Supplementary Information

Numerical analysis and design of light-driven liquid crystal polymer-based motorless miniature cart

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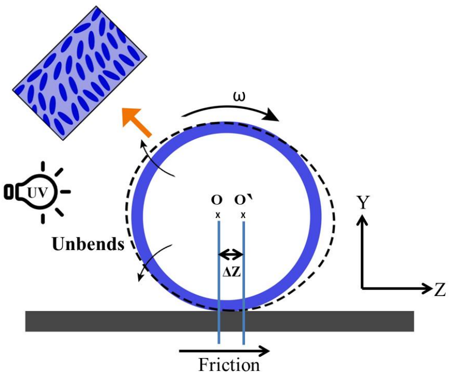

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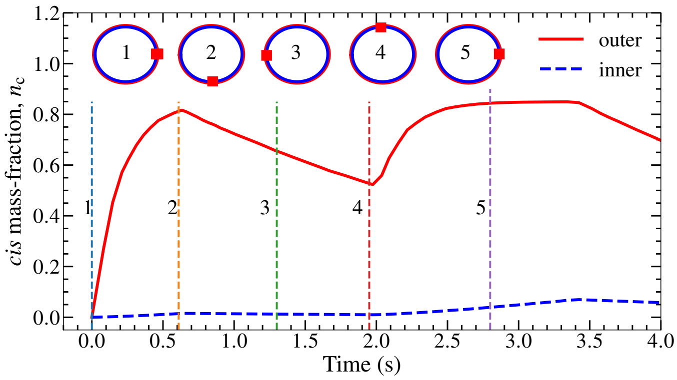
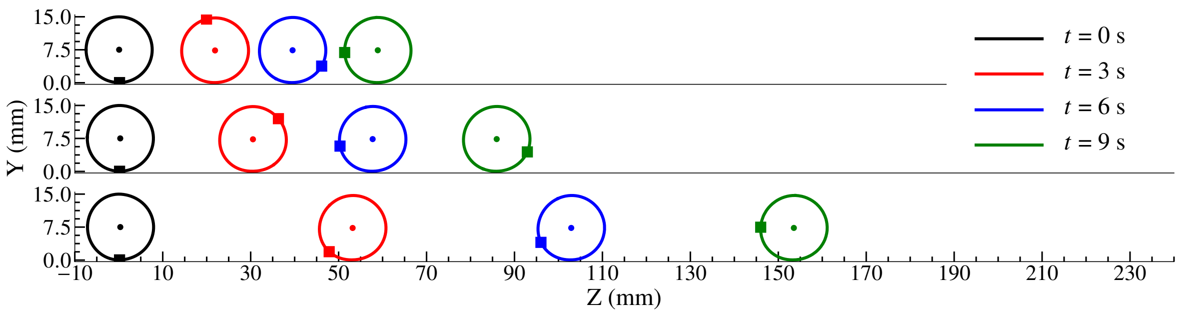


(b)

Fig S1: a) Schematic illustration of a splayed PH wheel showing the shift in the CG from O to O′ by ΔZ upon UV illumination. b) Cross-sectional view of mid-width of the splayed PH wheel with positions of the right node (at time t=0 s) highlighted at different time instances (1-5) and transient variation of the *cis* mass-fraction of the right node of the splayed PH wheel at outer ($z = 0\,\mu$m) and inner ($z = 80\,\mu$m) under illumination. (The isomerization parameters are $\alpha = 30$, $\beta = 3$, $d_t = 5\,\mu$m and $\tau = 3\,$s.)



