Families of tessellations of space by elementary polyhedra via retessellations of face-centered-cubic and related tilings

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Families of Tessellations of Space by Elementary Polyhedra via Retessellations of the FCC and Related Tilings

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Abstract

The problem of tiling or tessellating (i.e., completely filling) three-dimensional Euclidean space $\mathbb{R}^3$ with polyhedra has fascinated people for centuries and continues to intrigue mathematicians and scientists today. Tilings are of fundamental importance to the understanding of the underlying structures for a wide range of systems in the biological, chemical and physical sciences. In this paper, we list and investigate the most comprehensive set of tilings of $\mathbb{R}^3$ by any two regular polyhedra known to date. We find that among all of Platonic solids, only the tetrahedron and octahedron can be combined to tile $\mathbb{R}^3$. For tilings composed of only congruent tetrahedra and congruent octahedra, there seem to be only four distinct ratios between the side of the two polyhedra. These four canonical periodic tilings are respectively associated with certain packings of tetrahedra (octahedra) in which the holes are octahedra (tetrahedra). Moreover, we derive two families of an uncountably infinite number of periodic tilings of tetrahedra and octahedra that continuously connect the aforementioned four canonical tilings with one another, containing the previously reported Conway-Jiao-Torquato family of tilings [Conway, Jiao and Torquato, PNAS **108**, 11009 (2011)] as a special case. For tilings containing infinite planar surfaces, non-periodic arrangements can be easily generated by arbitrary relative sliding. We also find that there are three distinct canonical periodic tilings of $\mathbb{R}^3$ by congruent regular tetrahedra and congruent regular truncated tetrahedra associated with certain packings of tetrahedra (truncated tetrahedra) in which the holes are truncated tetrahedra (tetrahedra). Remarkably, we discover that part of the aforementioned tilings can be obtained by "retessellating" the well-known tiling associated with the face-centered-cubic (FCC) lattice i.e., by combining the aforementioned fundamental tiles (i.e., regular tetrahedra and octahedra) to form larger polyhedra.

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I. INTRODUCTION

The study of three-dimensional tilings by polyhedra is of fundamental importance to the understanding of a wide range of systems in the biological [1, 2], chemical [3, 4] and physical sciences [5, 6]. Tilings are naturally related to networks (underlying connected graphs) [7] and represent an alternative way to visualize three-dimensional structures. Systematic enumerations of tilings based on their symmetry have been made possible by the use of combinatorial methods [8]. These allow scientists to gather useful information on the possible ways of how matter aggregates both at the microscopic (e.g., atomic and molecular) and macroscopic length scales. For example, the combinatorial tiling theory, and algorithms and methods based upon it [9], represent a powerful tool for the study of the structure of zeolites, silicate networks, aluminophosphates, nitrides, chalcogenides, halides, carbon networks, clathrate hydrates and ice [10]. A wide range of systems, such as block copolymers, liquid crystals, colloids and metallic alloys, also form structures with various types of long-range order, both periodic [11] and aperiodic [12–14]. Macroscopic examples include arrangements of cells in living tissues [2], the structure of foams, and any aggregate of spherical soft particles appearing in nature and synthetic situations [1]. Additionally, exploring the connection between packings and tilings has the potential to deepen our understanding of packing problems [15–18]. For example, Conway and Torquato constructed dense packings of regular tetrahedra from the "Welsh" tiling of irregular tetrahedra [19], corresponding to the structure of $MgCu_2$, also referred as the Laves phase $C15$ by Frank and Kasper (with space group $Fd\bar{3}m$) [20].

In this paper, we mainly focus on the problem of tiling three-dimensional Euclidean space $\mathbb{R}^3$ *periodically* with regular polyhedra (i.e., the Platonic solids) including tetrahedron, octahedron, icosahedron, dodecahedron and cubes. (We also consider tilings by the Archimedean truncated tetrahedron and regular tetrahedron.) Except for cubes, none of the remaining four regular polyhedra can individually tile $\mathbb{R}^3$. Thus, we first investigate the tilings with two types of regular polyhedra other than the obvious tessellations that can be constructed by using cubes of two different sizes. From simple considerations based on their dihedral angles, no pair of regular polyhedra can completely fill $\mathbb{R}^3$ apart from tetrahedra and octahedra, either periodically or nonperiodically, which we show now. Consider an edge of a regular polyhedron, in order to have a space-filling structure consisting of pairs of Platonic

solids, the edge needs to be surrounded by other tiles, no matter whether the polyhedron has face-to-face contact with its neighbors or not. This means that dihedral angles taken from other Platonic solids should add up to either π (non face-to-face matching) or 2π (face-to-face matching). From the list of dihedral angles (see Table I), it is clear that the only possibilities of tiling $\mathbb{R}^3$ by a pair of regular polyhedra are given by either different sized cubes or a mixture of tetrahedra and octahedra.

TABLE I: The dihedral angles of the Platonic solids

Polyhedron	Dihedral Angle
Tetrahedron	$2\tan^{-1}(\sqrt{2}/2) \approx 0.392\pi$
Icosahedron	$2\tan^{-1}[(3+\sqrt{5})/2] \approx 0.768\pi$
Dodecahedron	$2\tan^{-1}[(1+\sqrt{5})/2] \approx 0.648\pi$
Octahedron	$2\tan^{-1}(\sqrt{2}) \approx 0.608\pi$
Cube	$\pi/2$

It is well known that a periodic tiling of $\mathbb{R}^3$ by congruent regular tetrahedra and congruent regular octahedra can be derived from the face-centered-cubic (FCC) lattice by connecting the nearest-neighbor lattice sites (i.e., the FCC tiling). The net associated with this tiling, called "octet truss" by Buckminster Fuller, is also known as the alternated cubic honeycomb, or tetrahedral-octahedral honeycomb (stored as *fcu* on the Reticular Chemistry Structure Resource [21]). A related family of tilings by octahedra and tetrahedra that are not as well known as the octet truss are those associated with the infinite number of Barlow packings of identical spheres [22]. We note that in this family of tilings, the number of nonperiodic tilings is overwhelmingly larger than the periodic ones. These tilings, together with the FCC tiling, are the only possible ones composed of regular octahedra and tetrahedra when face-to-face matching of polyhedra (i.e., the *tiles*) in the tiling is required.

When the face-to-face matching is not required, the polyhedra only share part of their faces with their neighbors. Very recently, Conway, Jiao and Torquato [23] have shown that one such tiling by congruent octahedra and small congruent tetrahedra can be derived from the densest known packing of regular octahedra [24], which has been conjectured to be the densest among all octahedron packings [25]. This new tiling consists of fundamental repeat

units composed of one octahedron and six tetrahedra whose edge length is one third of that of the octahedra. Moreover, these authors [23] also discovered an a *one-parameter* family of periodic tilings containing an uncountable number (i.e. a continuous spectrum) of tilings by congruent octahedra and small tetrahedra with two different sizes, connecting the tiling associated with the conjectured densest octahedron packing [25] at one extreme and the FCC tiling at the other extreme.

Are these the only possible tilings by regular octahedra and regular tetrahedra? In general, a complete enumeration of all possible tilings by tetrahedra and octahedra in $\mathbb{R}^3$ is a notoriously difficult problem. Given that the number of configurations is uncountable, any attempt to classify these tilings would only make sense if such a classification is subject to a set of restrictions. One natural constraint is that the tiles are congruent tetrahedra and octahedra, as in the FCC tiling and the tiling associated with the conjectured densest packing of octahedra [25], henceforth referred to as the "DO" structure.

