# Packing Nonspherical Particles: All Shapes Are Not Created Equal

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# Geometric Structure Approach to Jammed Particle Packings

**Torquato & Stillinger, Rev. Mod. Phys. (2010)**

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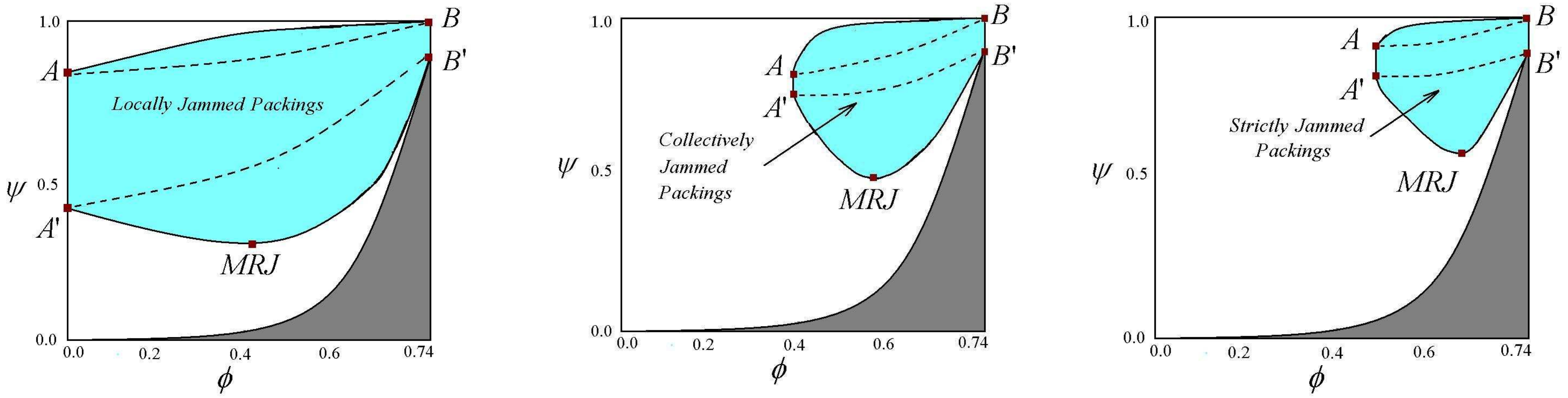
## Order Maps for Jammed Sphere Packings



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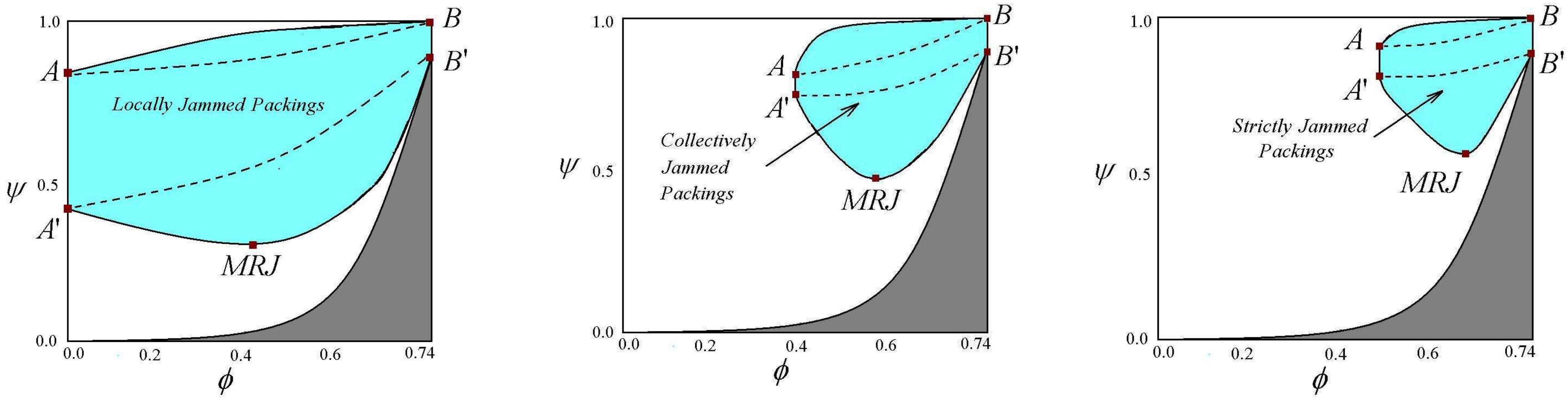
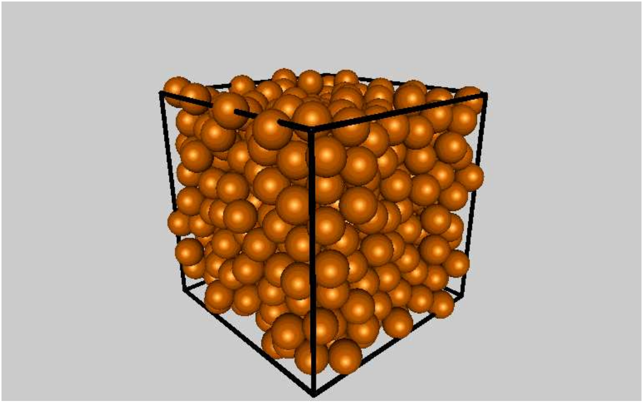
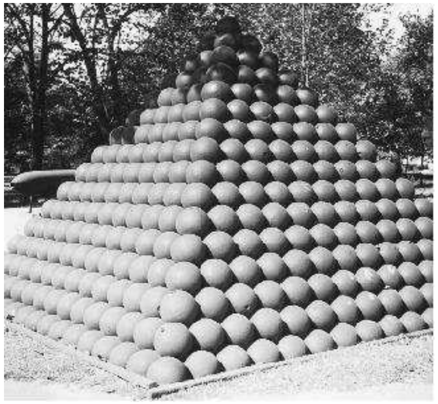



