Intrinsic structural features in jammed disordered packing of monodisperse spheres

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Abstract

A new tetrahedral structure model was developed and the geometrical structure of jammed disordered packings of monodisperse spheres with different friction coefficients was systematically characterized. An intrinsic structure feature is revealed for all jammed disordered packings, which is determined only by the packing fraction, independent of interparticle friction. Moreover, the structural configurations associated with crystal phases are more prevalent than the geometric frustrated ones. In addition, irregular simplexes are found to play a key role in an increase in density, rather than regular simplexes, in contrast to previous expectation. Our model provides an intrinsic structural basis for the random close packing.

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Finding the most efficient way to pack identical spheres is among the oldest puzzles known to scientists [1,2]. Apart from the mathematical significance [3-5], packings of spheres have been widely applied to the structural studies of living cells [6] and liquids [7-12], colloids [13,14], glass transition [15-19], phase transition between disordered and ordered states [20-29], and jamming system [30-36]. In 1611, Kepler conjectured that the densest packing of spheres could be achieved by stacking close-packed planes with packing fraction of $\frac{\pi}{\sqrt{18}} \approx 0.7405$, which was proved only recently [4]. However, for disordered sphere packings first explored by Bernal in 1960’s, the most compact way to pack spheres, that is, random close packing (RCP), results in a maximum packing fraction of $\phi_{\text{RCP}} \approx 0.64$, beyond which a packing contains crystalline regions inevitably [8-10,21,25,29,35]. Moreover, recent theoretical studies suggest that a phase diagram demarcated by an RCP line, random loose packing (RLP) line, and granular line can be constructed for frictional disordered packings characterized by interparticle friction coefficient [33]. This study demonstrates that RCP is not a unique point, but an RCP line from the frictionless point to the point with infinite friction coefficient. Although $\phi_{\text{RCP}}$ seems to be robust, its nature and physical origin are greatly disputed [5,8,21,22,24,27,31,32,35,37-42].

In 2000, Torquato et al. pointed out that the state with $\phi_{\text{RCP}}$ may correspond to the maximally random jammed state, where the systems are jammed with minimization of typical order parameters [31], such as bond-orientational order. Based on the energy landscape of systems of particles interacting with finite range, repulsive potential jam, a jamming threshold was found to be very close to 0.64 [32]. By developing a mean-
field approach of jammed disordered packings, the states lying in the RCP line can be interpreted as the ground states of hard spheres characterized by different interparticle friction coefficients [33]. Moreover, the entropy of the jammed disordered packings was also calculated to characterize the jammed structures and found to decrease with increasing packing fraction, indicating that the states in the RCP line is more ordered than others in the phase diagram [34,43]. However, no detailed structure feature in disordered sphere packings was investigated in the above studies, mainly due to the lack of good order parameters for the characterization of randomness [31], which is crucial for understanding the nature of RCP. Recently, by investigating tetrahedral configurations of frictionless hard spheres, polytetrahedral aggregates adjacent by faces are revealed to be most prevalent at RCP point and decreases as packing fraction exceeds $\phi_{RCP}$ [21,24]. While the polytetrahedral model provides a plausible structural perspective for densification mechanism in disordered packings and RCP, it cannot explain how the crystal nuclei formation starts in the disordered packings with such a geometric frustrated polytetrahedral configuration filled in everywhere as the density passes through the critical density [44]. Moreover, tetrahedron presents not only in polytetrahedral configurations, but also in the densest crystal structures [45]. Therefore, polytetrahedral structure might be only one-sided feature of disordered packings. Thus, a thorough structural model is highly desirable for comprehensively exploring structural features in disordered packings and nature of RCP.

In this Letter we numerically explored the structure of jammed disordered packings of monodisperse spheres with different interparticle friction coefficients by Voronoi-
Delaunay partitioning. Apart from tetrahedron (T), quartoctahedron (Q) and BCC Simplex (B) were also taken into account, so that one can investigate the local configurations associated with both crystal phases and geometric frustrated structures and their respective roles in RCP in disordered sphere packings. We show that the geometrical structure of jammed disordered packings depends only on packing fraction \( \phi \), not on friction coefficient. As packing fraction increases, although the geometric frustrated clusters increase slightly, the clusters associated with crystal phases formed by face-adjacent T, Q, and B increase more and are the characteristic features in the disordered packings. While all simplexes become denser with increasing packing fraction, it is the irregular simplexes rather than the regular ones (T, Q, and B) that dominate the increase in the density of the disordered packing.