In this paper, we report on the discovery of two additional distinct canonical tilings of $\mathbb{R}^3$ by *congruent* octahedra and *congruent* tetrahedra besides the DO and FCC and related tilings. Our tilings are respectively associated with a dense *uniform* packing [26] of regular tetrahedra reported in Ref. [19], henceforth referred to as the "UT", in which the holes are small congruent regular octahedra, and a dense packing of octahedra constructed here in which parallel layers of hexagonally packed octahedra are stacked one on the top of the other, henceforth referred to as the "LO" structure. Together with the FCC tiling and the tiling associated with the densest octahedron packing, these four distinct canonical tilings of $\mathbb{R}^3$ are the basic tessellations containing congruent octahedra and congruent tetrahedra.

When more than one type of octahedron or tetrahedron is allowed, one expects that the number of possible tilings should increase dramatically. Consider for instance a Sierpinski tetrahedron [27] at some intermediate stage, which is an example of how space can be filled by regular congruent tetrahedra and any given number of non-congruent octahedra.

Indeed, we show that there exist two families of periodic tilings of tetrahedra and octahedra that continuously connect the aforementioned four tilings (FCC, DO, UT and LO) with one another (see the figure in Sec. IV). Thus, this constitutes an uncountably infinite number of tilings for each family. The tiles include either congruent large octahedra and small different-sized tetrahedra or congruent large tetrahedra and small different-sized octahedra. Specifically, we find a two-parameter tiling family that connects the DO and LO tilings to
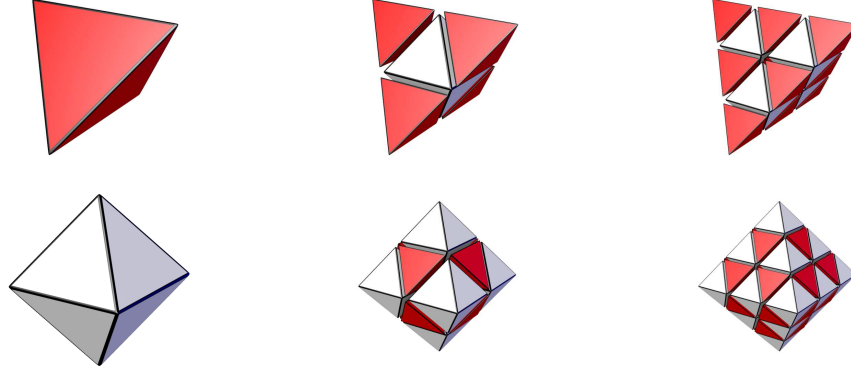
FIG. 1: (Color online) Scale-invariance property of the FCC tiling via the "retessellation" process. Each tile can be split into a self-similar tile cluster containing smaller tiles of the only two available types (either tetrahedra or octahedra). The top and bottom sets of images depict the two simplest possible decompositions or retessellations of a regular tetrahedron and a regular octahedron, respectively.

the FCC tiling, whose fundamental repeat unit is composed of one large octahedra and six small tetrahedra with three different sizes. This family contains the Conway-Jiao-Torquato family of tilings [23] as a special case. We also obtain a one-parameter family of tilings by large tetrahedra and small octahedra, connecting the UT tiling to the FCC tiling. The fundamental repeat unit of these tilings contains two congruent large tetrahedra and two small octahedra with different sizes.

Moreover, we introduce a unified description of the tilings by octahedra and tetrahedra using the idea of "retessellation", which we illustrate by examining the FCC tiling. First, we identify a useful and singular property of this tiling, namely, its self-similarity. In particular, each octahedron in the tiling can be dissected (i.e., retessellated) into T_{O} small tetrahedra and O_{O} small octahedra with the same edge length (see Fig. 1). In a similar way, each tetrahedron can be dissected into T_{T} small tetrahedra and O_{T} small octahedra. The number of tetrahedra and octahedra, each of unit edge length, contained in an octahedron of side n are:

$$
\begin{aligned}
T_{\mathrm{O}} &= \tfrac{4(n-1)n(n+1)}{3}, \\
O_{\mathrm{O}} &= \tfrac{n(2n^2+1)}{3},
\end{aligned}
\tag{1}
$$

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The number of unit tetrahedra and unit octahedra contained in a tetrahedron of side n are:

$$T_{\mathrm{T}} = \frac{n(n^2+2)}{3},$$
$$O_{\mathrm{T}} = \frac{(n-1)n(n+1)}{6}. \tag{2}$$

Extending this process, referred to as "retessellation", to the entire FCC tiling leads to a FCC tiling with smaller tiles whose side is $1/n$ of the original tiles. From a different point of view, one can also start with an infinitely large FCC tiling and single out large octahedra composed of O_{O} original octahedra and T_{O} original tetrahedra of the FCC tiling (see Fig. 1). This process, also referred to as retessellation, leads to a FCC tiling with larger tiles than those in the original tiling.

Remarkably, we find that this "retessellation" approach can be applied to construct all of the aforementioned basic tilings of regular tetrahedra and regular octahedra, including the four distinct canonical tilings and the two families of tilings. In other words, the tilings can be constructed by singling out a finite number of the octahedron and tetrahedron tiles in the FCC tiling to form compound octahedra and tetrahedra with different sizes that are tiles of the corresponding tilings. In addition, we report a tiling by large regular tetrahedra and small regular truncated tetrahedra that heretofore has not been identified. We find that this tiling, the tilings by large regular truncated tetrahedra and small regular tetrahedra associated with recently discovered dense packings of regular truncated tetrahedra [19, 23], and a tiling by irregular truncated tetrahedra associated with the β-tin structure [28] can also be obtained by retessellations of FCC tiling. Thus, the retessellation process provides a unified approach to determine the possible tilings of $\mathbb{R}^3$ by elementary polyhedra including regular octahedra, regular tetrahedra, as well as regular and irregular truncated tetrahedra.

The rest of the paper is organized as follows: In Sec. II, we present the four canonical periodic tilings of $\mathbb{R}^3$ by congruent regular tetrahedra and congruent regular octahedra (i.e., the FCC, DO, LO and UT tilings). In Sec. III, we construct two families of periodic tilings whose tiles contain congruent octahedra (tetrahedra) and tetrahedra (octahedra) of different sizes that continuously connect the aforementioned four distinct canonical tilings with one another. In Sec. IV, we present the general formulation of the retessellation process and show that it can be applied to obtain the most comprehensive set of tilings of $\mathbb{R}^3$ by octahedra, tetrahedra and truncated tetrahedra known to date. In Sec. V, we provide concluding remarks.

II.   TILINGS OF $\mathbb{R}^3$ BY CONGRUENT REGULAR TETRAHEDRA AND CONGRUENT REGULAR OCTAHEDRA

In this section, we describe the four distinct canonical tilings of $\mathbb{R}^3$ by congruent regular octahedra and congruent regular tetrahedra. These include the FCC tiling, the tiling associated with the conjectured densest packing of octahedra (the DO tiling), the tiling associated with the dense uniform packing of regular tetrahedra (the UT tiling) [19] in which the holes are small congruent octahedra, and the tiling associated with a layered packing of octahedra (the LO tiling) in which the holes are small congruent tetrahedra. Although the FCC tiling is well known, the tiling associated with the conjectured densest octahedron packing was only discovered recently [23]. The latter two tilings are derived here for first time to the best of our knowledge.