## Optimal Strictly Jammed Packings

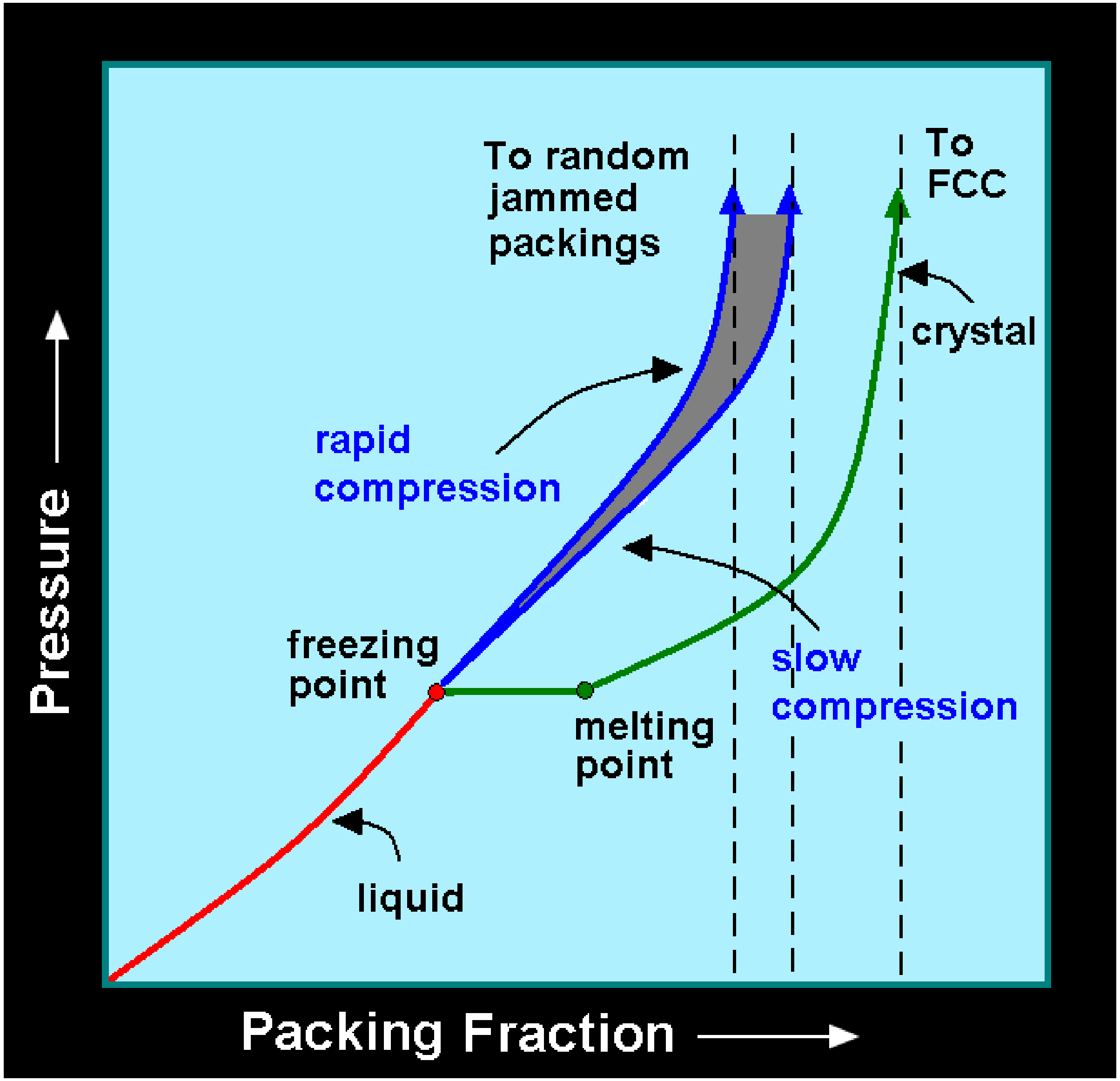




**A:** $Z = 7$ **MRJ:** $Z = 6$ **(isostatic)** **B:** $Z = 12$

- **MRJ packings are hyperuniform with quasi-long-range pair correlations with decay** $1/r^4$.

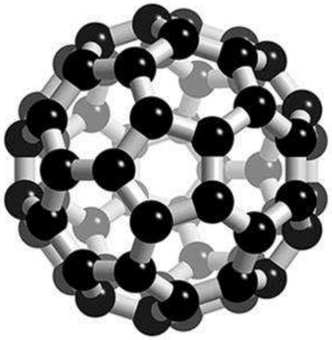
# 3D Hard Spheres in Equilibrium



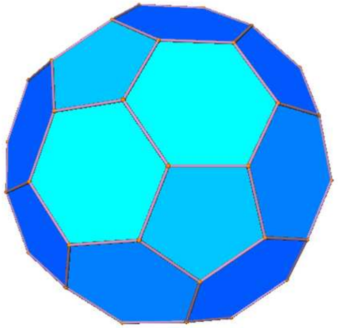

