Supplementary materials

I. Janus colloid in nematic LC

To test our method in simple geometries, we have simulated the spherical Janus particles in the nematic media. The resulting director distributions and defect profiles are presented in Fig. S-1. As one can see, the method fully reproduces the results published earlier in Ref. 3, with the only difference that we are using the smooth variation of the anchoring angle at the border between homeotropic anchoring and planar degenerate anchoring. As it follows from Fig. 5 for $d/p_0 = 0$, the minimum free energy corresponds to $\theta = \pi/2$ [the structure presented in Fig. S-1 (b)], exactly as in Fig. 10 of Ref. [3].

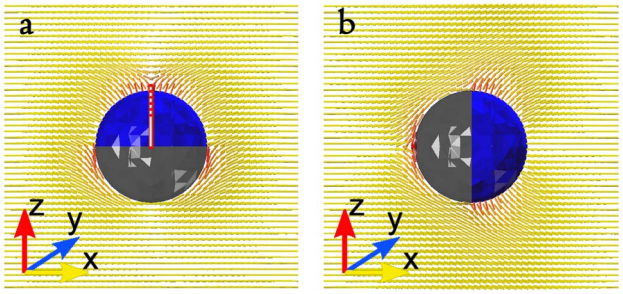

Fig. S-1 (Color online) Optimal director distribution and defect profiles in nematic LC with Janus colloid particle at $\theta = 0^\circ$ (a) and 90° (b). All definitions are the same as in Fig. 2.

II. Planar and homeotropic colloids in cholesteric LC

We have also simulated spherical particles with fully homeotropic anchoring (see Fig. S-2) and fully planar degenerate anchoring (see Fig. S-3) in both nematic and cholesteric medias (at various d/p_0 ratios). One can see from these figures that our method nicely reproduces the director distributions and structures of defects obtained previously in Refs. [7,8,11,16].

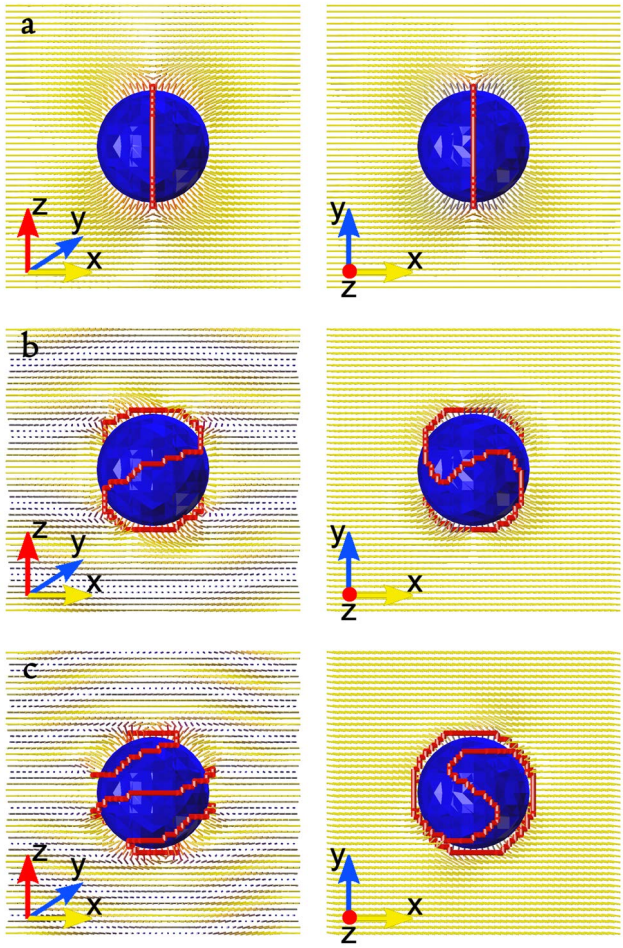

Fig. S-2 (Color online) Director distribution and structure of defects around homeotropic colloid particle in cholesteric LC for various d/p_0 ratios: (a) $d/p_0 = 0$ (nematic); (b) $d/p_0 = 0.8$; (c) $d/p_0 = 1.6$. Director vectors are colored in correspondence with the direction (yellow – along x-axis, blue – along y-axis, and red – along z-axis). Defect lines are shown with thick red lines.