A tiling of $\mathbb{R}^3$ by congruent octahedra and congruent tetrahedra can be classified based upon their side ratio s, which is defined as follows:

$$s = \frac{s_\text{O}}{s_\text{T}} \tag{3}$$

where s_O is the side of the octahedra and s_T is that of the tetrahedra in the tiling. Another relevant parameter is the tile ratio $t = n_\text{O}/n_\text{T}$, where n_O and n_T are respectively the number of octahedra and tetrahedra in the fundamental repeat unit of the tiling.

Interestingly, we find that for the aforementioned four distinct canonical tilings discussed in this section, the tile ratio t turns out to be inversely proportional to side ratio s:

$$t = \frac{n_\text{O}}{n_\text{T}} = \frac{1}{2s} \tag{4}$$

This leads to an explicit formula for the packing density ϕ (i.e., fraction of space covered by the polyhedra, also referred to as packing fraction) of either octahedra or tetrahedra, which can be expressed as a function of the side ratio s alone, i.e,

$$\phi_\text{O} = 1 - \phi_\text{T} = \frac{1}{1 + \frac{1}{2s^2}} \tag{5}$$

where ϕ_O and ϕ_T are respectively the packing density of octahedra and tetrahedra in the tiling. In Table II, we summarize the main features of the four tilings that will be described in detail below. Note that only the FCC tiling has cubic symmetry.

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TABLE II: The family of four tilings by regular tetrahedra and octahedra, i.e., the tiling associated with the uniform packing of tetrahedra (UT), the FCC tiling, the tiling associated with the layered packing of octahedra (LO), and the tiling associated with the conjectured densest octahedron packing (DO) [25]. Note the relationship between the side ratio s, tile ratio t and packing fraction of the octahedra. The space group associated with each tiling is also given.

Name	s	t	ϕ_o	Space Group
UT	1/2	1	1/3	P4/mmm
FCC	1	1/2	2/3	$Fm\bar{3}m$
LO	2	1/4	8/9	trig.
DO	3	1/6	18/19	$R\bar{3}$

A. The Tiling Associated with the Uniform Packing of Tetrahedra (UT Tiling)

In Ref. [19], Conway and Torquato constructed a dense periodic packing of regular tetrahedra, whose fundamental cell contains two tetrahedra forming partial face-face contacts. Specifically, the tetrahedra are arranged on a primitive tetragonal lattice [19] and oriented in two mutually orthogonal directions. The vertex coordinates of the two tetrahedra in the fundamental cell are given by:

$$
\begin{aligned}
P_{T1} &= \{0, 1/2, 0\}, \{1, -1/2, 0\}, \{1, 1/2, 1\}, \{0, -1/2, 1\} \\
P_{T2} &= \{-1/2, 0, 0\}, \{1/2, 1, 0\}, \{1/2, 0, 1\}, \{-1/2, 1, 1\}
\end{aligned}
\tag{6}
$$

And the lattice vectors of the uniform packing are given by:

$$
\mathbf{a}_1 = (1, 0, 0)^T, \quad \mathbf{a}_2 = (0, 1, 0)^T, \quad \mathbf{a}_3 = (1/2, 1/2, 1)^T.
\tag{7}
$$

The center of a contacting region is also the inversion center associated with the contacting tetrahedron pairs. Every tetrahedron in the packing can be mapped to another one by translation and center-inversion operation. Thus, this packing is referred to as the "uniform tetrahedron packing". At the time of this discovery, no mention was made of the holes in this packing.

Interestingly, we find that the holes in the uniform tetrahedron packing are in fact regular octahedra whose edge length is half of that of a tetrahedron. Filling the holes with octahedra of proper size leads to a novel tiling of $\mathbb{R}^3$ by tetrahedra and small octahedra. In the tiling,
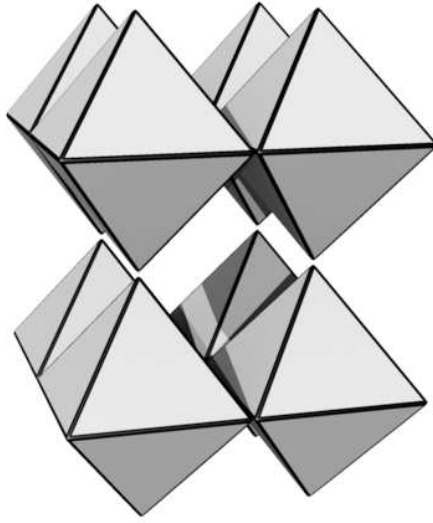
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FIG. 2: (Color online) The 8 octahedra surrounding each tetrahedron in the UT tiling, which is associated with the uniform packing of tetrahedra. Each octahedron shares four of its edges with four of its neighbors.

each tetrahedron has face contacts with 4 tetrahedra and 8 octahedra, and each octahedron shares its faces with 8 tetrahedra. The fundamental repeat unit contains two tetrahedra and two small octahedra. A portion of the net of the octahedra surrounding each tetrahedron are shown in Fig. 2. In the full, triply periodic net, each octahedron shares four of its edges with four different neighbors.

B. The FCC and Related Tilings

Consider an octahedron P_O defined by via the relation

$$P_O = \left\{ \mathbf{x} \in \mathbb{R}^3 : |x_1| + |x_2| + |x_3| \leq 1 \right\}. \tag{8}$$

which is placed on the lattice sites specified by

$$\mathbf{a}_1 = (1, 1, 0)^T, \quad \mathbf{a}_2 = (-1, 1, 0)^T, \quad \mathbf{a}_3 = (0, 1, 1)^T. \tag{9}$$

In this octahedron packing (with a density $\phi = 2/3$), four octahedra, each making contacts by sharing edges perfectly with the other three, form a regular-tetrahedron-shaped hole with the same edge length of the octahedra. If tetrahedra of proper size are inserted into the

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holes of the packing, the FCC tetrahedron-octahedron tiling is recovered (see Fig. 6). In this periodic tiling, each octahedron makes perfect face-to-face contacts with 8 tetrahedra. The fundamental repeat unit of this tiling contains one octahedron and two congruent tetrahedra. Individual layers of this tiling completely fill the space between two parallel planes at a distance equal to the diameter of an inscribed sphere in an octahedron (the distance between two opposite faces of an octahedron). This property allows the generation of an infinite family of tilings based on stackings of layers of the type described above, all having the same side ratio, but that can not be retessellated into the FCC tiling. One well-known example is HCP, but it is also possible to generate non-periodic arrangements.