**Torquato & Stillinger, Rev. Mod. Phys. (2010)**

# Dense Packings of Nonspherical Particles in $\mathbb{R}^3$

Granular Media



Bucky Ball: C$_{60}$



Truncated Icosahedron

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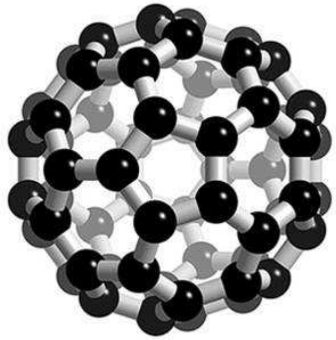

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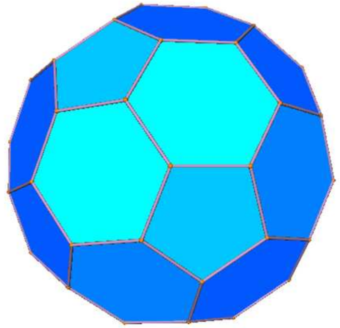
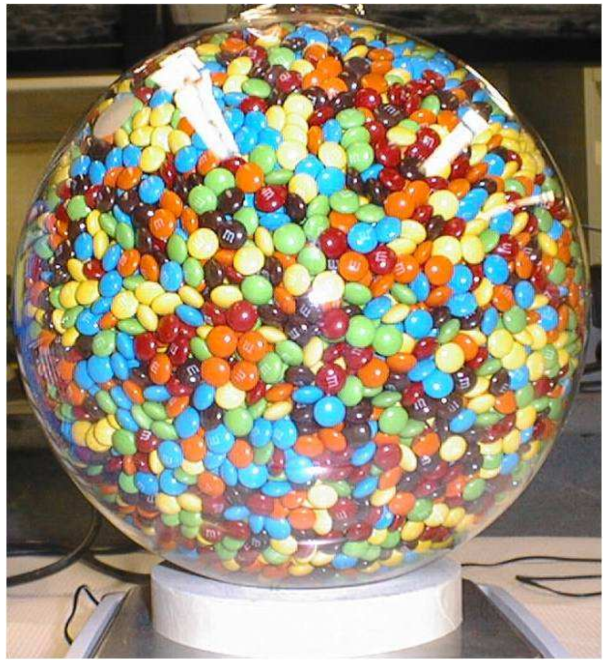


