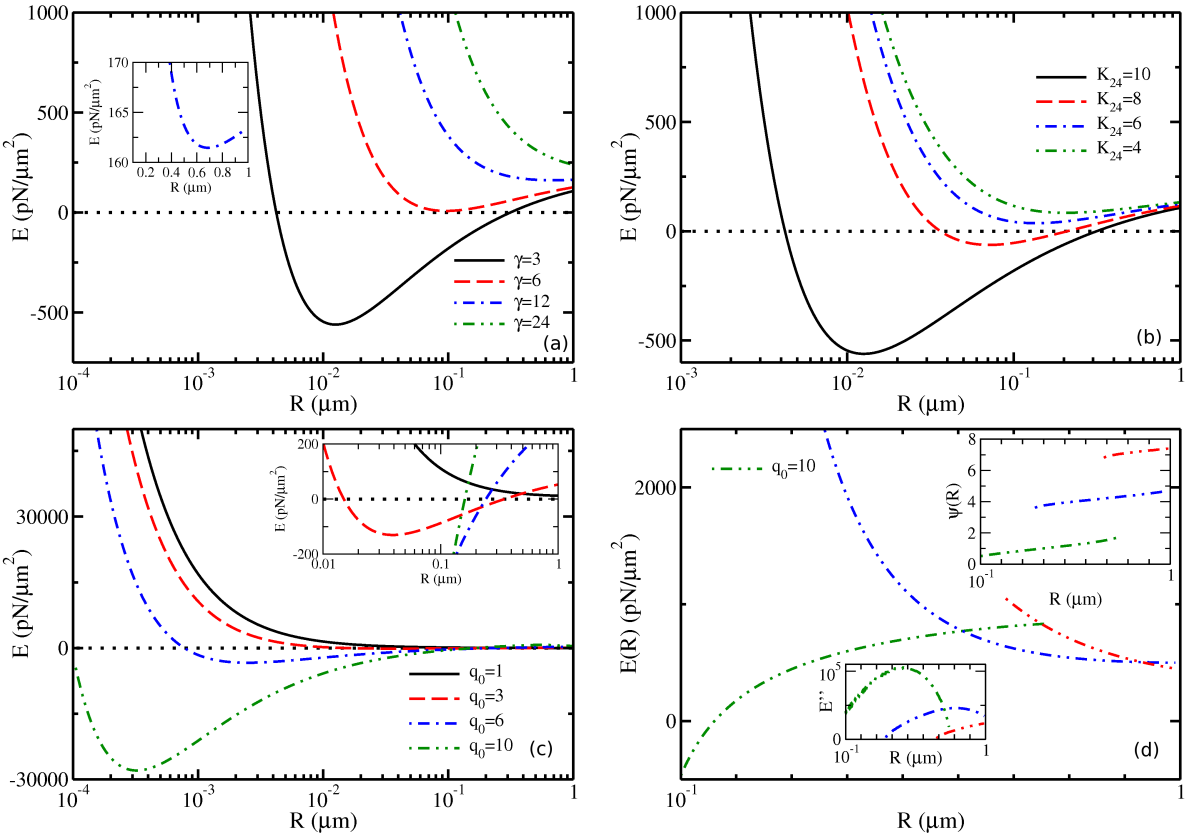

Figure S2 Total energy per unit volume $E(R)$ vs. fibril radius R for selections of different parameters (a) γ, (b) K_{24}, and (c) q_0. Insets of (a) and (c) highlight local minima that are not easily seen in the main plot. (d) highlights one region of the $q_0 = 10\ \mu\text{m}^{-1}$ curve from (c), with inset showing the twist-angle at the surface $\psi(R)$ for $q_0 = 10$. $E(R)$ is given by Eqn. 6, where the twist angle satisfies Eqns. 8 and 10 to result in the minimal bulk free-energy at a given R. In (a), (b), and (c) the dotted black line indicates $E = 0$. In (c) there is bifurcation of minima at large R for $q_0 = 10\ \mu\text{m}^{-1}$ — we only plot the bifurcation with the lowest energy at each R value, and the bifurcations are further explored in (d). The bifurcations exists because there are several minima in energy as $\psi'(0)$ is varied. The three bifurcations found are plotted in green, blue, and red. The upper-right inset shows each bifurcation has a different range of surface twist-angles. The lower-centre inset shows that the bifurcations end at radii at which the second derivative of energy with respect to $\psi'(0)$ (E'') goes to zero. The states plotted in blue and red are ruled out for collagen fibrils because of the large radii, the large twist-angles $\psi > \pi$ that would imply a change of axial fibril orientation, and the positive energies which would not be stable with respect to a cholesteric phase.