C. The Tiling Associated with the Layered Packing of Octahedra (LO Tiling)

Here, we derive a tiling of $\mathbb{R}^3$ by congruent octahedra and small congruent tetrahedra, which to our knowledge has not been presented before. Consider an octahedron defined by Eq. (8) that is placed at each lattice site specified by the lattice vectors $\mathbf{a}_1$, $\mathbf{a}_2$ and $\mathbf{a}_3$:

$$\mathbf{a}_1 = \left(-\tfrac{1}{2}, 1, \tfrac{1}{2}\right)^T, \quad \mathbf{a}_2 = (-1, 1, 0)^T, \quad \mathbf{a}_3 = \left(-\tfrac{1}{2}, \tfrac{1}{2}, 1\right)^T. \tag{10}$$

This lattice packing has a density of $\phi = 8/9$, in which each octahedron makes face-contact with 8 neighbors leading to small tetrahedral holes. The edge-length of the tetrahedral holes is a half of that of the octahedra. The coordinates of vertices for the tetrahedra can be written as $(n_1/2, n_2/2, n_3/2)$, where $n_1, n_2, n_3 = 0, \pm 1, \pm 2$. Inserting tetrahedra of the proper size into the holes leads to a new tiling of $\mathbb{R}^3$ by congruent octahedra and congruent tetrahedra. Each octahedron makes face-contact with 16 small tetrahedra (Fig. 3). The fundamental repeat unit of this tiling contains one octahedron and four small tetrahedra. As with FCC, individual layers of this tiling can arbitrarily slide one on the top of the other, leading to other periodic and non-periodic tilings with the same side and tile ratios.

D. The Tiling Associated with the Densest Packing of Octahedra (DO Tiling)

Consider an octahedron defined by Eq. (8) that is placed at each lattice site specified by the lattice vectors $\mathbf{a}_1$, $\mathbf{a}_2$ and $\mathbf{a}_3$ of the optimal lattice packing of octahedra:

$$\mathbf{a}_1 = \left(\tfrac{2}{3}, \tfrac{2}{3}, \tfrac{2}{3}\right)^T, \quad \mathbf{a}_2 = \left(-1, \tfrac{2}{3}, \tfrac{1}{3}\right)^T, \quad \mathbf{a}_3 = \left(-\tfrac{1}{3}, \tfrac{1}{3}, \tfrac{4}{3}\right)^T. \tag{11}$$
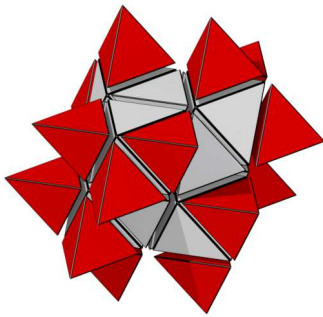
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FIG. 3: (Color online) The 16 tetrahedra surrounding each retessellated octahedron in the tiling associated with the layered packing of octahedra (i.e., the LO tiling). The tetrahedra share corners and each tetrahedron shares two of its edges with two of its neighbors.
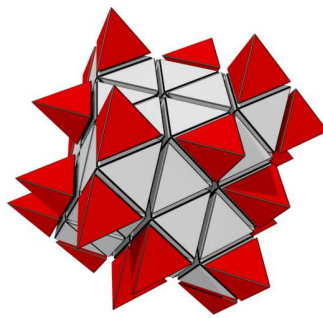

FIG. 4: (Color online) The 24 tetrahedra surrounding each retessellated octahedron in the conjectured densest packing of octahedra (i.e., the DO tiling). The tetrahedra only share corners.

This conjectured densest known packing of octahedra [25] has a density of $\phi = 18/19$. The octahedra make contact with one another in a complex fashion to form a dense packing with small regular tetrahedral holes. The edge length of a tetrahedron is only one third of that of the octahedron and therefore the ratio of the volume of a single octahedron to that of a tetrahedron is 108. The coordinates of vertices for the tetrahedra can be written as $(n_1/3, n_2/3, n_3/3)$, where $n_1, n_2, n_3 = 0, \pm 1, \pm 2, \pm 3$. Insertion of tetrahedra of appropriate size into the holes results in the new tetrahedron-octahedron tiling of $\mathbb{R}^3$ [23], in which each octahedron makes contacts with 24 small tetrahedra (Fig. 4). The fundamental repeat unit of this tiling contains one octahedron and six small congruent tetrahedra.

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III. FAMILIES OF PERIODIC TILINGS OF $\mathbb{R}^3$ BY REGULAR TETRAHEDRA AND REGULAR OCTAHEDRA

In this section, we present two families of an uncountably infinite number of periodic tilings of $\mathbb{R}^3$ by octahedra and tetrahedra, connecting the four distinct canonical periodic tilings discussed in the previous section. Specifically, we construct a two-parameter tiling family that continuously connects DO and LO tilings to the FCC tiling. This family contains the Conway-Jiao-Torquato family of tilings [23] as a special case. We also obtain a one-parameter continuous family of tilings, connecting the UT tiling to the FCC tiling, whose fundamental repeating unit contains two congruent large tetrahedra and two small octahedra with different sizes.

A. Family of Periodic Tilings Connecting the DO and LO Tilings to the FCC Tiling

In Ref. [23], the authors constructed a one-parameter continuous family of tilings of $\mathbb{R}^3$ by octahedra and tetrahedra, connecting the FCC tiling to the tiling associated with the densest octahedron packing. Each tiling in the family is obtained by inserting regular tetrahedra with proper sizes into the tetrahedral holes of the associated lattice packing of regular octahedra, whose lattice vectors are given by

$$
\begin{aligned}
\mathbf{a}_1 &= (1-\alpha,\ 1-\alpha,\ 2\alpha)^T, \\
\mathbf{a}_2 &= (-1+\alpha,\ 1,\ \alpha)^T, \\
\mathbf{a}_3 &= (-\alpha,\ 1-2\alpha,\ 1+\alpha)^T,
\end{aligned}
\tag{12}
$$

where $\alpha \in [0, 1/3]$. As α moves immediately away from zero, each octahedron in the packing makes partial face-to-face contact with 14 neighbors, leading to 24 tetrahedral "holes" for each octahedron, 3 on each faces of the octahedron, with edge length $\sqrt{2}\alpha$, $\sqrt{2}\alpha$ and $\sqrt{2}(1-2\alpha)$. Thus, the fundamental repeat unit of the tilings in this family contains one large octahedra and six small tetrahedra with two different sizes except for the extreme cases where $\alpha = 0$ and $1/3$. In the former case, the tiling unit contains one octahedron and two equal-sized tetrahedra; and in the later case, the tiling unit contains one octahedron and six equal-sized tetrahedra. As α increases from 0 to $1/3$, the octahedron packing continuously deforms from the FCC packing to the optimal lattice packing, during which every octahedron

moves relatively to one another in a particular way specified by the parameter α, without violating the nonoverlap constraints.

The aforementioned construction is based on the fact that the FCC packing of octahedra is not collectively jammed [23, 29], i.e., the particle in the packing can continuously move relative to one another without violating the nonoverlap conditions. As pointed out in Ref. [23], the particular collective octahedron motion leading to the continuous family of tilings is just one of an uncountably infinite number of unjamming collective motions of the packing.

In particular, the collective motion of octahedra specified by the following transformation brings the FCC tiling to the LO and DO tilings:

$$
\begin{aligned}
\mathbf{a}_1 &= (1 - \alpha, \ 1 - \beta, \ \alpha + \beta)^T, \\
\mathbf{a}_2 &= (-1, \ 1 - \beta, \ \beta)^T, \\
\mathbf{a}_3 &= (-\alpha, \ 1 - \alpha - \beta, \ 1 + \beta)^T,
\end{aligned}
\tag{13}
$$

where $\alpha, \beta \in [0, 1]$. For $\alpha = \beta = 0$, one has the FCC tiling. When $\alpha = 1/2$ and $\beta = 0$, the LO tiling is obtained. During the transformation, the octahedra slide relative to one another along the edges, maintaining face contact. This leads to four tetrahedral holes of two different sizes associated with each octahedra. At the LO limit, the tetrahedral holes are of the same size. Since this configuration can be split along parallel planes, an infinite number of tilings of $\mathbb{R}^3$ by octahedra and tetrahedra can be constructed from the LO tiling by relative translations and rotations of these layers. When $\alpha = \beta = 1/3$ the DO tiling is formed. During the transformation from the FCC tiling to the DO tiling, three types of tetrahedral holes are observed. The sum of their side lengths coincides with the side length of the octahedron.