In this work, the jammed disordered packings with different interparticle friction coefficients were investigated [33,43,46]. Different friction coefficients may produce different mechanical coordination numbers which characterizes the mechanical features at the grain scale in disordered packings. Each packing contains 10000 identical spheres in a cubic box with periodic boundary conditions. The details of the algorithm for packing preparation can be found in Refs. [33,43], according to which, the jammed disordered packings with mechanically stable and force-equilibrated at different packing fractions can be generated. To obtain Delaunay simplexes, Voronoi-Delaunay method was employed to decompose three-dimensional structures [47], so that Voronoi network can be constructed, in which each vertex is incident to four spheres, defining the Delaunay simplex. Thus, all Delaunay simplexes of the system can be determined,
and their geometric characteristics can be analyzed.

To quantitatively evaluate the shape of a Delaunay simplex, Procrustean distance (PD) approach was used to estimate the proximity of a simplex to a given template by the degree of coincidence upon their superposition [48] (see Supplementary Information section I). Small PD value indicates that the shape of the simplex is close to the template. In our work, three templates of perfect tetrahedron (T), quartoctahedron (Q) and BCC Simplex (B) were employed to calibrate the Delaunay simplexes in disordered packings (see Supplementary Figure 1). PD distribution of the Delaunay simplexes are broad, and shifts to smaller distance with increasing packing fraction. In addition, the distribution at around zero distance increases. These indicate that the simplexes in disordered packings become more and more regular, and more T, Q, and B are formed with the increase of density.

In order to assign a Delaunay simplex to a given template shape, a cutoff distance needs to be specified for T, Q, and B, respectively, i.e., \( d_T \), \( d_Q \), and \( d_B \), below which a simplex is considered to be a particular shape. In our work, \( d_T^2 = 0.01 \), \( d_Q^2 = 0.01 \), and \( d_B^2 = 0.01 \) are employed in the calibration of all simplexes (see Supplementary Information section II for details). All selected simplexes are regarded as regular simplexes. Simplexes with \( d^2 > 0.01 \) to all three templates are denoted as irregular simplexes (I).

Figure 1 shows the volume fraction of regular simplexes (T, Q, and B) as a function of packing fraction \( \phi \) and mechanical coordination number \( Z \) for the jammed disordered packings in the phase diagram (see Supplementary Movie 1 for more details).
The volume fraction is about 12% at the RLP point of $\phi = 0.539$ and increase continuously with increasing packing fraction, reaching about 41% as packing fraction is close to $\phi_{\text{RCP}}$. It is also found that in the disordered packings of the same $\phi$, the population of the regular simplexes is almost the same, independent of $Z$ value. Moreover, the fraction of T, Q, and B in the packings at the same $\phi$ is also independent of mechanical coordination number $Z$ (see Supplementary Figure 3 and Movie 2). This reveals that the geometric structure features in the jammed disordered packings are intrinsic, independent of interparticle friction or preparation protocol. It has been shown that fluctuation density as a function of $\phi$ is also the same for packings with different friction coefficients [34,43]. Our results reveal the underlying intrinsic structure basis in the jammed disordered packings of monodisperse spheres. This finding also provides a new understanding of RCP. The disordered packings at RCP line keep the random feature without crystal phases and contain maximal number of regular simplexes compared to the disordered packings below $\phi_{\text{RCP}}$. Therefore, from the structural point of view, RCP may be well-defined.

As shown in Supplementary Figure 3, the volume fraction of T, Q and B increases from 3%, 7% and 4% at $\phi \approx 0.54$ to 14%, 20% and 11% at $\phi \approx 0.64$, respectively. The volume fraction of T at $\phi \approx 0.64$ is much less than 30% reported in Ref. [21] where T was identified by the difference of the maximal edge lengths $e_{\text{max}}$ from unit $\delta = e_{\text{max}} - 1 < 0.255$. Because the condition of $\delta < 0.255$ used in Ref.[21] to identify T from Delaunay simplexes is relatively loose, some “quasi-regular tetrahedron” are also included [45,49]. Thus, the population of T in disordered packings is
overestimated. The method and calibration employed in our work are much more rigorous, so that the simplexes with much more regular shapes can be selected, and T, Q, and B can be maximally distinguished (see Supplementary Information section I and II).