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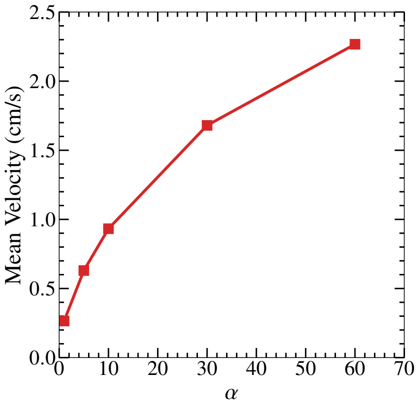

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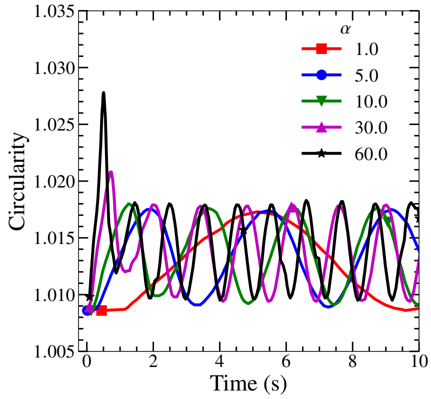


(c)

Fig S2: a) Cross-sectional view of ALCN splayed PH wheel illuminated by light with different forward reaction coefficients, $\alpha = 5$ (top), $\alpha = 10$ (middle), $\alpha = 30$ (bottom) at various time instants. Effect of forward reaction coefficient, α on the b) mean-velocity and c) circularity of splayed PH wheel under illumination. (The isomerization parameters are $\alpha/\beta = 10$, $d_t = 5\,\mu m$ and $\tau = 3\,s$.)

S1. Influence of isomerization and geometric parameters on the rolling motion of ALCN wheel

S1.1. Effect of attenuation length, d_t

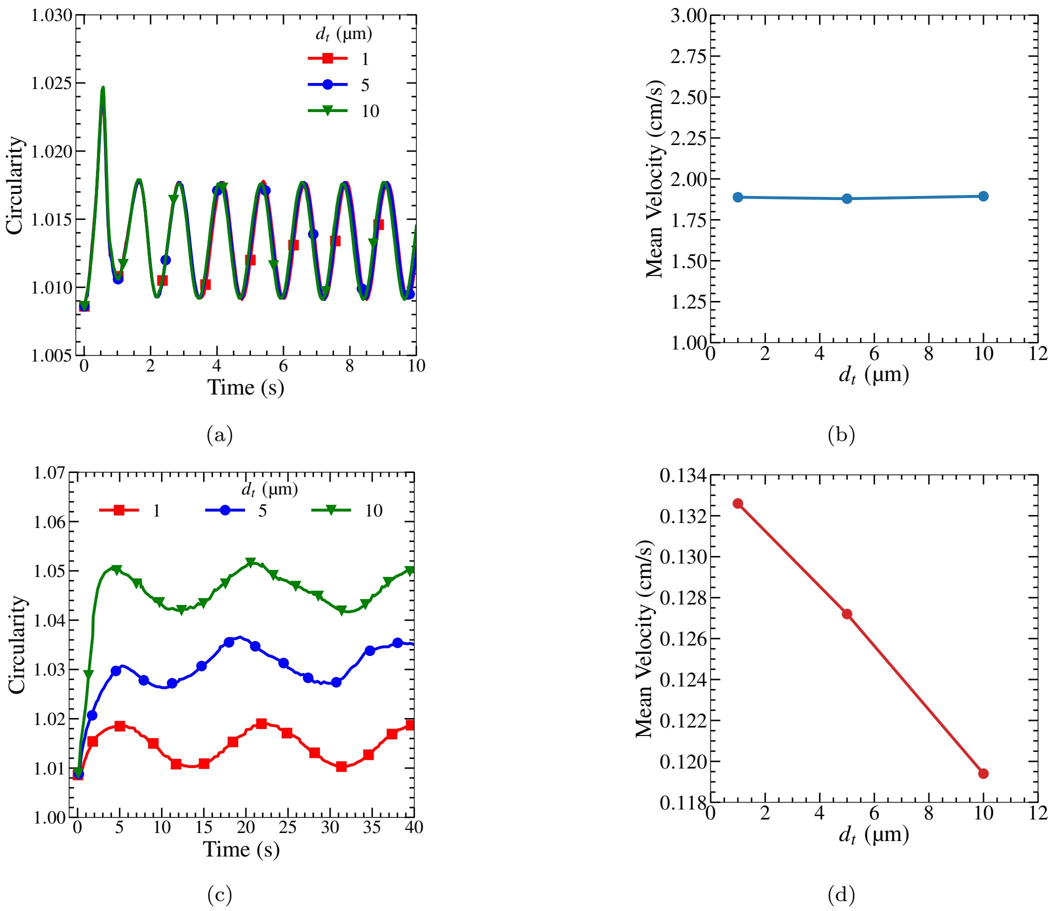
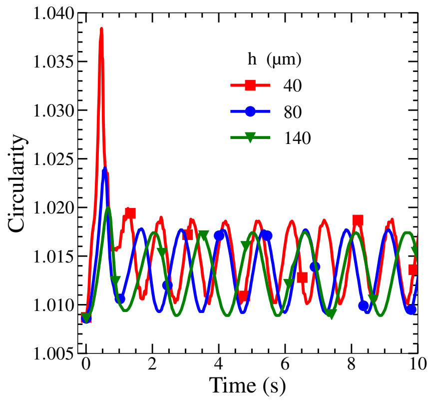