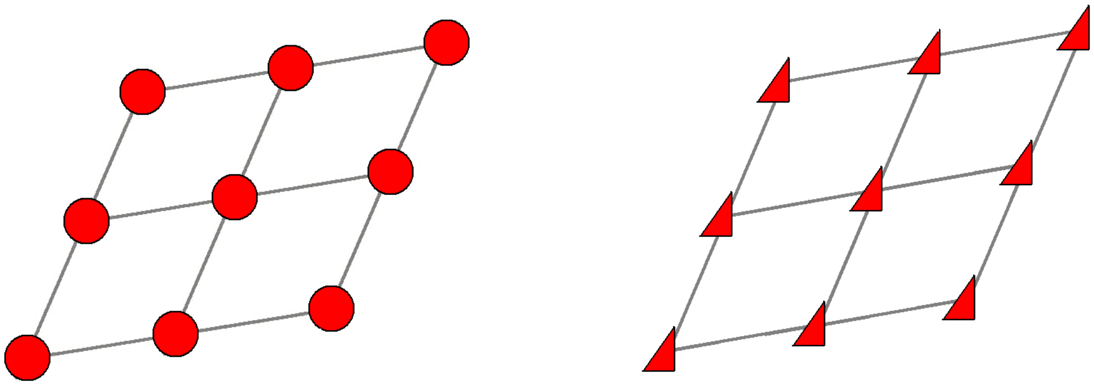
**Truncated Icosahedron**

**Ellipsoids: Donev et al., Science (2004)**

# Definitions

- A collection of nonoverlapping congruent particles in $d$-dimensional Euclidean space $\mathbb{R}^d$ is called a **packing** $P$.
- The **density** $\phi(P)$ of a packing is the fraction of space $\mathbb{R}^d$ covered by the particles.
- **Lattice packing** $\equiv$ a packing in which particle centroids are specified by integer linear combinations of basis (linearly independent) vectors. The space $\mathbb{R}^d$ can be geometrically divided into identical regions $F$ called **fundamental cells**, each of which contains just one particle centroid. For example, in $\mathbb{R}^2$:

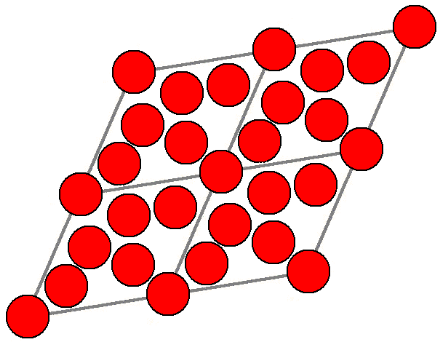


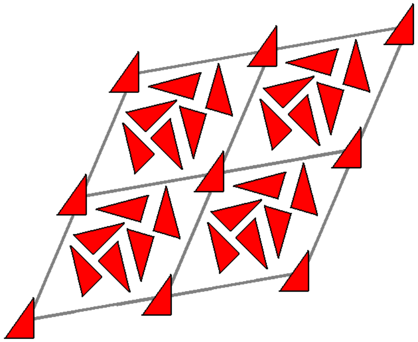
Thus, if each particle has volume $v_1$:

$$\phi = \frac{v_1}{\mathrm{Vol}(F)}.$$

# Definitions

- **A periodic packing is obtained by placing a fixed nonoverlapping configuration of $N$ particles in each fundamental cell.**