III. Box size effects

Since computer simulations are always limited in time, the optimal choice of the box size is very important. In the main part of the paper we were using the box size equal to 2.5 particle diameters d. The question arises, whether this size is large enough for simulation of "infinite" media? To answer this question, in the present section we study the dependency of results on the simulations box size in two ways.

Firstly, we have produced calculations for various box size to particle diameter ratios l/d for particular fixed value of $d/p_0 = 1.6$ at various tilt angles θ (from 0° to 90°) and fixed azimuthal angle $\varphi = 80^\circ$ corresponding to the free energy minimum obtained for the box size $l/d = 2.5$ used in the main part of the paper. It is natural to suppose that variation of the box size will not change the free energy minimum position with respect to azimuthal angle φ, while minimization of the free energy with respect to both angles θ and φ takes much computational time, especially for the large boxes. The dependencies of the total free energy on the tilt angle θ for various l/d ratios are presented in Fig. S-4, and one notices that all of them are similar and have the same global minimum position.

As it was discussed in [17], where our calculation method is explained in details, several independent optimization runs are

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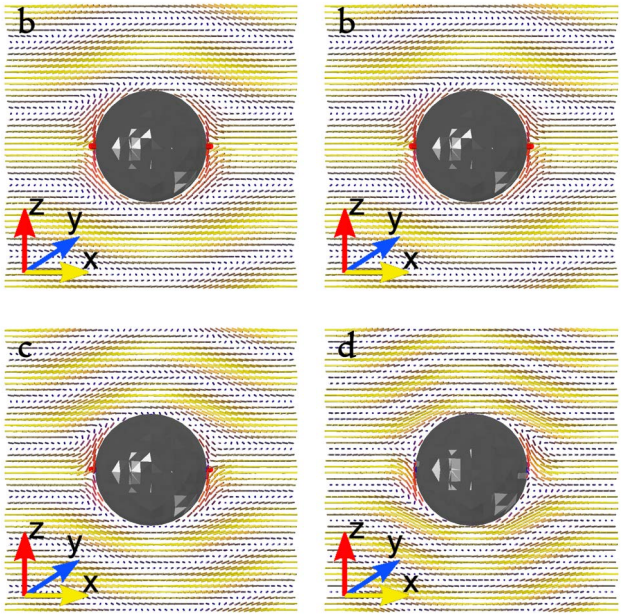


Fig. S-3 (Color online) Director distribution and position of defects around planar degenerate colloid particle in cholesteric LC for various d/p_0 ratios: (a) $d/p_0 = 0$ (nematic); (b) $d/p_0 = 0.8$; (c) $d/p_0 = 1.2$; (d) $d/p_0 = 1.6$. Director vectors are colored in correspondence with the direction (yellow – along x-axis, blue – along y-axis, and red – along z-axis). Point defects on poles of the particle are shown with thick red points.

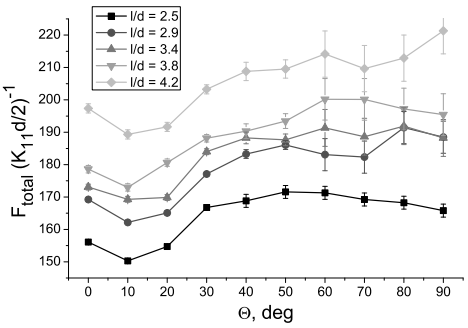
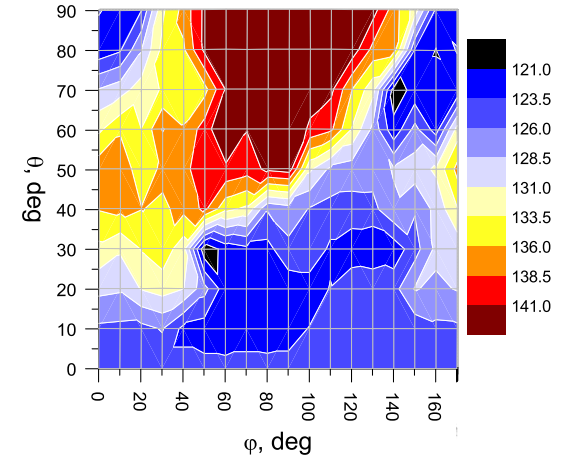


Fig. S-4 Dependence of the dimensionless total free energy on the tilt angle for various values of box size to particle diameter ratio l/d. Here $d/p_0 = 1.6$ and φ was chosen equal to 80° corresponding to the global free energy minimum position at $l/d = 2.5$.