Next, we explored the local configurations associated with both crystal phases and geometric frustrated structures by characterizing the clusters formed by face-adjacent packings of the regular simplexes (T, Q, and B) [8,21,24,45]. In FCC crystal, every T is adjacent by faces only to four Q, and every Q is adjacent to two T and two Q, so that there are two types of five face-adjacent clusters \{T:QQQQ\} and \{Q:TTQQ\}. Here the first letter in {} represents the central simplex, while the others represent the face-adjacent simplexes to the central one. In HCP crystal, there are three types of clusters: \{T:TQQQ\}, \{Q:TQQQ\} and \{Q:TTQQ\}. In BCC crystal, however, there is only one type of cluster \{B:BBBB\}. In these crystal-type clusters, if one or two simplexes adjacent to the central one do not satisfy the crystal-type cluster configurations, such clusters are classified as defective clusters and denoted as defective I and defective II, respectively. In addition, one T may be adjacent to two or more T, i.e., \{T:TTTT\}, \{T:TTT*\} and \{T:TT**\} (*∈(Q, B, I)) which characterize the typical geometric frustrated structures for dense amorphous phase [8,21,24,45,50]. Here the number of clusters was defined by the number of central simplexes, and the fraction of one type cluster was obtained by the number of clusters divided by the total number of simplexes in disordered packings.

Figure 2 shows the volume fraction of crystal-type, defective and geometric
frustrated clusters as a function of packing fraction for the jammed disordered packings with different mechanical coordination numbers, respectively. They all increase with increasing packing fraction. It can be clearly seen that the population of the clusters associated with crystal phases, i.e., crystal-type and defective clusters increases more quickly and is much higher than the geometric frustrated ones, dominating the local ordering in all jammed disordered packings. The population of each type cluster in the packings lying in the RLP line can be found in Supplementary Figure 4. In specific, FCC- and HCP-type clusters increase more significantly. This indicates that the structures associated with FCC and HCP crystal phases may play a much more important role than the geometric frustrated structures in the disorder-order transition as packing fraction goes beyond $\phi_{\text{RCP}}$ [26,39]. The spatial distribution of the central simplexes of the crystal-type, defective, and geometric frustrated clusters in the packing at RCP point is illustrated in Supplementary Figure 5. It is clearly seen that the clusters associated with crystal phases are more prevalent in the packing at RCP point, and the geometric frustrated clusters are embedded in. This demonstrates that the configurations associated with crystal phases may be more important in the geometrical structure in the jammed disordered packings and disorder-order transition as packing fraction passes through the RCP density. On the other hand, only small fraction of T has the geometric frustrated configurations. As shown in Supplementary Figure 6, while the volume fraction of T reaches about 12% at $\phi_{\text{RCP}}$, the fraction of T with geometric frustrated configurations is only about 4.5%. This indicates that the geometric frustrated structure feature may not be as significant as expected in previous studies [7,8,18,21,24].
In contrast, the configurations associated with crystal phases are much more important in jammed disordered packings. Such structure feature in the packings at RCP line can naturally explain the crystal nuclei formation and disorder-order transition near $\phi_{RCP}$. These can be further understood by exploring the densification mechanism in disordered packings within our structure model.

In previous studies, the increase in the density of disordered packings below $\phi_{RCP}$ was attributed to the increase of T that coalesce into polytetrahedral aggregates [21]. However, as shown above, the population of T is much lower than that reported in Refs. [21,24], and only small fraction of T has the geometric frustrated configurations. Thus, the increase of T is unlikely to account for the density increase in disordered packings.

To explore the densification mechanism in disordered packings with increasing packing fraction, we analyzed the mean packing density of different types of simplex in disordered packings, which allows to evaluate how each type of simplex contributes to the density increase. The packing fraction of a simplex is defined by the ratio of the occupied volume of the simplex to its total volume [51]. The mean packing fraction of one type of simplex is given by the harmonic mean method [28,29]. For example, the mean packing fraction of T can be expressed as $\phi_T = \frac{N_T}{\sum_{i=1}^{N_T} 1/\phi_T^i}$, with $\phi_T^i$ being the packing fraction of $i$th T and $N_T$ the total number of T. As shown in Figure 3(a), the mean packing fraction of all types of simplex increases as packing fraction increases. Thus, all types of simplex become denser and denser, making contributions to the density increase. It can be seen that the mean packing fraction of T, Q, and B is more than 0.6 even in the packing at RLP point, much higher than irregular simplex.
showing the nature of dense packing in T, Q, and B. Although the mean packing fraction of T, Q, and B continuously increases, the increase rate is getting slower, and the mean packing fraction becomes almost saturated far below $\phi_{RCP}$, especially for T and Q. As shown in Figure 3(a), the mean packing fraction of T, Q, and B changes little for $\phi > 0.6$. In contrast, however, the mean packing fraction of irregular simplexes (I) increases linearly and exceeds 0.6, as packing fraction approaches $\phi_{RCP}$. Therefore, the density increase in I is more significant than that in T, Q, and B.