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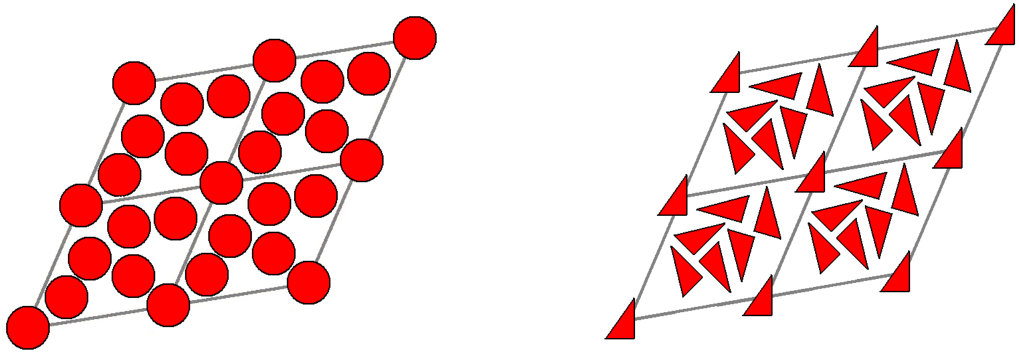
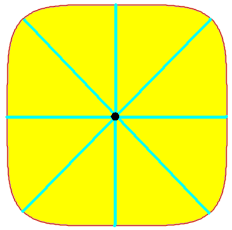


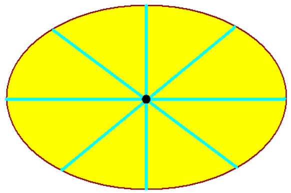
Thus, the density is

$$\phi = \frac{N v_1}{\mathrm{Vol}(F)}.$$

- A particle is **centrally symmetric** if it has a center $C$ that bisects every chord through $C$ connecting any two boundary points.



centrally symmetric
2 equivalent $\perp$ axes



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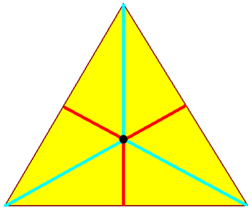
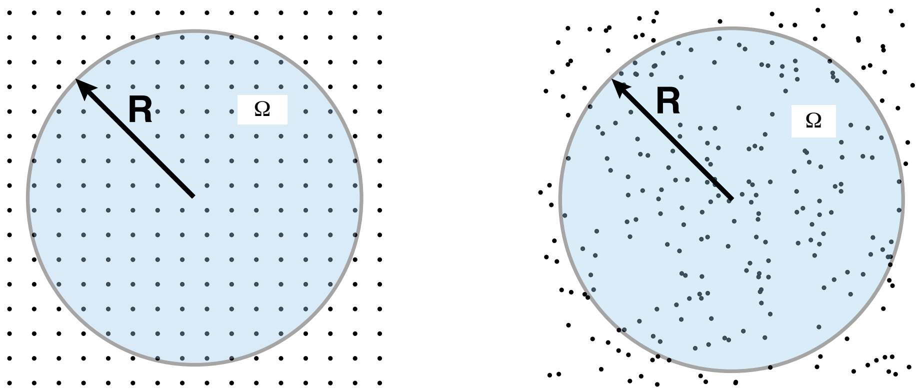


non-centrally symmetric

# Hyperuniformity for General Point Patterns

Torquato and Stillinger, PRE (2003)




- Denote by $\sigma^2(R) \equiv \langle N^2(R)\rangle - \langle N(R)\rangle^2$ the number variance.
- For a Poisson point pattern and many correlated point patterns, $\sigma^2(R) \sim R^d$.
- We call point patterns whose variance grows more slowly than $R^d$ hyperuniform (infinite-wavelength fluctuation vanish). This implies that structure factor $S(k) \to 0$ for $k \to 0$.
- The hyperuniformity concept enables us to classify crystals and quasicrystals together with special disordered point processes.
- All crystals and quasicrystals are hyperuniform such that $\sigma^2(R) \sim R^{d-1}$ – number variance grows like window surface area.
- Many different MRJ particle packings are hyperuniform with $S(k) \sim k$ for $k \to 0$.

Donev, Stillinger & Torquato, 2005; Berthier et al., 2011;

Zachary, Jiao & Torquato, 2011; Kurita and Weeks, 2011.