Fig S3: Effect of attenuation length, d_t on a) circularity b) mean velocity of planar wheel illuminated by light. Effect of attenuation length, d_t on c) circularity d) mean velocity of HP wheel illuminated by light. (The isomerization parameters are $\alpha = 30$, $\beta = 3$ and $\tau = 3\,\text{s}$.)

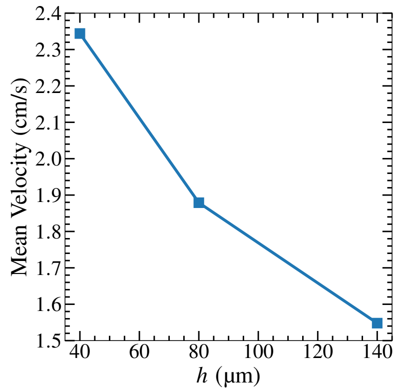
It is known that the attenuation length d_t subsumes the absolute number of azo-chromophores in the LC network [1]. The polymer network with higher azo dye concentrations will have less attenuation length due to higher absorption probability. The values of attenuation length, d_t are found to be in the range of 1 µm to 10 µm in the literature.[2–4] Hence, in this work $d_t = 1$, 5 and 10 are considered. The polymer network with higher attenuation length will make the light to penetrate deeper, giving rise to a uniform distribution of *cis* mesogens through the depth. In Planar wheels, the change in strain gradient with different attenuation lengths do not lead to distinct shapes as depicted in Fig. S3a owing to the restrictive nature of unbending deformation. Hence the mean velocity of planar wheels for different attenuation lengths (see Fig. S3b) are almost identical as the circularity does not vary much. In contrast, the splayed HP wheel with higher d_t has higher photo-induced strain and hence, circularity changes with change in d_t as shown in Fig. S3c.

The rolling resistance increases with an increase in d_t for HP wheels as the shape becomes more non-circular and therefore reduces the corresponding mean velocity as shown in Fig. S3d.

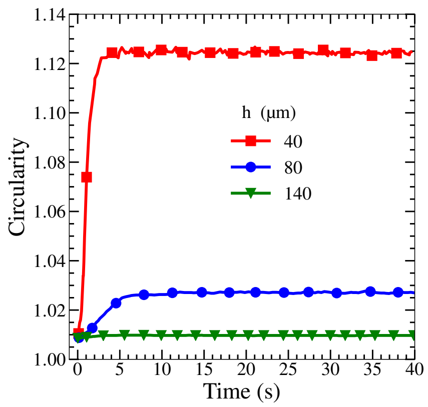
S1.2. Effect of film thickness, h



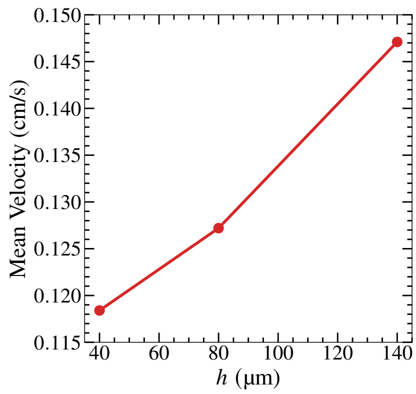
(a)