To more precisely evaluate the densification of each type of simplexes, we analyzed the volume change of each Delaunay simplex between two successive packing fractions of $\phi_1$ and $\phi_2$ ($\phi_1 < \phi_2$). We classified all simplexes in $\phi_1$ into three parts: the existing regular simplexes (T, Q, and B) in $\phi_1$, irregular simplexes (I) in $\phi_1$ transformed into regular simplexes (T, Q, or B) in $\phi_2$, and the remaining of I in $\phi_1$. We estimated the volume change of three part of simplexes as packing fraction increases from $\phi_1$ to $\phi_2$. Figure 3(b) shows the ratio of volume change in three parts to the total volume change between two successive packing fractions. Surprisingly, the remaining of I contributes more than 70% increase in the density. However, the existing and newly transformed T, Q, and B make a very little contribution to the density increase. The above results elucidate that instead of regular simplexes (T, Q, and B), the irregular simplexes (I) dominate the increase in the density, playing more important role in the density increase in disordered packings. Previous studies reported that an increase in the number of tetrahedral configurations that coalesce into polytetrahedral clusters is responsible for the increase in the density of a disordered packing before $\phi_{RCP}$.
[21,24,45]. However, our analysis clearly shows that instead of the simplexes with regular shapes, those with irregular shapes dominate the densification in disordered packings. Our results suggest a new mechanism in density increase in disordered packings. In general, all simplexes in disordered packings become denser as packing fraction increases. However, the density increase in the regular simplexes of T, Q, and B is very limited, especially in the disordered packings of $\phi > 0.6$, because they are already very dense. Although more T, Q, and B are formed with increasing packing fraction, their increase between two successive packing fractions is also very limited, which cannot account for the density increase, either. In contrast, irregular simplexes are loosely packed, and their population is much higher, compared to T, Q, and B, so that they can easily change shapes and become more regular and denser with increasing packing fraction, making greater impact on the density increase. This is elucidated more clearly in Supplementary Figure 7, showing the local packing fraction distribution of different types of simplexes. The distribution of irregular simplexes as well as all simplexes shifts to higher density and becomes much narrower with increasing packing fraction. Our results suggest that the density increase in disordered packings relates to a continuous change in structures.

Note that the mean packing fraction of I exceeds 0.6 near $\phi_{RCP}$, very close to the value of B at RLP point, as shown in Fig. 3(a). This implies that the whole structure in the packings close to $\phi_{RCP}$ has been very regular, and may be ready for the formation of crystal phase, as packing density further increases. Another interesting phenomenon is that the mean packing fraction of regular simplexes (T, Q, and B) at RLP point is just
around 0.64 (see Fig.3(a)), coincident with $\phi_{RCP}$, which could have some implications on the critical density.

We should emphasize that lying in $\phi_{RCP}$, four packings with $Z \approx 4$ contain relatively higher population of the crystal-type and defective clusters, compared to others with $Z>4$ (see Figure 2(a) and (b)). This may result from the preparation of disordered packings. As mentioned in Ref.[33,43], the smaller the mechanical coordination number $Z$ is, the more difficultly the mechanically stable disordered packings are prepared. This also demonstrates that our structural model is very sensitive and able to efficiently detect local ordering in disordered structures. In addition, our model can be applied to not only jammed disordered packings, but also other disordered sphere packing systems, even the packings with packing fraction beyond $\phi_{RCP}$, so that the disorder-order transition in hard sphere packings can be explored by our model. In addition, this model can be potentially applied to simple metallic liquids, since they can be regarded as disordered packing of hard spheres [52].