# Outline

- **Organizing principles for maximally dense packings of nonspherical particles.**
- **Organizing principles for MRJ packings of nonspherical particles (e.g., isostatic or not; hyperuniformity, etc.).**
- **Tunability capability via particle shape to design novel crystal, liquid and glassy states.**

# Packings of the Platonic and Archimedean Solids

- **Difficulty in obtaining maximally dense packings of polyhedra: complex rotational degrees of freedom and non-smooth shapes.**

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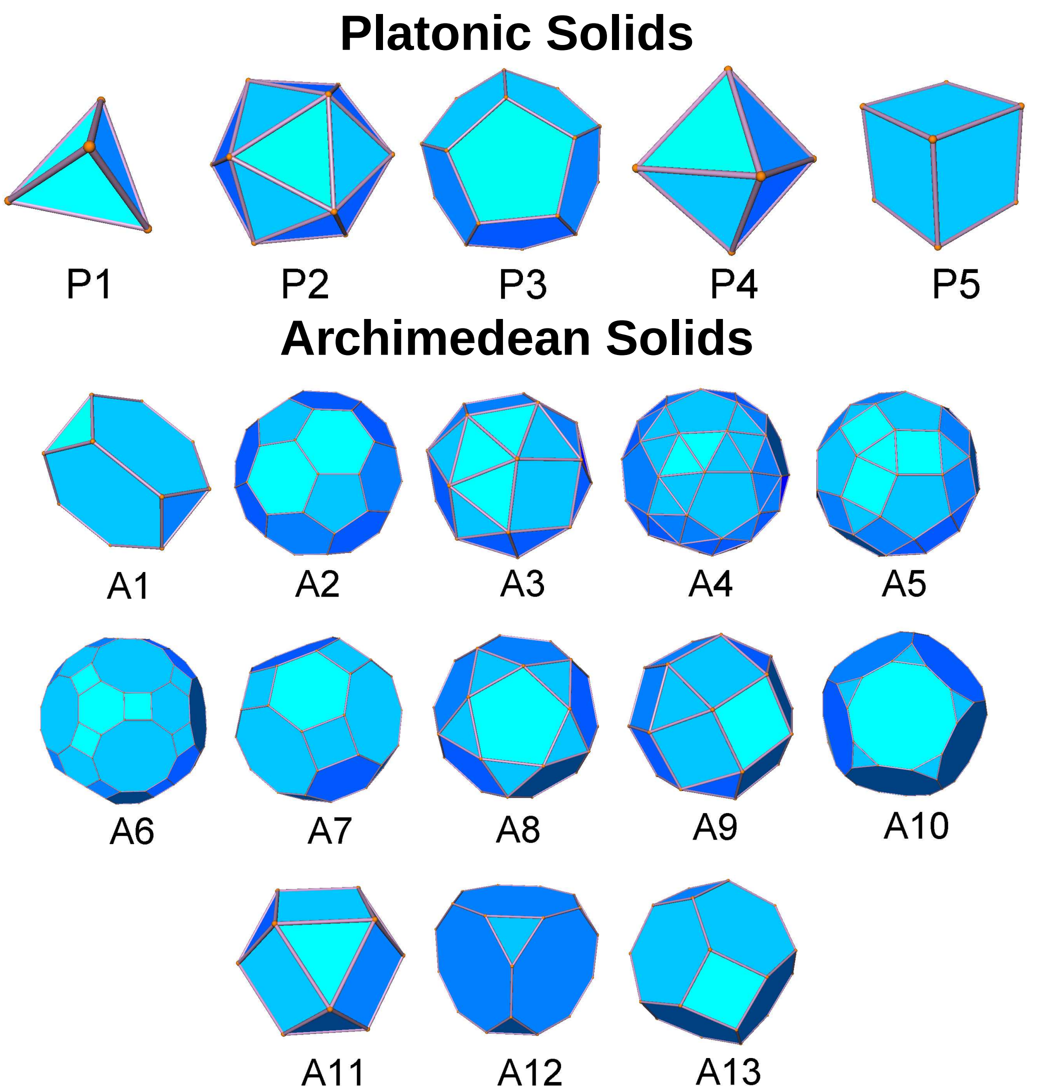
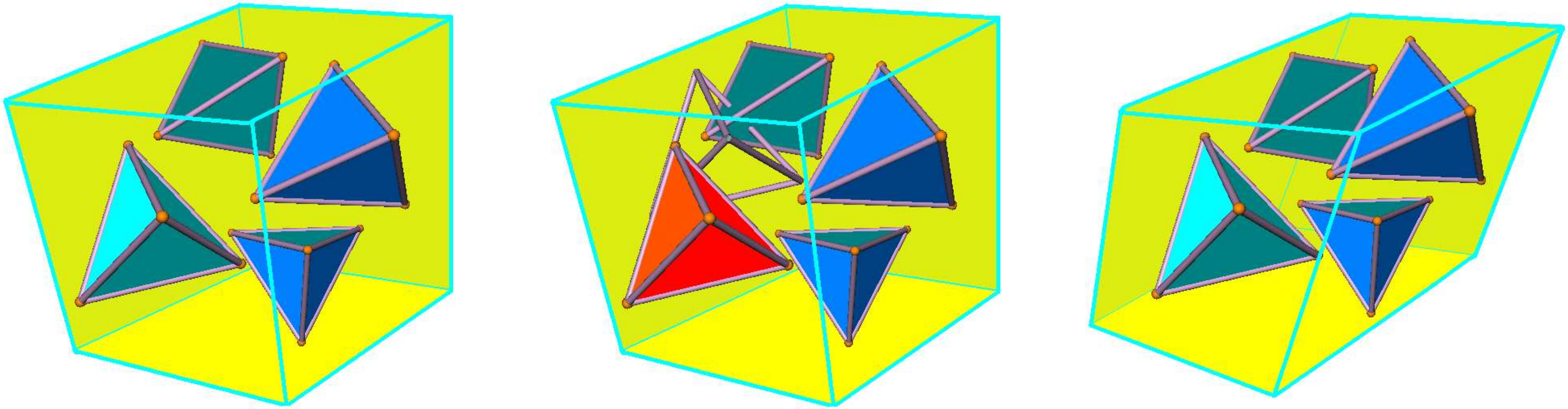
- **Torquato & Jiao, Nature (2009); PRE (2009); PRE (2010)**



