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Communication: A packing of truncated tetrahedra that nearly fills all of space and its melting properties

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Dense polyhedron packings are useful models of a variety of condensed matter and biological systems and have intrigued scientists and mathematicians for centuries. Here, we analytically construct the densest known packing of truncated tetrahedra with a remarkably high packing fraction $\phi = 207/208 = 0.995192\dots$, which is amazingly close to unity and strongly implies its optimality. This construction is based on a generalized organizing principle for polyhedra lacking central symmetry that we introduce here. The “holes” in the putative optimal packing are perfect tetrahedra, which leads to a new tessellation of space by truncated tetrahedra and tetrahedra. Its packing characteristics and equilibrium melting properties as the system undergoes decompression are discussed. © 2011 American Institute of Physics. [doi:10.1063/1.3653938]

Dense particle packings are useful models for a variety of condensed matter systems, including liquids, glasses and crystals,^{1–5} granular media,^{3,6} and heterogeneous materials.³ Understanding how nonspherical particles pack in space is a first step toward a better understanding of how biological cells pack.⁷ Probing the symmetries and other mathematical properties of the densest packings is a problem of interest in discrete geometry and number theory.⁸ In general, a packing is defined as a large collection of nonoverlapping solid objects (particles) in d -dimensional Euclidean space \mathbb{R}^d . Associated with a packing is the packing fraction ϕ defined as the fraction of space \mathbb{R}^d covered by the particles.

The three-dimensional Platonic and Archimedean polyhedra possess beautiful symmetries and arise in many natural and synthetic structures. An original investigation of dense packings of regular tetrahedra, one of the five Platonic solids, by Conway and Torquato⁹ has spurred a flurry of subsequent research activity, including studies to obtain dense packing of hard polyhedra^{10–15} and to understand the phase behavior of colloidal systems made of such solid objects.^{12,16,17} General organizing principles have been established for the densest packings of polyhedra in \mathbb{R}^3 .^{10,11} For centrally symmetric Platonic and Archimedean solids, it has been conjectured that the densest packings can be achieved by arranging the polyhedra on an appropriate Bravais lattice (see definition below) with the same orientation.¹⁰ (A centrally symmetric solid has a center of inversion symmetry.) For non-centrally symmetric polyhedra, the optimal packings are generally not Bravais lattice packings.¹¹ For example, a tetrahedron lacks central symmetry, and it is known that its densest packing must exceed that of the densest Bravais lattice packing.⁹

The Archimedean analog of the regular tetrahedron is the truncated tetrahedron, whose densest packing has been shown

to be a non-Bravais lattice packing.⁹ An Archimedean truncated tetrahedron has four regular hexagonal faces and four regular triangular faces, as obtained by truncating the corners (small tetrahedra with edge length $1/3$ of that of the original tetrahedra) of a tetrahedron (see Fig. 1(a)). In particular, a truncated tetrahedron does not possess central symmetry and its dihedral angle (i.e., the angle between two faces) is the same as that of a tetrahedron $\theta = \cos^{-1}(1/3) \approx 0.392\pi$. Since θ is not a sub-multiple of 2π , one cannot tile (i.e., completely fill) the three-dimensional Euclidean space \mathbb{R}^3 with truncated tetrahedra.

Betke and Henk showed that the optimal Bravais lattice packing of truncated tetrahedra possesses a packing fraction $\phi = 207/304 = 0.680921\dots$ ¹⁸ Conway and Torquato constructed a dense packing of truncated tetrahedra with $\phi = 23/24 = 0.958333\dots$,⁹ which proved that the optimal packing must be a non-Bravais lattice packing. Recently, de Graaf, van Roij, and Dijkstra¹⁹ showed via numerical simulations that truncated tetrahedra can pack at least as dense as 0.988, suggesting the existence of even denser packings.

Indeed, in this paper, we find an exact construction for the densest known packing of truncated tetrahedra with a remarkably high packing fraction $\phi = 207/208 = 0.995192\dots$ ²⁰ which nearly fills all of space. This implies its optimality, which is supported by additional numerical maximization studies, as explained below. This construction is based on a generalized organizing principle for polyhedra that lack central symmetry that we introduce here. We show that the “holes” in the putative optimal packing are perfect tetrahedra and hence taken together with the truncated tetrahedra lead to a new tessellation of \mathbb{R}^3 . Moreover, we investigate the equilibrium melting properties of the putative optimal packing.

