Supplementary Information for

Towards understanding of shape formation mechanism of mesoporous silica particles

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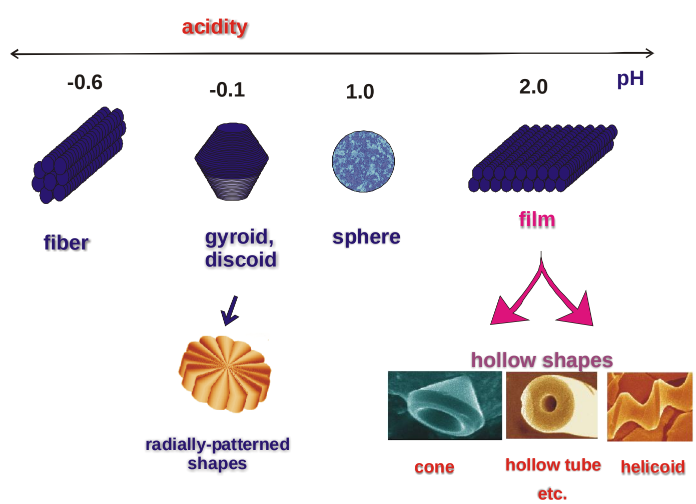
Universality of the assembly mechanism

It is conceivable to say that the variability of shapes described in the manuscript, including the fibers analyzed in the manuscript, are self-assembled through a similar mechanism (see refs. [1-4] for more detail). **SI Fig.1** shows an example of classification of "zoo" of these shapes. Specifically, the synthesized shapes shown are classified by the acidity of the synthesizing bath.

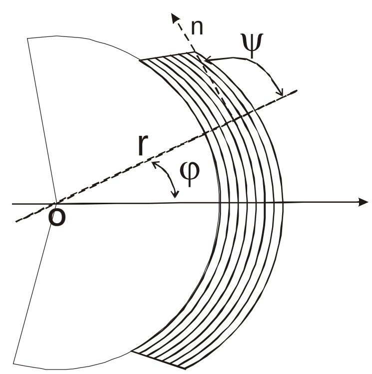


SI Fig.1. Variety of nanoporous shapes that were prepared by using CTACl as surfactant micellar template and TEOS as silica precursor. [1]

Besides the fundamental interest in explaining the formation mechanism, there is a lot of interest in the controlled assembly of nontrivial shapes because it can carry different functionalities, [5,6] and can be used for drug delivery, as parts of future micromachines, nano reactors or microcatalysis, as the matrix for new nanostructured materials.

Calculation of **Free energy of the fibers**

Assuming that the energy of freshly formed fibers, which have p6mm symmetry, is described by Frank Landau formula, eq. (1) of the main text, integration over the fiber volume can be done analytically. **SI Fig.2** shows the notations used in the derivation.



SI Fig. 2. Polar coordinate notation for a fiber-like liquid crystal, where $\vec{n}$ is the vector of the director-field. Vertical ***z*** axis is perpendicular to the page.

Because we do not observe experimentally the fiber twisted around the axis of symmetry or splayed fibers, the terms with K_1 and K_2 vanish, and the resulting energy is given by $\mu^0 = K_3 f(l, R, d)$, where l is the length of a fiber, d is the diameter of the fiber, R is the radius of the bent fiber.

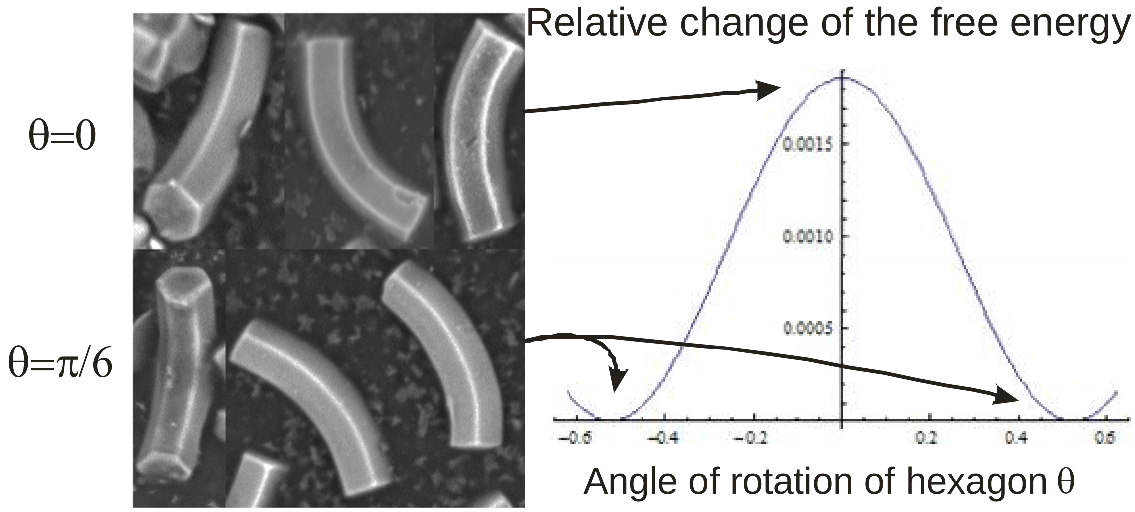
Using cylindrical coordinate system, SI Fig.2, one can rewrite Eq. (1) as follows:

$$\mu_0 = K_3 \int_R^{R+d} dr \int_{hex\ boundary} dz \int_{\varphi_0}^{\varphi_1} d\varphi \left[1 - \cos(2\psi)\right] \left[1 + \left(\frac{\partial \psi}{\partial \varphi}\right)^2\right] \qquad \text{(SI1)}$$

where $\varphi 0$ ($\varphi 1$) is the polar angle corresponding to the beginning (end) of the fiber. To take the above integrals, we used Mathematica (the integrand was simplified in similar to refs.[3, 6] manner). The used code is attached at the end of the Supplementary materials. Finally, the free energy for a hexagonal fiber reads

$$\mu^0 = \frac{\sqrt{3} l K_3}{2R}\left[d\, ln\left[\frac{d-4R}{3d-4R}\right] + 4R\, ln\left[\frac{4R}{4R-d}\right] - 2\left(d-2R\right) ln\left[\frac{d-4R}{2d-4R}\right]\right] \qquad \text{(SI2)}$$

