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Slightly broken icosahedral symmetry advances Thomson problem

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ABSTRACT

To advance Thomson problem we generalize physical principles suggested by Caspar and Klug (CK) to model icosahedral capsids. Proposed simplest distortions of the CK spherical arrangements yield new-type trial structures very close to the lowest energy ones. In the region $600 \leq N \leq 1000$, where N is the number of particles in the structure, we found 40 new spherical crystals with the lowest ever seen energies and curvature-induced topological defects being not the well-known elongated scars but flatten pentagons. These crystals have N values prohibited in the CK model and demonstrate a new way to combine the local hexagonal order and spherical geometry.

Self-organization of repelling particles retained on a spherical surface is under discussion for more than a century and is called Thomson problem [1] after J.J. Thomson who suggested his model of atom 110 years ago. Now we know that Thomson problem arises on different levels of the matter self-organization. Arrangements in multi-electron bubbles in superfluid helium [2] almost perfectly correspond to structures formed by charged particles in the frame of the problem. Some of the Thomson structures (TSs) are similar to spherical viral capsids [3]. Simplest repelling potentials $1/r_{ij}^{\alpha}$, where r_{ij} is the distance between ith and jth particles and $\alpha \geq 1$, are used to describe colloidal crystals occurring at the interface between two fluids [4–7] and porous dried colloidosomes [8–10]. If $\alpha \to \infty$ then the TSs tend to densest packings of spherical caps on a sphere. This problem is named after Tammes [11] and has a significant number of applications [12].

Experimental and theoretical studies of spherical crystals and physical properties of 2D order [4,7,13–15] support a new wave of interest in the Thomson problem in the past years [16–19]. The low-energy structures formed by repelling particles retained on spherical and other curved surfaces are actively used to study and classify the curvature-induced extended topological defects and reactions between them [7,18,20] in 2D colloidal crystals with unconventional geometry. However, the classical spherical TSs corresponding to the global energy minima are also very interesting [6,21–23]. Their search is a challenging work since the equilibrium energies of structures corresponding to global and local-minima are very close. Moreover, the difference between the equilibrium energies is strongly reduced and the number of equilibrium structures grows exponentially with the number N of particles in the structure [24]. The list of spherical TSs with the lowest ever seen energy is constantly updated [23] by the Bowick group of physicists.

Note that some of the TSs with $N < 400$ demonstrate icosahedral symmetry [22] and up to the numerical optimization correspond to the Caspar and Klug (CK) structures of viral capsids [3]. Here, we adapt and develop the initial CK geometrical model to search for the lowest-energy TSs which have slightly broken icosahedral symmetry and numbers of particles prohibited in the CK capsid model. These TSs appear to be much more spread and our approach allows replacing about 10% of structures from the list [23] in the interval $600 \leq N \leq 1000$. We analyze this interval since the related arrangements of particles are sufficiently complicated, but simultaneously these crystals are well investigated by other authors.

Large ($N > 400$) known TSs are simply connected hexagonal lattices with 12 extended topological defects [23] induced by the sphere curvature. Most of spherical viral capsids are also described in terms of hexagonal lattices [3,25]. Quasiequivalence [3] of proteins in capsids makes their global symmetry the icosahedral one. However, icosahedral arrangements of particles are possible only at the particular N values. Moreover, even for these N values there is not any physical reason (like entropy contribution into free energy) which favors the high symmetry of sufficiently

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large TSs. Therefore, slight distortions of icosahedral lattices can simultaneously increase admitted N values and make the distorted structures energetically favorable. Following this idea we constructed and optimized several hundred of trial structures from the interval $600 \leq N \leq 1000$ during a few hours of calculation with laptop. As a result of this work for 40 values of N we found new spherical crystals with energies lower than those of earlier seen energetically best structures. All the TSs found belong to the same new type of the ground states, where the minimal-size topological defects are the identical flattened pentagons and their vacant geometric centers are located at the vertices of regular or slightly deformed spherical icosahedron.

The proposed below geometric method to construct spherical hexagonal lattices with slightly broken icosahedral symmetry doesn't depend on the explicit form of the particles coupling. However, to compare our results with the previous ones we put $\alpha = 1$ and choose the energy F of the particles interaction in the form:

$$F = \sum_{j>i}^{N} \frac{1}{r_{ij}}. \tag{1}$$

Let us recall that sufficiently large TSs with $N > 400$ demonstrate the local hexagonal order and contain 12 extended topological defects [6,26] (ETDs), located near the vertices of regular or slightly irregular icosahedron covered by a simply connected hexagonal lattice. The ETDs are induced by curvature and the hexagonal order in their areas is strongly distorted. Each ETD carries a total topological charge $+1$. After a triangulation the ETDs are presented as linear scars [4] consisting of closely located particles with different surroundings. Particles having 5 or 7 nearest neighbors alternate in the scars, therefore they are usually treated as sequences of elementary 5-fold and 7-fold disclinations. Note that like the TSs the spherical colloidal crystals also possess 12 scars located similarly [26].