Some important definitions are in order here before describing our new packing. A lattice Λ in \mathbb{R}^3 is an infinite set of points generated by a set of discrete translation operations defined by integer linear combinations of a basis of \mathbb{R}^3 ,

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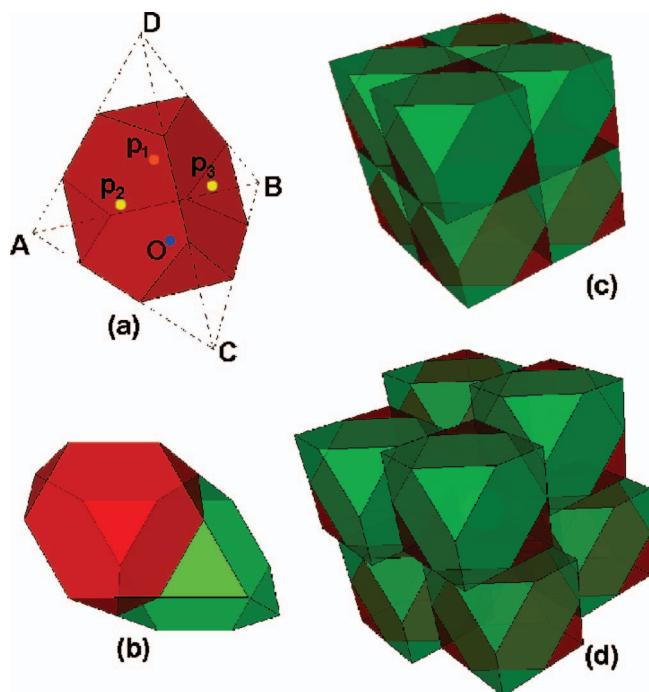


FIG. 1. Truncated tetrahedron and portions of its packings. (a) A truncated tetrahedron with its associated tetrahedron shown. The labels are described in the text. (b) A dimer (pair) of truncated tetrahedra making perfect contact through hexagonal faces. Such a dimer is also a truncated regular rhombohedron. (c) A portion of the Conway-Torquato packing of truncated tetrahedra with a packing fraction $\phi = 23/24 = 0.958333\dots$. The holes in this packing are regular tetrahedra with the same edge length as the truncated tetrahedra. (d) A portion of the densest known packing of truncated tetrahedra with $\phi = 207/208 = 0.995192\dots$. The holes in this densest known packing are regular tetrahedra whose edge length is $1/3$ of that of truncated tetrahedra.

i.e., \mathbf{a}_1 , \mathbf{a}_2 , and \mathbf{a}_3 .⁸ The vectors \mathbf{a}_i ($i = 1, 2, 3$) are called lattice vectors for Λ . A (Bravais) lattice packing associated with Λ is one in which the centroids (geometric centers) of the nonoverlapping particles are located at the points of Λ , each oriented in the same direction. The space \mathbb{R}^3 can then be geometrically divided into identical regions F called fundamental cells, each of which contains just the centroid of one particle. Hence, the packing fraction of a lattice packing is given by $\phi = \frac{V_p}{\text{Vol}(F)}$, where V_p is the volume of a particle and $\text{Vol}(F) = |\mathbf{a}_1 \times \mathbf{a}_2 \cdot \mathbf{a}_3|$ is the volume of a fundamental cell. A periodic (non-Bravais lattice) packing is obtained by placing a fixed nonoverlapping configuration of N particles (where $N \geq 1$) with arbitrary orientations in each fundamental cell of a lattice Λ . Hence, the packing is still periodic under translations by Λ , but the N particles can occur anywhere in the chosen cell subject to the nonoverlap condition. The packing fraction of a periodic packing is given by $\phi = \frac{NV_p}{\text{Vol}(F)}$.

Since a truncated tetrahedron lacks central symmetry, its optimal (maximally dense) packing can only be a non-Bravais lattice packing.⁹ Based on our principles developed for determining the densest polyhedron packings,^{10,11,14} we argue more generally that the fundamental cell of the optimal packing of truncated tetrahedra should contain a simple compound object composed of truncated tetrahedra that itself is centrally symmetric. The fact that the aforementioned Conway-Torquato packing (henceforth referred to as the “CT packing”) possesses such a fundamental cell con-

taining a centrally symmetric dimer (defined below) of truncated tetrahedra with a high packing fraction $\phi = 23/24 = 0.958333\dots$ suggests that it can be used as a starting point to find the optimal packing. Indeed, in the ensuing discussion, we provide a construction of the densest known packing of truncated tetrahedra by optimizing the CT packing.

