Supporting Information

Thermal Properties of Lauric Acid Confined in Carbon Nanotubes as Shape-stabilized Phase Change Materials

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MD of phase change temperatures: The C-form crystal structure [1] of LA was used in the simulation (Fig. S1(a)), with lattice parameters of a = 9.524 ± 0.02 Å，b = 4.965 ± 0.01 Å，c = 35.39 ± 0.07 Å，and β = 129⁰13'±1'.

The melting process was from 295K to 355K with a temperature increment of 10K under NPT ensemble. At each temperature, the system was pre-equilibrated with a 200ps run before the data collection in the next 200 ps. The phase change temperatures were obtained based on the change of self-diffusion coefficients at different temperatures. As Fig. S1(b) shows, there are turning points in the curve of self-diffusion coefficients as a function of temperature, regarded as the phase change temperatures. The three turning point of 53.5℃, 52.0℃，and 41.9℃ of LA, 5-10nmCNTs/LA1, and 2-5nmCNTs/LA1, respectively, qualitatively agree with the DSC results.
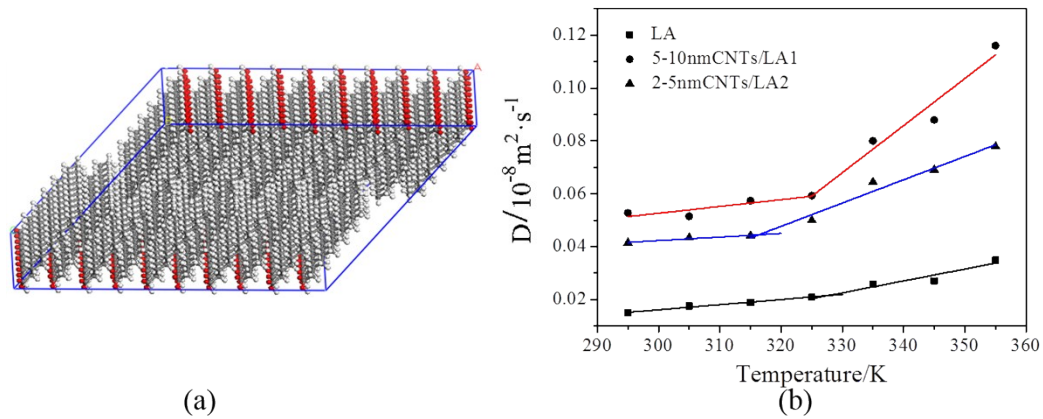

(a)   (b)

Fig. S1 (a) C-form crystal structure of LA. (b) The self-diffusion coefficients as a function of temperature.

MD of structure of LA molecules confined in CNTs: The order parameter was used to characterize the orientation relative to the axis of CNTs, which is defined as follows [2]:

$$S = \frac{3}{2} < COS^2(\theta) > - \frac{1}{2}$$
(S1)

where θ is the angle between the vector of the end-to-end C atoms and the axis of CNT.

For the molecules on the wall, most values of *S* are close to 1, which means that the LA molecules distribute along the axis, and those of the inner molecules are closer to -0.5, which indicate that LA molecules spread on the radial plane and can easily undergo crystallization (Fig. S2).
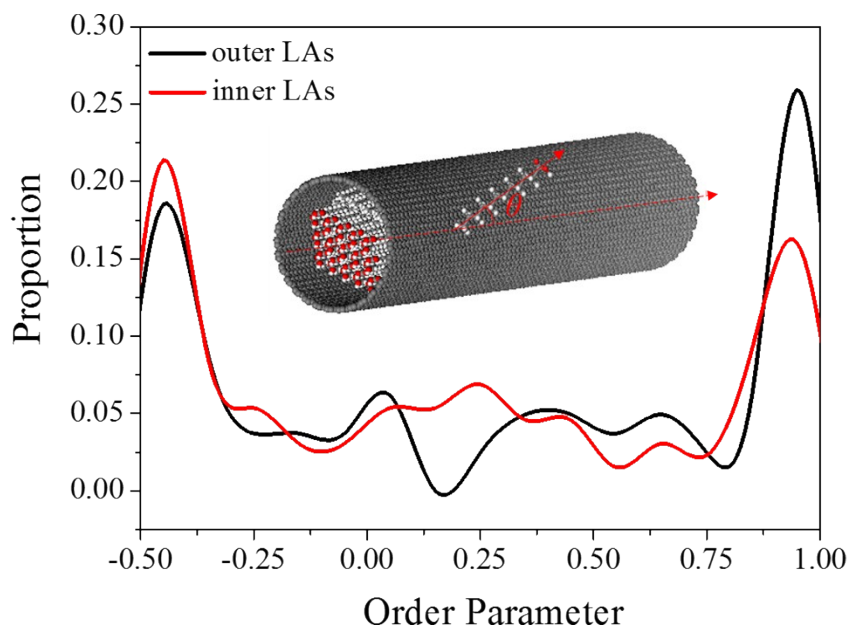

Fig. S2 Order parameter of LA molecules confined in CNTs.