In conclusion, we developed a new tetrahedral structural model. It is revealed that disordered packings of monodisperse spheres possess intrinsic structure feature, which depends only on packing fraction. Instead of geometric frustrated structures, the local configurations associated with crystal phases are the essential features in disordered packings at the RCP line, which ensures that the crystal phases may naturally form as density passes through $\phi_{RCP}$. Our study provides the underlying structural basis for the random close packing.

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**Figure 1.** Volume fraction of regular simplexes (T, Q, and B) in jammed disordered packings with different packing fractions $\phi$ and mechanical coordination number $Z$. The color of dots represents the volume fraction as indicated by the color bar. The dashed lines in $Z - \phi$ plane illustrate the random loose packing (RLP) line, random close packing (RCP) line, and granular line, respectively, which demarcate the phase diagram of all the jammed disordered packings of monodisperse hard spheres with different packing fraction and friction coefficients producing different mechanical coordination number $Z$ [33,43].
**Figure 2.** Comparison of the volume fraction of the crystal-type, defective (I and II), and geometric frustrated (\{T:TTTT\}, \{T:TTT*\} and \{T:TT**\} (\*\in\{Q, B, I\})) clusters in the jammed disordered packings with different packing fraction \(\phi\) and mechanical coordination number \(Z\). The fraction of each crystal-type and defective cluster is presented in Supplementary Figure 4. The color of each symbol represents \(Z\) value as indicated by the color bar in (b).
Figure 3. (a) Mean local packing density of T, Q, B, and I as a function of packing fraction. The mean local packing density of regular simplexes (T, Q, and B) was also presented. The horizontal dashed line marks the local packing density of BCC Simplex at RLP point. (b) The ratio of volume change to the total volume change between two successive disordered packings for the existing regular simplexes (T, Q, and B), irregular simplexes (I) transformed into regular simplexes (T, Q, or B), and remaining of I, respectively.
SUPPLEMENTARY INFORMATION

Intrinsic structural features in jammed disordered packing
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I. Procrustean distance

To identify tetrahedron (T), quartoctahedron (Q) and BCC Simplex (B) in disordered packings, the proximity of an arbitrary Delaunay simplex to a given template can be quantitatively characterized by the square of Procrustean distance [1,2]

\[ d^2 = \min_{c,R,t,P} \left\{ \frac{1}{n} \sum_{i=1}^{n} \| x_i - (cR y_i + t) \|^2 \right\}, \]

where \( \{x_1, x_2, \ldots, x_n\} \) and \( \{y_1, y_2, \ldots, y_n\} \) are the coordinates of \( n \) spheres in a Delaunay simplex and the template, respectively. The minimum is calculated over all three-dimensional rotations \( R \), translations \( t \), size scaling \( c \), and all possible combinatorial mapping between the two sets of coordinates \( P \). From the definition, it is obvious that smaller values of \( d \) indicate more regular simplex to the template. For an arbitrary Delaunay simplex, \( d^2 \) can be calculated for the template of T, Q, and B, respectively. Supplementary Figure 1 shows the \( d^2 \) distribution of Delaunay simplexes in disordered packings at different packing fraction to the template of T, Q, and B, respectively. We use \( d^2 \) as an order parameter to define the emergence of T, Q, or B in disordered packings when it is below a cutoff value in the following.
Supplementary Figure 1. Square of Procrustean distance distribution of Delaunay simplexes in disordered packings of monodisperse spheres on random loose packing (RLP) line at different packing fractions to the template of T (a), Q (b), and B (c), respectively. The vertical dashed lines mark the cutoff distances of $d_T^2=0.01$, $d_Q^2=0.01$, and $d_B^2=0.01$, respectively.