B. Family of Periodic Tilings Connecting the FCC Tiling to the UT Tiling

Consider the packing of regular tetrahedra associated with the FCC lattice, in which each fundamental cell contains two tetrahedra and an octahedron. The density of this packing is $\phi = 1/3$. It is clear that this packing is not collectively jammed and the tetrahedra can slide relatively to one another with fixed orientations.

Specifically, we find a collective motion of tetrahedra that continuously transform the FCC packing to the uniform packing of tetrahedra, during which the holes in the packing

are regular octahedra of two sizes. For the tetrahedra with orientations specified by Eq. (6), the transformation of the UT tiling to the FCC tiling is specified by the centers of the two tetrahedra in the fundamental cell, i.e.,

$$T_1 = \left(-\tfrac{1}{2}, \tfrac{\alpha-1}{2}, \tfrac{1}{2}\right)$$
$$T_2 = \left(\tfrac{1-\alpha}{2}, -\tfrac{1}{2}, \tfrac{1}{2}\right) \tag{14}$$

and the associated lattice vectors:

$$\mathbf{a}_1 = (1, \ 1-\alpha, \ 0)^T,$$
$$\mathbf{a}_2 = (\alpha-1, \ 1, \ 0)^T, \tag{15}$$
$$\mathbf{a}_3 = (\alpha/2, \ 1-\alpha/2, \ 1)^T,$$

where $\alpha \in [0, 1]$. When $\alpha = 0$, one obtain the UT tiling; and when $\alpha = 1$, one has the FCC tiling.

IV. "PHASE DIAGRAM" FOR OCTAHEDRON-TETRAHEDRON TILINGS

The aforementioned two families of tilings enable one to continuously connect any of the four tilings with congruent octahedra and congruent tetrahedra to one another via an infinite number of tilings associated with non-congruent octahedra or tetrahedra. During the transformation from one tiling to another, one of the polyhedron tiles change in size. For example, the tiling associated with the uniform packing of tetrahedra (the UT tiling) and the tiling associated with the layered packing of octahedra (the LO tiling) can be transformed into FCC and vice versa by sliding a subset of tiles along their edges as described above.

A schematic "phase diagram" showing the connections between the octahedron packing fractions octahedron-tetrahedron tilings is given in the left panel of Fig. 5. The vertical axis in the plot of the diagram is the density of the octahedron packings ϕ_{o} associated with the tilings. The horizontal axis is the side ratio s of the tilings. The quantitative relationship between ϕ_{o} and s is specified by the following equations for transformations from FCC to UT tiling and from FCC to LO and DO tilings, respectively,

$$\phi_o = 1 - \frac{1}{3(2s^2 - 2s + 1)}, \tag{16}$$

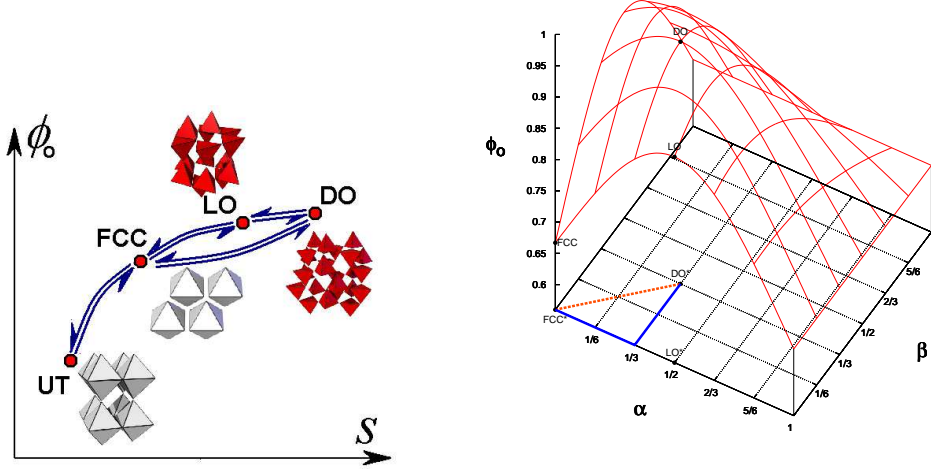$$\phi_o = \frac{1}{1 + \frac{\alpha^3 + \beta^3 + (1-\alpha-\beta)^3}{2}}. \tag{17}$$

15

FIG. 5: (Color online) Left panel: A schematic phase diagram showing the continuous paths between the four canonical octahedron-tetrahedron tilings (UT, FCC, LO and DO tilings). The vertical axis in this plot is the density of the octahedron packings ϕ_O associated with the tilings. The horizontal axis is the side ratio s of the tilings. Right panel: Detailed phase diagram depicting the ϕ_o-α-β surface as obtained from the packing density formula (17) associated with the octahedron packings associated with the FCC ($\phi_0 = 2/3$), LO ($\phi_o = 8/9$) and DO ($\phi_o = 18/19$) tilings. One path to go from the LO to DO structure involves a two-step process (solid blue line in the α-β plane): first the parameter α is increased from 0 to 1/3 to, leading to an intermediate tiling configuration (shown in Fig. 9). The continuously transformation from the FCC tiling to the DO tiling discovered by Conway, Jiao and Torquato [23] is also shown (dashed orange line in the α-β plane). Then β is increased from 0 to 1/3, leading to the DO tiling. The projections of the three canonical points FCC, LO and DO on the surface to the α-β plane are marked with asterisks.

where $\alpha = s$ and $\beta \in [0, s]$. In the right panel of Fig. 5, a detailed sub-diagram showing the transformation from FCC to LO and DO tilings specified by Eq. (17) is given. The density of the octahedron packings vary across all the possible intermediate configurations in the FCC-LO-DO family, reaching its maximum value of $\phi_o = 18/19 \approx 0.947368\ldots$ in the DO packing.

We note that although direct transformations are possible between any tiling and FCC, a transition between the tiling associated with the uniform packing of tetrahedra and the tiling associated with the layered packing of octahedra (or the tiling associated with the densest packing of octahedra) without passing through the FCC configuration is not possible.
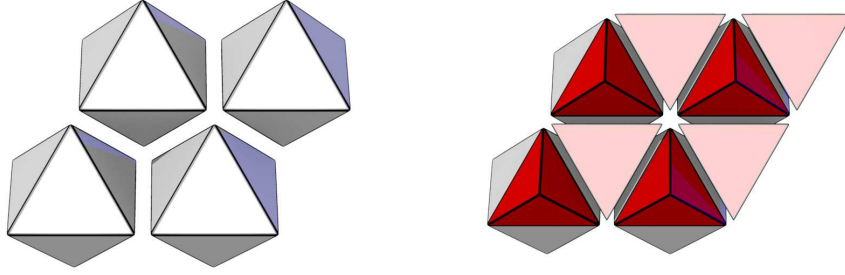
FIG. 6: (Color online) The FCC tiling with side ratio 1 and tile ratio is 1/2.