It is convenient to describe a truncated tetrahedron from its associated tetrahedron with vertices labeled A, B, C, and D [see Fig. 1(a)]. The centers of the four hexagonal faces of the truncated tetrahedron are denoted by \mathbf{p}_1 , \mathbf{p}_2 , \mathbf{p}_3 , and \mathbf{O} , which can be expressed in terms of the vectors associated with the vertices of the original tetrahedra, i.e.,

$$\begin{aligned} \mathbf{p}_1 &= \frac{(\mathbf{v}_A + \mathbf{v}_B + \mathbf{v}_D)}{3} - \mathbf{O}, & \mathbf{p}_2 &= \frac{(\mathbf{v}_A + \mathbf{v}_C + \mathbf{v}_D)}{3} - \mathbf{O}, \\ \mathbf{p}_3 &= \frac{(\mathbf{v}_B + \mathbf{v}_C + \mathbf{v}_D)}{3} - \mathbf{O}, \end{aligned} \quad (1)$$

where \mathbf{v}_i ($i = A, B, C, D$) are the vectors associated with the vertices and the origin $\mathbf{O} = \frac{1}{3}(\mathbf{v}_A + \mathbf{v}_B + \mathbf{v}_C)$. In the aforementioned CT packing,⁹ each fundamental cell contains two truncated tetrahedra, making a perfect contact through one of the hexagonal faces of each particle (i.e., forming a *dimer*), which are center-inversion images of each other through \mathbf{O} [see Fig. 1(b)]. Such a repeat unit is centrally symmetric and can be considered to be a regular rhombohedron with two sharper corners (with in-face angle $\pi/3$) truncated. The truncated rhombohedron has six pentagonal faces and two triangular faces [Fig. 1(b)]. The CT packing then corresponds to removing the sharp corners (tetrahedra with half edge-length of the rhombohedron) of each rhombohedron in its tiling [see Fig. 1(c)], leading to $\phi = 23/24$ with the lattice vectors

$$\mathbf{a}_1 = -2\mathbf{p}_3, \quad \mathbf{a}_2 = -2\mathbf{p}_2, \quad \mathbf{a}_3 = 2\mathbf{p}_1. \quad (2)$$

Both the truncated-tetrahedron dimer (i.e., the truncated regular rhombohedron) and the CT packing possess 3-fold rotational symmetry, with the symmetry axes being the long body-diagonal of the rhombohedron. Each dimer makes contacts with six neighbors through its six pentagonal faces.

It is noteworthy that the CT packing is not “collectively” jammed and can be continuously deformed until the packing fraction reaches a (local) maximum. Following Torquato and Stillinger,²¹ a packing is *locally* jammed if no particle in the system can be translated while fixing the positions of all other particles. A *collectively* jammed packing is a locally jammed packing such that no subset of particles can simultaneously be continuously displaced so that its members move out of contact with one another and with the remainder set. A packing is *strictly* jammed if it is collectively jammed and all globally uniform volume non-increasing deformations of the system boundary are disallowed by the impenetrability constraints. Readers are referred to Ref. 21 for further details.

The truncated-tetrahedron dimers in the CT packing can slide relative to one another along directions of certain edges, while the 3-fold rotational symmetry of the packing is maintained (see Fig. 2). Such a deformation can be achieved via continuously varying the lattice vectors

$$\begin{aligned} \mathbf{a}_1 &= -2\mathbf{p}_3 + \gamma(\mathbf{v}_D - \mathbf{v}_C), & \mathbf{a}_2 &= -2\mathbf{p}_2 + \gamma(\mathbf{v}_D - \mathbf{v}_A), \\ \mathbf{a}_3 &= 2\mathbf{p}_1 + \gamma(\mathbf{v}_B - \mathbf{v}_D), \end{aligned} \quad (3)$$