II. Determination of the Procrustean distance cutoff

To determine the Procrustean distance cutoff for T, Q, and B, thermal effect on crystal structures was also taken into account in our calibration. First, we carried out MD simulations to anneal FCC (Cu), HCP (Zr), and BCC (V) crystal structures at 300K for 1ns, respectively. Due to the thermal effect, the atoms in each crystal structure are vibrating around their equilibrium positions, so that the simplexes in each crystal structure deviate from their perfect shapes. Second, we performed the calculations of the Procrustean distance for the annealed crystal structures with respect to each template, and a distance distribution in an annealed crystal structure for each template can be obtained. Supplementary Figure 2(a-c) shows the Procrustean distance distributions for the template of T, Q, and B in the annealed FCC, HCP, and BCC crystal structures, respectively. To determine the best cutoff for T, Q, and B, the following issues have to
be taken into account simultaneously: (1) the cutoff should be as small as possible, so that more regular simplexes to the corresponding templates can be selected; (2) the cutoff should lead to the minimum overlap of T, Q, and B, so that they can be maximally distinguished. Based on the above considerations, the cutoff of $d^2=0.01$ was chosen in the calibration of all Delaunay simplexes to the templates of T, Q, and B, respectively, as shown in Supplementary Figure 2. The vertical dashed lines indicate that the simplexes with $d^2 \leq 0.01$ can be regarded as T, Q, or B. For an arbitrary Delaunay simplex $i$, $d^2_i$ was calculated for the template of T, Q, and B, respectively, so that $d^2_{iT}$, $d^2_{iQ}$, and $d^2_{iB}$ were obtained. If only one value is smaller than 0.01, the Delaunay simplex is assigned to the corresponding shape. If there are two or three values are smaller than 0.01, the smallest one is chosen and the corresponding shape is assigned to the Delaunay simplex. If they are all larger than 0.01, the Delaunay simplex is classified into irregular simplex (I).

![Supplementary Figure 2](image)

**Supplementary Figure 2.** The Procrustean distance distributions of Delaunay simplexes to the template of T(red), Q(blue), and B(green) in FCC (a), HCP (b), and BCC (c) crystals annealed at 300K, respectively. The vertical dashed line in each panel indicates that the simplexes with $d^2 \leq 0.01$ can be regarded as T, Q, or B.
Supplementary Figure 3. The volume fraction of tetrahedron (a), quartohedron (b), and BCC simplex (c) in jammed disordered packings with different packing fractions $\phi$ and mechanical coordination number $Z$, respectively. The color of dots represents the volume fraction as indicated by the color bar. The dashed lines in $Z - \phi$ plane is random loose packing (RLP) line, random close packing (RCP) line, and granular line, respectively, which demarcate the phase diagram of all the jammed disordered packings of monodisperse spheres with different packing fraction and friction coefficients producing different mechanical coordination number $Z$ [3]. The spatial distribution of regular simplexes (T, Q and B) in disordered packings at $\phi = 0.539$ (d), $\phi = 0.603$ (e) and $\phi = 0.636$ (f), respectively. The size of box slice is $0.2x \times y \times z$. 
**Supplementary Figure 4.** Population of crystal-type clusters (a), and clusters with one (b) and two (c) simplexes adjacent to the central one do not satisfy the crystal-type cluster configurations as a function of packing fraction in the packings lying in the RLP line, respectively. The population of the geometric frustrated clusters of \{T:TTTT\}(a), \{T:TTT\*\}(b) and \{T:TT**\} (\*∈(Q, B, I)) (c) was also presented with purple pentagons. The population of HCP-type clusters of \{T:TQQQ\} and \{Q:TQQQ\} is even higher than the FCC-type clusters, indicating that HCP phase may be formed as disordered packings are crystallized. On the other hand, the population of \{B:BBBB\} clusters is almost zero, although the fraction of B is similar to T as shown in Supplementary Figure 3 and Supplementary Movie 2. This implies that BCC crystal phase is hardly formed in disordered sphere packings, consistent with previous studies [2,4].
Supplementary Figure 5. The spatial distribution of the central simplexes in the crystal-type, defective (I and II) and geometrical frustrated (\{T:TTTT\}, \{T:TTT*\} and \{T:TT**\} (∗∈(Q, B, I))) clusters in disorder packing at RCP point (ϕ = 0.636). The volume fraction of defective clusters is about three times that of geometrical frustrated ones. The size of box slice is 0.2x * y * z.
Supplementary Figure 6. (a) Volume fraction of total tetrahedron (circle) and the geometric frustrated clusters (pentagon) as a function of packing fraction in disordered packings lying in the RLP line. The geometric frustrated clusters include \{T:TTTT\}, \{T:TT^*\} and \{T:TT^{**}\} (\*\in(Q, B, I)). (b) The spatial distribution of all tetrahedra in the packing at RCP point ($\phi = 0.636$) including the geometric frustrated clusters with purple and others with red. The size of box slice is 0.2x * y * z.
Supplementary Figure 7. Packing fraction distribution of tetrahedron (T), quartoctahedron (Q), BCC Simplex (B), irregular simplexes (I) and all simplexes in disordered packings at $\phi = 0.539$ (a), $\phi = 0.603$ (b), and $\phi = 0.636$ (c) lying in the RLP line, respectively.

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