V.   UNIFIED DESCRIPTION OF TILINGS BY RETESSELLATING THE FCC TILING

In Sec. I, we introduced the idea of the "retessellation" of the FCC tiling, which is based on a remarkable property of the FCC tiling (see Fig. 6), i.e., self-similarity. Specifically, each tile (an octahedron or a tetrahedron) can be dissected into a large number of smaller tiles which are associated with a "rescaled" FCC tiling with finer tiles. This retessellation process is shown in Fig. 1. On the other hand, one can single out large octahedra and tetrahedra composed a large number of the original tiles of the FCC tiling to obtain a "rescaled" FCC tiling with coarser tiles.

The retessellation process provides an extremely useful unified means to investigate periodic tilings by elementary polyhedra. In this section, we show that besides the FCC tiling, all of the aforementioned two families of tilings by octahedra and tetrahedra can be obtained by certain retessellations of the FCC tiling. In addition, we report a tiling of large regular tetrahedra and small regular truncated tetrahedra for the first time here. We show that this tiling, together with the tilings by regular truncated tetrahedra and regular tetrahedra associated with the recently discovered dense packings of regular truncated tetrahedra, and a tiling by irregular truncated tetrahedra associated with the β-tin structure can also be obtained by retessellations of FCC.
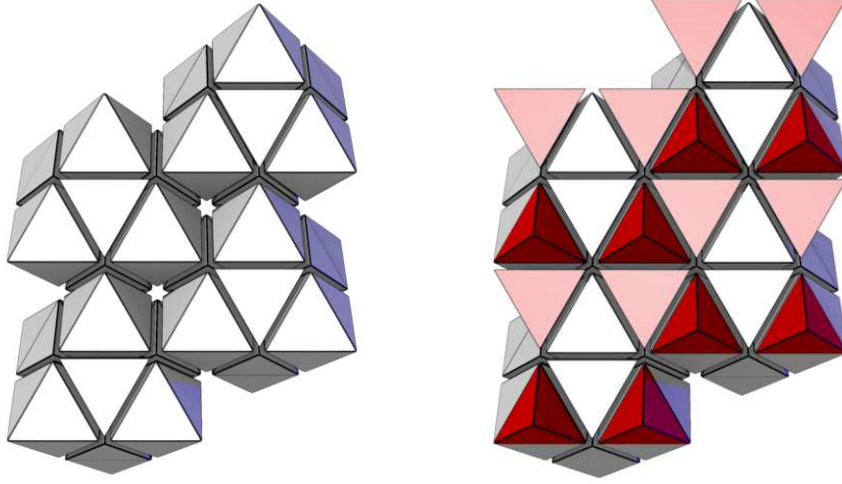
17

FIG. 7: (Color online) Dissected view of the LO tiling with side ratio is 2. The associated packing by regular octahedra contains tetrahedral holes of side 1/2. The associated tile ratio is 1/4.

A. Tilings Associated with Octahedron Packings via Retessellations of the FCC Tiling

For the LO tiling (i.e., the tiling associated with the dense lattice packing of octahedra), each repeat unit contains 4 tetrahedra and 1 octahedron. As shown in Fig. 7, also this tiling can be dissected into an FCC tiling (Fig. 6), by splitting each octahedron into 6 smaller octahedra and 8 smaller tetrahedra. Note that octahedra layers can be freely stacked on the top of each other with arbitrary orientations, leading to a family infinite number of tilings with the same tiles. In this family, the number of nonperiodic tilings is overwhelmingly larger than that of the periodic ones.

The DO tiling (i.e., the tiling associated with the densest packing of octahedra) can be obtained by retessellating the FCC tiling. Each repeat unit of this tiling contains one octahedron and six tetrahedra (Fig. 8). Specifically, each octahedron is dissected into 32 small tetrahedron tiles and 19 small octahedron tiles, whose edge length is the same as that of the small tetrahedra in the original packing. A three-dimensional model of the net by the tetrahedra only can be viewed online [30].

Tilings of $\mathbb{R}^3$ by congruent octahedra and small tetrahedra with different sizes are shown in Fig. 9. These tilings are rational approximants of intermediate configurations during the continuous transformations that bring respectively LO and DO tilings to the FCC tiling. The
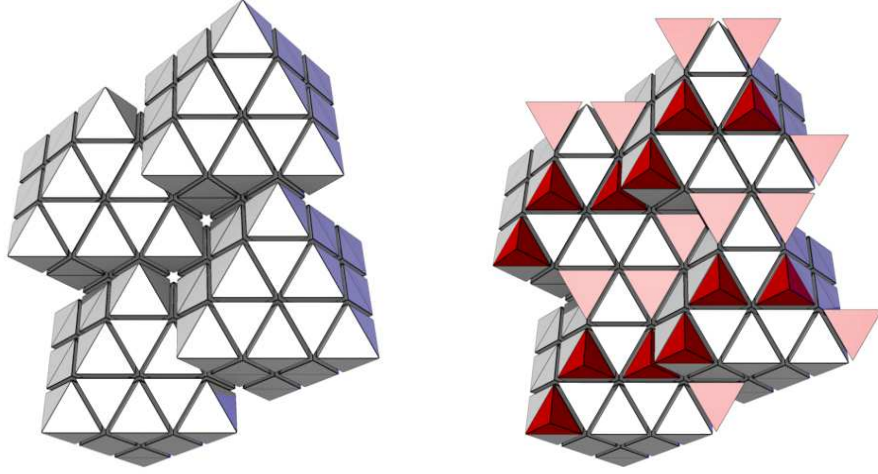
18

FIG. 8: (Color online) Dissected view of the DO tiling [23] with side ratio 1/3. This is associated with the conjectured densest known packing of octahedra [25], which is a lattice packing [24]. The image shows the net of vertex-sharing tetrahedra filling the gaps of the packing by octahedra.
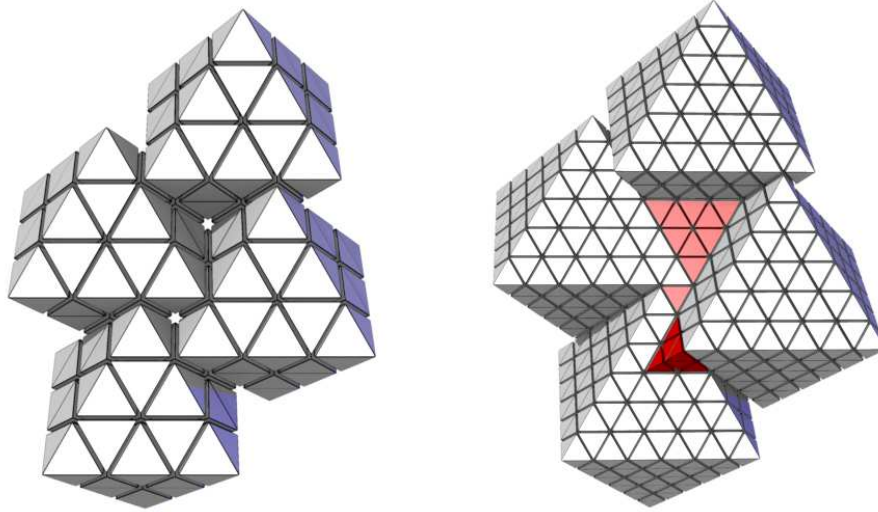