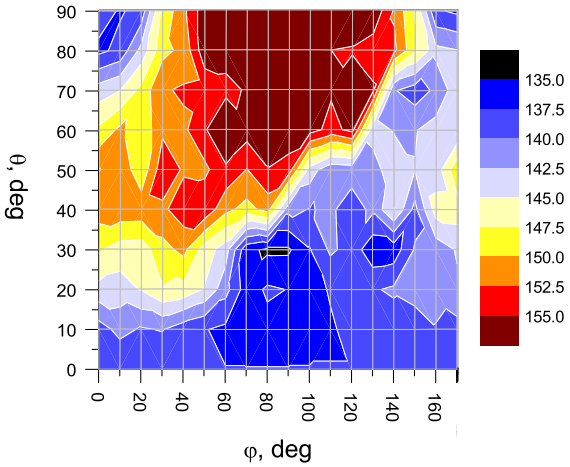
essentially used in our software to obtain the structure as close as possible to the one corresponding to the global free energy minimum at each point. The error bars presented in Fig. S-4 correspond to the RMS deviations of the free energy from the minimal value (obtained at particular run) over the whole set of runs. From the first round of calculation we approximately know the global free energy minimum position. On the next stage, we run our software many times in the vicinity of the global minimum position obtained at previous runs. In particular, at $l/d = 2.5$ (corresponding to the box size used in the main part of the paper) we run it 40 times at each $\theta < 40^\circ$, while at each $\theta > 40^\circ$ we run it only 20 times to save computational time. Obviously, the error obtained at $\theta < 40^\circ$ [about ± 0.5 dimensionless energy units (e.u.)] is smaller than the error obtained at $\theta > 40^\circ$ [about ± 2 e.u.]. At larger box size to particle diameter ratios l/d we are generally using the smaller number of runs, since the target is only to show that the global minimum position does not change, when the box size changes. Thus, for larger l/d, we run our software 20 times at each $\theta < 40^\circ$ and 8 times at each $\theta > 40^\circ$. The corresponding error appears to be larger. At $\theta < 40^\circ$ it varies between ± 0.7 e.u. for $l/d = 2.9$ and ± 1.4 e.u. for $l/d = 4.2$. At $\theta > 40^\circ$ it varies between ± 5.0 e.u. for $l/d = 2.9$ and ± 7.1 e.u. for $l/d = 4.2$. Although fig. S-4 does not pretend to precise description at large θ, the data presented in fig. S-5 and fig. S-6 (see details below), show good overall agreement between the data obtained for various box sizes, in particular at large θ.

Secondly, we have calculated and compared the free energy profiles in the $\theta - \varphi$ space for the box size to particle diameter ratio $l/d = 2.5$ used in the main part of the paper and for sufficiently larger ratio 3.8. The resulting profiles are presented in fig. S-5 for $d/p_0 = 1$ and in fig. S-6 for $d/p_0 = 2$. One can see from these figures that the free energy profiles for small and large box sizes are topologically very similar as at relatively large cholesteric pitch ($d/p_0 = 1$), as at relatively small cholesteric pitch ($d/p_0 = 2$). In particular, the exact positions of the free energy minima in the $\theta - \varphi$ space for small and large boxes are very close to each other.

The director distributions and defect profiles for various box sizes at $\theta = 10^\circ$ and $\varphi = 80^\circ$ are presented in Fig. S-7 for visual comparison of the results at various box sizes. Generally, one notices a miserable difference between these structures, and, in particular, the defect structure remains the same for each box size. From all these observations we finally conclude that the box size $l/d = 2.5$ used in the main part of the paper is large enough to study the orientational ordering of Janus colloid particle in cholesteric media.