It should be noted that formula SI2 is derived for the case of the fiber that is shown in SI Fig. 2, the case of $\theta = 0$. Rotation of the hexagon to its maximum different configuration corresponding to $\theta = \pi/6$ gives only ~0.002% difference in the free energy, see **SI Fig. 3**. Therefore we will not consider the difference in the rotation angle of the fibers in our measurements.



SI Fig. 3. The relative change all the free energy is shown for different angles of bending of the hexagonal fiber.

The most probable parameter K_3 with respect to the Boltzmann distribution

Any parameter of a statistical distribution can be defined from the experimental data. Maximum likelihood method allows one to do that. In the maximum likelihood method, each parameter of the statistical distribution maximizes the probability to find the experimental data from the point of view of the particular distribution. Therefore, one has to find the extremum, zero derivative of the probability with respect to the parameter (for example, K_3) of the statistical distribution (for example, the Boltzmann distribution). The probability of recording of all set of N measured data is a multiplication of individual probabilities given by the Boltzmann distribution:

$$\boldsymbol{P}\left(\boldsymbol{X}_1, \boldsymbol{X}_{2,} .. \boldsymbol{X}_N \mid \boldsymbol{K}_3\right) = \boldsymbol{C}^N \mathbf{exp}\left[-\sum_{i=1}^{i=N} \boldsymbol{\mu}^0{}_i / \boldsymbol{k}_B \boldsymbol{T}\right], \qquad \text{(SI3)}$$

where $C = \sqrt{\frac{1}{K_3\left(kT\right)}} e^{-\frac{\mu}{kT}}$ is the normalization constant.

Putting the derivative of equation (SI3) with respect to K_3 equal to zero, one can find that $K_3 = \frac{kT}{\sum_{i=1}^{i=N}\left(\frac{\mu_i^0}{K_3}\right)\frac{1}{N}}$. It is worth noting here that function $\left(\frac{\mu_i^0}{K_3}\right)$ is experimentally determined. As one can see from eq. (SI2), it does not depend on K_3.

Mathematica code for calculation of free energy of hexagonal fiber

```
theta=.;
r01:=-(1/2)*d;
z01:=0;
r02:=-
(1/4)*d;z02:=(1/4)*d*Sqrt[3];r03:=(1/4)*d;z03:=(1/4)*d*Sqrt[3];r04:=(1/2)*d;z04:=0;r05:=(1/
4)*d;z05:=-(1/4)*d*Sqrt[3];r06:=-(1/4)*d;z06:=-(1/4)*d*Sqrt[3];r1:=R-d/2+r01*Cos[theta]-
z01*Sin[theta];z1:=r01*Sin[theta]+z01*Cos[theta];r2:=R-d/2+r02*Cos[theta]-
z02*Sin[theta];z2:=r02*Sin[theta]+z02*Cos[theta];r3:=R-d/2+r03*Cos[theta]-
z03*Sin[theta];z3:=r03*Sin[theta]+z03*Cos[theta];r4:=R-d/2+r04*Cos[theta]-
z04*Sin[theta];z4:=r04*Sin[theta]+z04*Cos[theta];r5:=R-d/2+r05*Cos[theta]-
z05*Sin[theta];z5:=r05*Sin[theta]+z05*Cos[theta];r6:=R-d/2+r06*Cos[theta]-
z06*Sin[theta];z6:=r06*Sin[theta]+z06*Cos[theta];z1max:=(z1*(r-r2)-z2*(r-r1))/(r1-
r2);z1min:=(z1*(r-r6)-z6*(r-r1))/(r1-r6);z2max:=(z2*(r-r3)-z3*(r-r2))/(r2-
r3);z2min:=z1min;z3min:=(z6*(r-r5)-z5*(r-r6))/(r6-r5);z3max:=z2max;z4max:=(z3*(r-r4)-
z4*(r-r3))/(r3-r4);z4min:=z3min;z5min:=(z5*(r-r4)-z4*(r-r5))/(r5-r4);z5max:=z4max;
I1:=Assuming[0<theta && theta<(1/6)*Pi,NIntegrate[Integrate[(1/r),{z,z1min,
z1max}],{r,r1,r2}]];
I2:=Assuming[0<theta && theta<(1/6)*Pi,NIntegrate[Integrate[(1/r),{z,z2min,
z2max}],{r,r2,r6}]];
I3:=Assuming[0<theta && theta<(1/6)*Pi,NIntegrate[Integrate[(1/r),{z,z3min,
z3max}],{r,r6,r3}]];
I4:=Assuming[0<theta && theta<(1/6)*Pi,NIntegrate[Integrate[(1/r),{z,z4min,
z4max}],{r,r3,r5}]];
I5:=Assuming[0<theta && theta<(1/6)*Pi,NIntegrate[Integrate[(1/r),{z,z5min,
z5max}],{r,r5,r4}]];
Itotal:=l*(I1+I2+I3+I4+I5)/R;
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SI References

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