FIG. 9: (Color online) Rational approximants of intermediate configurations during the continuous transformations that bring respectively the LO and DO tilings into the FCC tiling. The two tetrahedral holes of different size are visible in the LO tiling. The three types of tetrahedra have been added to the DO configuration for clarity. Note how each intermediate configuration, although now composed of more than two kinds of tile (voids are not identical), can still be retessellated as an FCC tiling. Animations showing the relative motion of the octahedra in the tiling can be viewed online [31, 32].
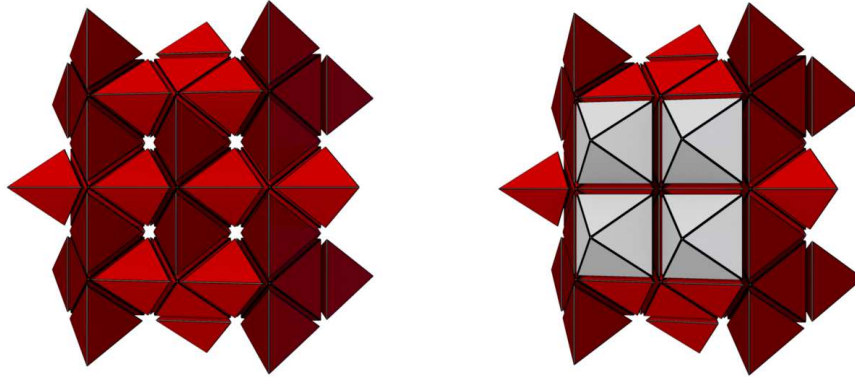
FIG. 10: (Color online) Dissected view of the UT tiling. The gaps in the uniform packing by tetrahedra described in [19] are regular octahedra of side 1/2, whose centers lie on a primitive tetragonal lattice. Note that each larger regular tetrahedron can be dissected into 5 smaller units as shown in Fig. 1, leading to the FCC tiling. The repeating unit contains 2 tetrahedra and 2 octahedra (tile ratio is 1).

edge length of the tetrahedra compared to the edge length of the octahedra are respectively 1/3 and 2/3 for the tiling shown in the left panel of Fig. 9 and 1/2, 1/3 and 1/6 for tiling shown in the right panel of Fig. 9.

B. Tilings Associated with Tetrahedron Packings via Retessellations of the FCC Tiling

In the UT tiling (i.e., the tiling associated with the uniform packing of tetrahedra), each tetrahedron tile is associated with one octahedron tile whose side length is 1/2 of that of the tetrahedron with centers lying on a primitive tetragonal lattice [19]. The fundamental repeat unit of this tiling contains 2 tetrahedra and 2 octahedra (with tile ratio $t = 1$). Note that each large tetrahedron tile can be dissected into five smaller tiles (one octahedron and four tetrahedra) as shown in Fig. 1. Together with the small octahedra, the tiles associated with the dissected tetrahedra lead to the FCC tiling (see Fig. 10).

A tiling of $\mathbb{R}^3$ by large tetrahedra and small noncongruent octahedra obtained via retessellation is shown in Fig. 11. The side length of the small octahedra are respectively 1/3, 2/3 of that of the tetrahedra. This tiling is a member of the family described in Sec. IIIB, with the parameter $\alpha = 1/3$. Together with the smallest octahedra, the tiles associated with
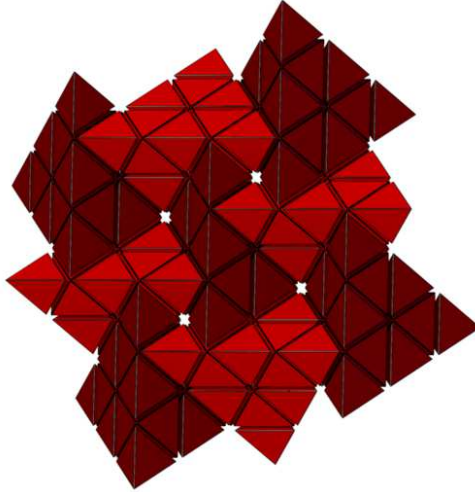
20

FIG. 11: (Color online) A rational approximant of an intermediate configuration during the continuous transformation that brings UT into FCC. Each intermediate configuration can still be retessellated as an FCC tiling. An animation showing the relative motion of the tetrahedra can be viewed online [33].

the dissected tetrahedra and the intermediate octahedra lead to the FCC tiling.

C. Tilings by Truncated Tetrahedra and Tetrahedra via Retessellation of the FCC Tiling

It has recently been shown that Archimedean truncated tetrahedra can pack to the extremely high density of $\phi = 207/208 = 0.958333\ldots$ [34]. It was shown that this packing can be achieved by a continuous deformation of the packing of truncated tetrahedra discovered by Conway and Torquato [19] with $\phi = 23/24 = 0.958333\ldots$. It was observed that the holes in both of these packings are regular tetrahedra and so both also are associated with tilings of $\mathbb{R}^3$ by the Archimedean truncated tetrahedron and regular tetrahedron. We note here that tiling associated with the Conway-Torquato packing is the same as the tiling associated with the cristobalite structure (referred to as CRS, see Fig. 12) discovered over a century ago by Andreini [35, 36]. Notice that although the CRS structure was previously known [35, 36], the observation that it corresponds to a dense packing of truncated tetrahedra with density $\phi = 23/24$ was only recently made [19].

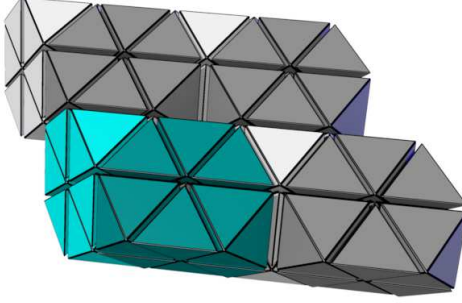In the Conway-Torquato packing, each truncated tetrahedron in the fundamental cell is

FIG. 12: (Color online) Retessellation of the quarter cubic honeycomb, the tiling associated with the structure of cristobalite CRS in the RCSR database). As in FCC, the tiling contains four sets of planar surfaces along which each layer can slide relatively to its neighbors without affecting packing density.

associated with a tetrahedral hole whose edge length is the same as the truncated tetrahedron. Here we show the existence of an additional packing by truncated tetrahedra that contains large tetrahedral holes (referred to as the "TH" tiling). The packing and the associated retessellated tiling are shown in Fig. 13. Its periodic unit contains six truncated tetrahedra and two tetrahedra with edge length 3.

In the densest known packing of truncated tetrahedra, each particle in the fundamental cell is associated with three small tetrahedral holes, whose edge length is one third of that of the truncated tetrahedron. If tetrahedra with proper sizes are inserted in the holes of these packings, one obtains tilings by truncated tetrahedra and regular tetrahedra (referred to as the "TT" tiling). A truncated tetrahedron can be retessellated into small regular octahedra and tetrahedra. Due to the arrangement of the polyhedra, the aforementioned tilings by truncated tetrahedra and regular tetrahedra can also be obtained from the retessellations of the FCC tiling (Fig. 14).