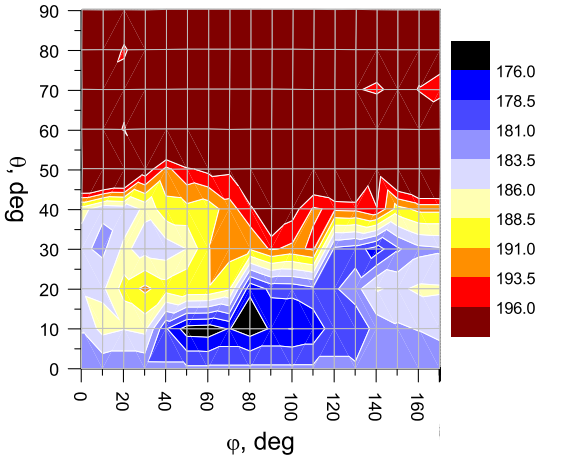


(a)

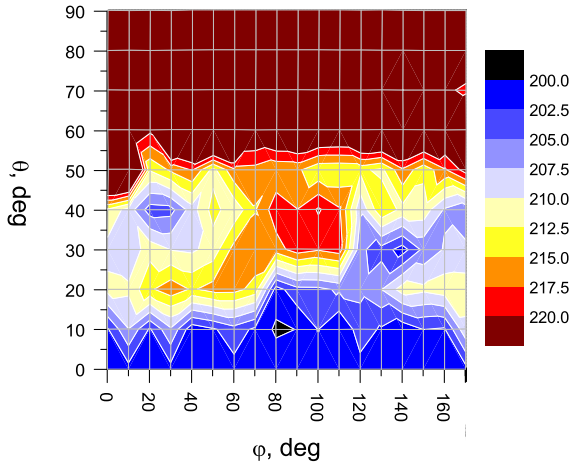


(b)

Fig. S-5 (Color online) Dimensionless free energy $F_{total}(K_{11}d/2)^{-1}$ profile for diameter-to-pitch ratio $d/p_0 = 1.0$ for various box size to particle diameter ratios l/d: (a) 2.5; (b) 3.8. In both cases the primary minimum is at $\theta = 30^\circ$, and the secondary minimum is at $\theta = 70^\circ$.



(a)



(b)

Fig. S-6 (Color online) Dimensionless free energy $F_{total}(K_{11}d/2)^{-1}$ profile for diameter-to-pitch ratio $d/p_0 = 2.0$ for various box size to particle diameter ratios l/d: (a) 2.5; (b) 3.8. In both cases the primary minimum is at $\theta = 10^\circ$.

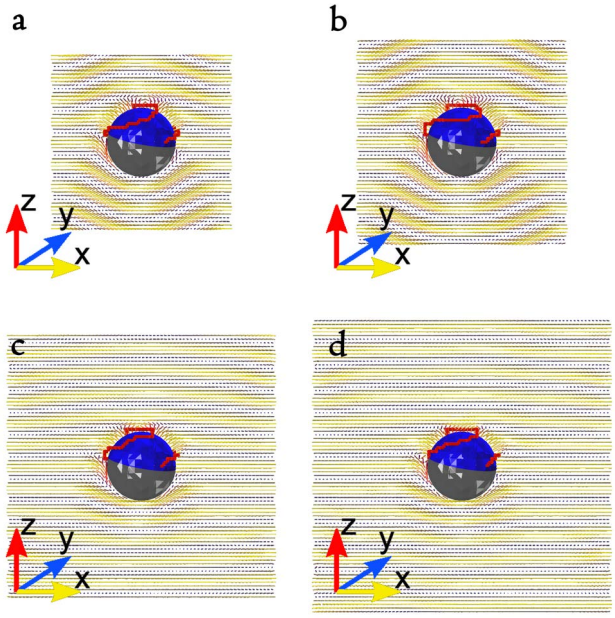


Fig. S-7 (Color online) Director distribution and position of defect lines around Janus colloid particle in cholesteric LC for various box size to particle diameter ratios l/d: (a) 1.0; (b) 1.34; (c) 1.51; (d) 1.68. Director vectors are colored in correspondence with the direction (yellow – along x-axis, blue – along y-axis, and red – along z-axis). Defect lines are shown with thick red lines. System configuration is fixed to $\theta = 10^\circ$, $\varphi = 80^\circ$.