Electronic Supplementary Information for

Close packings of identical proteins in small spherical capsids and similar proteinaceous shells

Sergei B. Rochal.*[a], Olga V. Konevtsova,[a] Ivan Yu. Golushko,[a] Rudolf Podgornik** [b,c,d]

[a]Physics Faculty, Southern Federal University, Rostov-on-Don, Russia.
[b]School of Physical Sciences and Kavli Institute for Theoretical Sciences, University of Chinese Academy of Sciences, Beijing 100049, China.
[c]CAS Key Laboratory of Soft Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China.
[d]Wenzhou Institute of the University of Chinese Academy of Sciences, Wenzhou, Zhejiang 325000, China.
* Corresponding author. E-mail: rochal_s@yahoo.fr
** Corresponding author. E-mail: podgornikrudolf@ucas.ac.cn

Packings of anisotropic particles with a symmetry of equilateral triangle

Another interesting special case of packings of weakly anisotropic SUs that can be obtained using the theory developed above (see eqn (3) in the main text) is packings of slightly deformed disks with a symmetry of equilateral triangle C_{3V}. In this case the interaction energy reads:

$$U = \sum_{i>j, r_{ij}<1} \left(\frac{1 + \alpha \left(\frac{3(\boldsymbol{r}_i \boldsymbol{n}_j + \boldsymbol{r}_j \boldsymbol{n}_i)}{\left(1 - (\boldsymbol{r}_i \boldsymbol{r}_j)^2\right)^{1/2}} - 4 \frac{(\boldsymbol{r}_i \boldsymbol{n}_j)^3 + (\boldsymbol{r}_j \boldsymbol{n}_i)^3}{\left(1 - (\boldsymbol{r}_i \boldsymbol{r}_j)^2\right)^{3/2}} \right)}{r_{ij}} \right)^n , \qquad \text{(S1)}$$

where $\boldsymbol{r}_i$, $\boldsymbol{r}_j$ are coordinates of the interacting particles, $\boldsymbol{n}_i, \boldsymbol{n}_j$ are their directors lying in the planes tangent to the sphere surface, and r_{ij} is the distance between the centers of the SUs. As in the case of elliptically deformed disks (see the main text) the degree of anisotropy equals $S_{max}/S_{min} = (1+2\alpha)/(1-2\alpha)$, where $\alpha > 0$, S_{max}, S_{min} are maximal and minimal radii of the particle, accordingly.
Figure S1 shows three such packings. The structure in the panel (a) was obtained by minimizing the energy of N=150 randomly distributed and oriented SUs. Starting coordinates for packings (b) and (c) correspond to the nodes of the spherical lattices (h=2, k=1, N=60) and (h=3, k=1, N=120); the initial orientations of directors were random but preserving icosahedral symmetry. During energy minimization no symmetry constrains were applied.

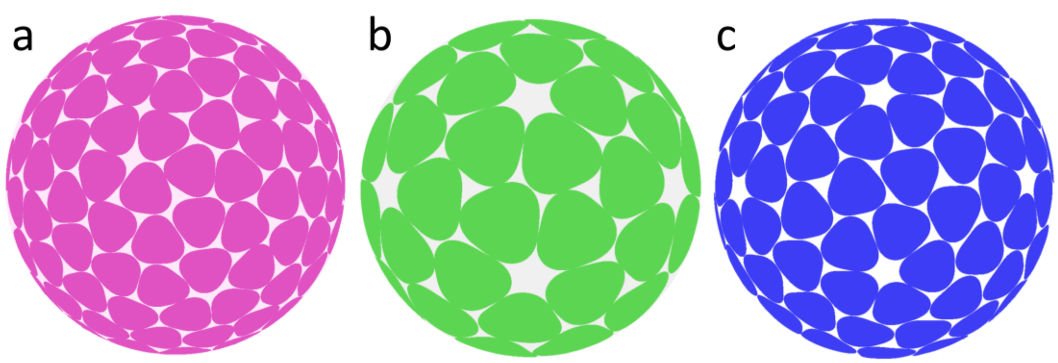

Fig. S1. Asymmetrical (a) and icosahedral (b and c) packings of weakly anisotropic particles with symmetry C_{3V}.