(b)



(c)



(d)

Fig S4: Effect of thickness, h on a) circularity, b) mean velocity of planar wheels illuminated by light. Effect of thickness, h on c) circularity d) mean velocity of HP wheels illuminated by light. (The isomerization parameters are $\alpha = 30$, $\beta = 3$, $\tau = 3\,\text{s}$ and $d_t = 5\,\mu\text{m}$.)

The thickness of the hollow wheel (Planar and HP) influences the amount of deformation (bending/unbending) and hence affects the mean velocities of wheels under illumination. The planar wheels with lower thickness unbend faster, causing the peak in circularity to be reached earlier as seen in Fig. S4a. As the changes in shape are faster for planar wheels of lower thickness, the rolling motion is initiated earlier, leading to higher mean velocities. Moreover, the mean of circularities with wheels of different thicknesses is similar and low enough so as not to generate any unwanted resistance. Hence, for planar wheels, the mean velocity of the wheels is inversely proportional to the thickness of the wheels as shown in Fig. S4b. In contrast, this higher deformation for lower thickness affects the splayed HP wheels adversely as they are prone to bend more (aided by gravity) and lead to high values of circularity as seen in Fig. S4c. Such high values of circularity for lower values of thickness reduces the mean velocity of the splayed HP wheels as higher circularity implies higher rolling resistance. Hence, the mean velocities of splayed HP wheels are proportional to the thickness of the wheel as seen in Fig. S4d. The circularity of the planar wheel is lesser compared to splayed HP wheels as shown in Figs. S4a and S4c. Hence for planar wheels, higher unbending deformation aids the motion and for splayed HP wheels, higher bending deformation inhibits the motion.

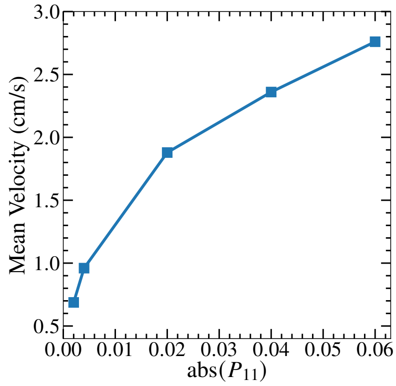


Fig S5: Mean velocity of planar wheel for different photo-expansion tensor values ($P_{11}, P_{22} = P_{33}$, $P_{22}/P_{11} = -0.6$). (The isomerization parameters are $\alpha = 30$, $\beta = 3$, $\tau = 3\,\mathrm{s}$ and $d_t = 5\,\mu\mathrm{m}$.)

S1.3. Effect of photo-expansion tensor, P_{ij}

For a particular thickness of the film, the increase (decrease) in the P_{ij} values will increase (decrease) the strain gradient through thickness. Hence the mean velocity of the wheels can either increase or decrease depending on the shape change of the wheels. In our work, we have observed an optimum value of P_{ij} ($P_{11} = -0.06, P_{22} = P_{33} = 0.036$) for planar wheels for which the mean velocity seems to be highest as shown in Fig. S5. For $P_{11} = -0.001$, the shape change was minimal upon light illumination, and hence starting torque was not enough to start the rolling motion. For $P_{11} = -0.2$, the wheel almost collapsed in the simulations due to significant shape change.

References

[1] D. Corbett, M. Warner, Bleaching and stimulated recovery of dyes and of photocantilevers, Physical Review E 77 (2008) 051710.

[2] M. L. Dunn, Photomechanics of mono-and polydomain liquid crystal elastomer films, Journal of Applied Physics 102 (2007) 013506.

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[4] D. Liu, L. Liu, P. R. Onck, D. J. Broer, Reverse switching of surface roughness in a self-organized polydomain liquid crystal coating, Proceedings of the National Academy of Sciences 112 (2015) 3880–3885.