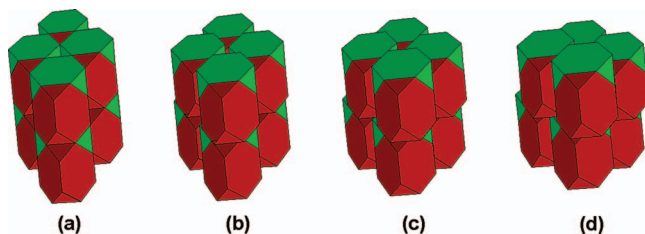


FIG. 2. Structures along the continuous deformation path that bring the Conway-Torquato packing of truncated tetrahedra with $\phi = 23/24$ to the putative optimal packing with $\phi = 207/208$. The associated deformation parameter γ for each packing is (a) $\gamma = 0$ (the Conway-Torquato packing), (b) $\gamma = 2/27$, (c) $\gamma = 4/27$, and (d) $\gamma = 2/9$ (our current putative optimal packing).

where $\gamma \in [0, 2/9]$ is the deformation parameter determined by the nonoverlapping constraints. For $\gamma = 0$, one has the CT packing, and $\gamma = 2/9$ corresponds to the densest known packing of truncated tetrahedra. By explicitly choosing a set of coordinates for \mathbf{v}_i ($i = A, B, C, D$), e.g., $\mathbf{v}_A = (-1, -1, -1)$, $\mathbf{v}_B = (1, 1, -1)$, $\mathbf{v}_C = (-1, 1, 1)$, $\mathbf{v}_D = (1, -1, 1)$, the packing fraction can be obtained using Eqs. (1) and (3)

$$\phi = \frac{2V_p}{\text{Vol}(F)} = \frac{2 \times (184/81)}{76\,544/16\,767} = \frac{207}{208} = 0.995192\dots \quad (4)$$

To obtain the densest known packing from the CT packing, the dimers must slide relative to one another such that each dimer now contacts two neighbors through one pentagonal face. Moreover, each dimer makes contacts with two additional neighbors along the direction of its long body-diagonal (i.e., $\mathbf{a}_1 + \mathbf{a}_2 - \mathbf{a}_3$) through the two triangular faces [see Fig. 1(d)]. Thus, each dimer has 14 face-to-face contacts in the densest known packing. We note that the formation of the additional triangular-face contacts prevents further deformations of the packing. The contacting equilateral triangular faces are center-inversion images of each other and share a common face center. This leads to six tetrahedron holes (with edge length $1/3$ of that of truncated tetrahedra) associated with each triangular face-to-face contact and, thus, each truncated-tetrahedron dimer. Let the volume of the holes $V_H = 1$, then the volume of a truncated tetrahedron $V_T = 621$. Alternatively, the packing fraction can easily be obtained via

$$\phi = \frac{V_T + V_T}{V_T + V_T + 6V_H} = \frac{621 + 621}{621 + 621 + 6} = \frac{207}{208}, \quad (5)$$

which is amazingly close to unity, given the fact that truncated tetrahedra can not tile \mathbb{R}^3 . Numerical maximization methods¹⁴ have been employed to verify that the densest known packing is indeed optimal among packings with similar structures. In fact, its remarkably high packing fraction, highly symmetric structure, and the numerical maximization results all suggest that this packing would be the optimal among all packings of truncated tetrahedra.

We note that by inserting regular tetrahedra of proper size into the holes of the optimal packing of the truncated tetrahedra, one completely fills the space without any gaps. This leads to a new tiling (or tessellation) of \mathbb{R}^3 by regular tetrahedra and truncated tetrahedra. Since the holes in the CT packing are also regular tetrahedra, a tiling associated with

this packing can be obtained in a similar way. Interestingly, it has recently been shown that the optimal packing of regular octahedra, which can be obtained by continuously deforming a sub-optimal face-centered-cubic packing of octahedra, corresponds to a new tiling of \mathbb{R}^3 by regular tetrahedra and octahedra.²² In fact, each octahedron packing in the family of packings obtained by the aforementioned continuous deformation is associated with a tiling of tetrahedra and octahedra unlike the situation for truncated tetrahedra where only the two “extremes” of the deformation correspond to tilings.

Once again, we see the important role that central symmetry plays in dense packings: although truncated tetrahedra are not centrally symmetric, they form centrally symmetric dimers, which then densely pack on a Bravais lattice. This is also the case for the densest tetrahedron packing, whose centrally symmetric unit has four particles forming two dimers. This suggests a generalization of the organizing principle we proposed for centrally symmetric Platonic and Archimedean solids. Specifically, we conjecture that the densest packings of convex polyhedra with equivalent principal axes are either a Bravais lattice packing of the polyhedra themselves that possess central symmetry or a Bravais lattice packing of centrally symmetric compound solids that are made of the polyhedra that lack central symmetry.