Specifically, for the tiling associated with the Conway-Torquato packing of truncated tetrahedra, if the size of the tetrahedra in the tiling is chosen to be the same as the fundamental tetrahedra for the retessellation, the truncated tetrahedron in the tiling can be retessellated into 4 fundamental octahedra and 7 fundamental tetrahedra (see Fig. 12). For the tiling associated with the densest packing of truncated tetrahedra, if the size of the
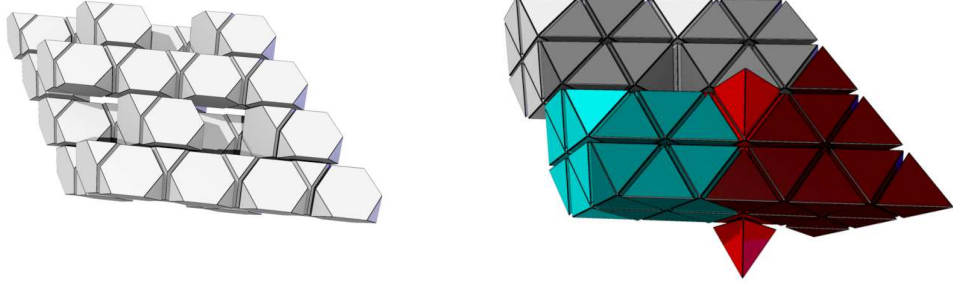
FIG. 13: (Color online) A low density packing by truncated tetrahedra and tetrahedra with side ratio 1/3. A subset of the packing showing the tetrahedral holes of side 3 and a periodic unit of the tiling. There are no variants to this tiling, since it is not possible to slide layers relatively to each other. Tile ratio is 3.
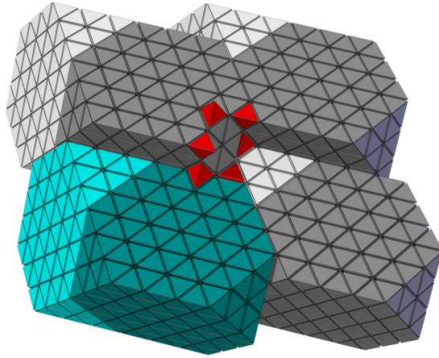

FIG. 14: (Color online) The tiling associated with the densest known packing by truncated tetrahedra (i.e., the TT tiling) can be built based upon the FCC tiling. The image shows four dimers belonging to the packing. The six tetrahedral holes per dimer are clearly visible at the center of the picture. Similar to the TH tiling, there are no variants associated with the TT tiling, since it is not possible to slide layers relatively to each other in the TT tiling.

small tetrahedra in the tiling is chosen to be the same as the fundamental tetrahedra for the retessellation, the large truncated tetrahedron in the tiling can be retessellated into 104 fundamental octahedra and 205 fundamental tetrahedra (see Fig. 14).

As a final example, we show that a recently discovered periodic tiling by irregular truncated tetrahedra associated with the β-tin structure [28] can be dissected into an FCC tiling.

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TABLE III: The three canonical tilings by regular truncated tetrahedra and regular tetrahedra. Note the relationship between side ratio s, tile ratio t and packing fraction of the truncated tetrahedra ϕ_{tt}. The space group associated with each tiling is also given.

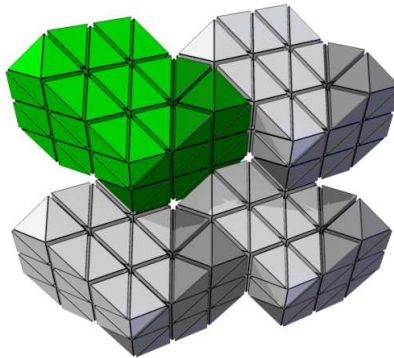| Name	s	t	ϕ_{tt}	Space Group
TH	1/3	3	23/32	trig.
CRS	1	1	23/24	$Fd\bar{3}m$
TT	3	1/3	207/208	trig.

FIG. 15: (Color online) The tiling by irregular truncated tetrahedra associated with the β-tin structure can be dissected into an FCC tiling.

Specifically, the irregular truncated tetrahedron is obtained by chopping the four corners of a regular tetrahedron with edge length 1/4 of that of the original tetrahedron. The FCC retessellation of this tiling is shown in Fig. 15, in which each truncated tetrahedron contains 20 tetrahedra and 10 octahedra.

VI. CONCLUSIONS AND DISCUSSION

In this paper, we enumerated and thoroughly examined the most comprehensive set of tilings of $\mathbb{R}^3$ by a number of elementary polyhedra, including simplices (regular tetrahedra), cross-polytopes (regular octahedra) and the simplest among the Archimedean solids (regular truncated tetrahedra) known to date. Importantly, we presented a fundamental link between all these configurations, which is the underlying FCC tessellation that forms the basis for

their constructions. Continuous transformations can bring each known configuration into the FCC tiling and vice versa, and each intermediate state can be represented by a tiling that can itself be dissected into an FCC tiling.

Since it is not possible to tile space using a single regular polyhedron (i.e., Platonic solids) other than the cube, we thoroughly investigated the possibility of constructing tilings containing two different regular polyhedra. We found that the only pair of regular polyhedra that tile $\mathbb{R}^3$ are the octahedron and tetrahedron. This is because only the dihedral angles of these two polyhedra can add up to integer multiples of π, a necessary condition for tilings as we discussed in Sec. I. Moreover, if we require that the tilings only contain congruent octahedra and congruent tetrahedra, there seem to be only four possible side ratios for two polyhedra. (In future work, we will explore a possible proof of this statement.) The four canonical periodic tilings associated with the aformentioned side ratios, i.e., the FCC, UT, DO and LO tilings, were discussed in detail. We also found that there are three distinct canonical periodic tilings of $\mathbb{R}^3$ by congruent regular tetrahedra and congruent regular truncated tetrahedra, i.e., the TH, CRS and TT tilings. In future work, we will pusue a possible proof of this statement.

We note that the main focus of the current work is periodic tilings of $\mathbb{R}^3$ by regular polyhedra other than the cube. As mentioned in Sec. III, a family of an uncountably infinite number of tilings associated with the LO tiling can be derived, in which the number of nonperiodic tilings is overwhelmingly larger than that of the periodic ones. In general, these tilings can not be obtained via the retessellation of the FCC tiling. However, they could result from retessellating the tilings associated with the stacking variants of FCC.

An outstanding question is whether there exist aperiodic tilings by congruent regular octahedra and tetrahedra with prohibited crystallographic symmetry (e.g., icosahedral or 12-fold rotational symmetry) [14], i.e., three-dimensional quasicrystal tilings. We can provide a partial answer to this question. For the four canonical tilings discussed in the paper, the side ratios s between the octahedra and tetrahedra are all rational numbers. In the case that $s = 1$, it is clearly impossible to obtain quasicrystal tilings due to the dihedral angles of the two polyhedra, as discussed in the Introduction. This should also be true for the other three side ratios for the other three canonical polyhedra, although currently a rigorous proof is lacking. If the side ratios are allowed to be irrational numbers, we cannot rule out the possibility that octahedra and tetrahedra can tile $\mathbb{R}^3$ aperiodically with prohibited

crystallographic symmetry, although we doubt it.

In future work, we would like to investigate these possibilities and generalize the retessellation idea to investigate nonperiodic tilings. In addition, it would be interesting to study tilings in high-dimensional Euclidean spaces using the retessellation idea.

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