Comparison between spherical structures corresponding to more or less deep energy minima of Eq. (1) shows [20] that when the spherical hexagonal order tends to its ground state, it becomes more perfect, the areas occupied by the extended defects become smaller, and the ETD structures becomes simpler. Nevertheless, the limit of this simplification representing a point disclination is not achieved and the lowest energy spherical structures cannot be reduced to the CK icosahedral lattices having 12 point topological defects.

According to the CK theory [3], the structures of a large number of spherical viral capsids is interpreted in terms of the icosahedron net decorated by a periodic hexagonal lattice with nodes containing capsomers constructed from proteins. The edges of the icosahedron assembled from the net are hexagonal translations, which are symmetrically equivalent to each other. Only two indexes (h, k) are sufficient to determine the icosahedron edges and to distinguish between the different capsid structures. The geometry of CK model provides the maximal equivalence of proteins in the viral capsid and imposes a restriction $10T + 2$ on the total number of capsomeres in it. The triangulation number T is the square of the icosahedron edge length: $T = h^2 + k^2 + hk$. The capsomers can contain five or six proteins. Each capsid includes 12 pentamers located in the icosahedron vertices. The pentamers in the model are the isolated topological defects, since they have not 6, but 5 nearest neighbors. The other capsomers are hexamers and their number is $10(T - 1)$.

Note, that in spite of huge advances in the interpretation of the viral capsids structures [25], the use of original CK geometric model to generate trial TSs is very limited. The icosahedral arrangements of particles are possible at the particular N values only. Moreover, the largest TS with the lowest ever seen energy [23], which yet correspond to the CK model, contains $N = 392$ particles and is indexed as $(2, 5)$. However, as it is shown below, some simple and clear modifications of the CK model make it suitable for larger structures and simultaneously increase essentially the list of admitted N values.

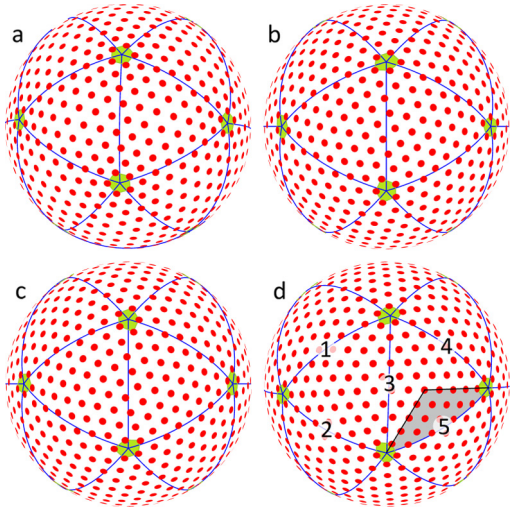

Fig. 1. Examples of structures arising due to exclusion of nodes in the icosahedrons vertices and containing $N = 10(T - 1)$ particles. (a) Ideal spherical CK $(7, 3)$ icosahedron with 12 vacant positions in its vertices. (b–c) In the optimized structures regular pentagons surrounding the vertices become flatten and the icosahedral symmetry is broken. The structures differ from each other by the flattened pentagons orientations and are extremely close in energy. The spherical icosahedra (shown in blue) preserve the regular shape since the optimization does not shift the ETDs centers. (d) The lowest-energy structure with $N = 800$ obtained in Ref. [23] is based on an irregular icosahedron with different edges. Triangulation indices of the edges enumerated by numbers from 1 to 5 are $(5, 6)$, $(5, 5)$, $(5, 6)$, $(4, 6)$, $(5, 5)$, respectively. These indices are determined by the side lengths of triangulation triangles. For the 5th edge, this triangle is highlighted with gray. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

To introduce our approach, let us note that in larger spherical structures the ETDs decrease energy (1) because they reduce increased density of particles appearing on the sphere near the projections of the icosahedron vertices. To obtain new 40 most favorable energetically structures in the region $600 \leq N \leq 1000$ it is sufficient to introduce identical simple topological defects by exclusion of particles in the vertices of regular or *specifically irregular* icosahedra. To obtain the lowest-energy structures with $N > 1000$ particles the more complicated ETDs arising due to exclusion of a larger number of particles near the icosahedrons vertices may be used. In a similar way several energetically favorable large structures with icosahedral symmetry were constructed [6]. Below we consider the case of regular icosahedra and then we pass to the problem how to construct energetically favorable structures based on slightly irregular icosahedral arrangements of particles.

Exclusion of 12 nodes in vertices of CK icosahedrons leads to a series of trial structures indexed like capsids by integer (h, k) and containing $N = 10(T - 1)$ particles. We started our computations for fifteen trial structures corresponding to the interval $600 \leq N \leq 1000$, which contains only fourteen different values of N from this series, since $9^2 + 9 \cdot 1 + 1 = 6^2 + 6 \cdot 5 + 5^2$. Before the gradient decent we changed randomly and very slightly the initial coordinates of particles. It induces bifurcations between the energy (1) minima. The arising low-symmetry structures (see examples in Fig. 1) have extremely close but different energies. The deepest energy minima are more frequent and about 10 variations of the initial conditions are sufficient to see the deepest minimum again. After the numerical optimization performed for all the trial structures we found 8 unknown earlier crystals with the lowest ever seen energies (see Table 1 and Supplementary materials) and