Although a comprehensive study of the equilibrium phase behavior is beyond the scope of the present paper, we conclude our investigation by examining the equilibrium melting properties of our putative optimal packing of truncated tetrahedra. At infinite pressure, the putative optimal packing of truncated tetrahedra constructed here is the thermodynamic equilibrium phase for these particles. Colloidal particles with shapes similar to that of truncated tetrahedra have been fabricated via different techniques.^{23,24} Thus, it is useful to see to what extent this solid phase is stable under finite pressures.

We have carried out Monte-Carlo (MC) simulations²⁵ to “melt” the optimal packing structure (i.e., the highest-packing-fraction “crystal”) via a decompression process. In particular, a periodic simulation box containing $N = 686$ particles is employed, whose size and shape are allowed to change.^{10,14} The volume of the simulation box is slowly increased to decrease the pressure and density (i.e., packing fraction) of the system. At each density, 10 000 000 MC trial moves are applied to each particle and 100 000 trial volume-preserving deformations are applied to the simulation box to equilibrate the system. Equilibrium structural characteristics, such as the pair-correlation function g_2 (see Fig. 3) and the number of dimers n_2 , are collected. We use such descriptors to gauge the remaining crystalline order in the system during the decompression process. We find that above $\phi \approx 0.68$, the crystal configurations associated with the optimal packing of truncated tetrahedra is the stable solid phase for these particles. Interestingly, when $0.53 < \phi < 0.68$, the crystal configurations associated with the CT packing becomes the stable phase. Below $\phi \approx 0.53$, the pair correlation function g_2 suddenly changes from a long-ranged function to an exponential decaying function (see Fig. 3) and n_2 quickly drops from $N/2$ to almost zero, indicating the occurrence of a first-order crystal-liquid transition.

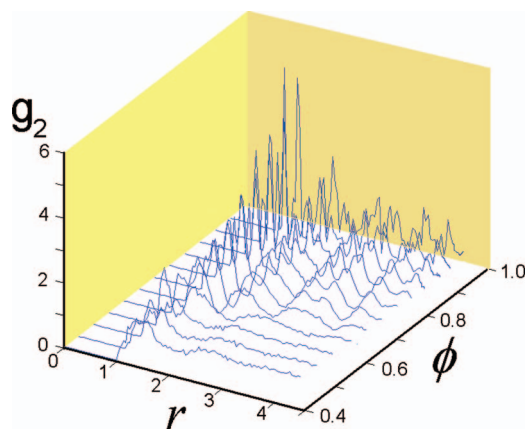


FIG. 3. Pair correlation function $g_2(r)$ associated with the centroids of the truncated tetrahedra at different densities in the range from 0.99 to 0.38 during the melting of the highest-packing-fraction crystal. At very high densities, $g_2(r)$ is a long-ranged function. Below $\phi \approx 0.53$, $g_2(r)$ suddenly changes from a long-ranged function to an exponential decaying function, indicating the occurrence of a first-order crystal-liquid transition.

Our simulations suggest that the crystal phases associated with the optimal packing and the CT packing of truncated tetrahedra are stable over a wide range of densities $\phi \in (0.53, 0.995)$ upon melting (decompression). This wide range of stability for the crystal phase is due to the fact that the dimers of truncated tetrahedra (in both the CT packing and the putative optimal packing) fill space very efficiently. This means that the free volume associated with crystals of the truncated tetrahedra is readily maximized in the dimer arrangement, leading to a lower free energy of the system. Since a dimer is formed by a pair of truncated tetrahedra contacting through the a common large hexagonal face, it is relatively easy for such local clusters to form in a dense liquid. Once such dimers nucleate, the system is expected to crystallize easily upon further compression. Thus, we expect the phase diagram of truncated tetrahedra to involve a single first-order liquid-solid phase transition. Of course, the exact coexistence range of ϕ and whether there are higher order solid-solid phase transitions can be precisely explored by carrying out free-energy calculations, which we intend to do in future work.

In summary, we have discovered a packing of truncated tetrahedra that nearly fills all of space, i.e., $\phi = 207/208$

$= 0.995192\dots$, via exact analytical construction and discussed its melting properties. We are not aware of any packing of a nontiling regular or semi-regular polyhedron with ϕ that is nearly unity. While a rigorous proof of its optimality is highly nontrivial, the fact that its packing fraction is amazingly close to unity in conjunction with our generalized organizing principle introduced here as well as our numerical maximization studies leads us to conclude that the packing is likely optimal.

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