# Adaptive Shrinking Cell

- **Optimization scheme that explores many-particle configurational space and the space of lattices to obtain a local or global maximal density.**

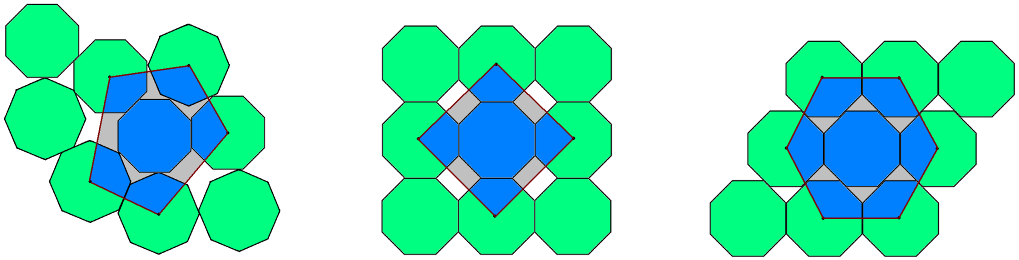


**(a)** **(b)** **(c)**

- **ASC scheme can be solved using a variety of techniques, depending on the particle shape, including MC and linear-programming methods. For spheres, the latter is very efficient [Torquato and Jiao, PRE (2010)].**

# Kepler-Like Conjecture for a Class of Polyhedra

- **Face-to-face contacts allow higher packing density.**
- **Central symmetry enables maximal face-to-face contacts when particles are aligned – consistent with the optimal lattice packing.**



- **For any packing of nonspherical particles of volume $v_{particle}$:**

$$\phi_{max} \le \phi_{max}^{upper\ bound} = \textbf{min}\left[\frac{v_{particle}}{v_{sphere}}\ \frac{\pi}{\sqrt{18}}, 1\right],$$

**where $v_{sphere}$ is the volume of the largest sphere that can be inscribed in the nonspherical particle.**

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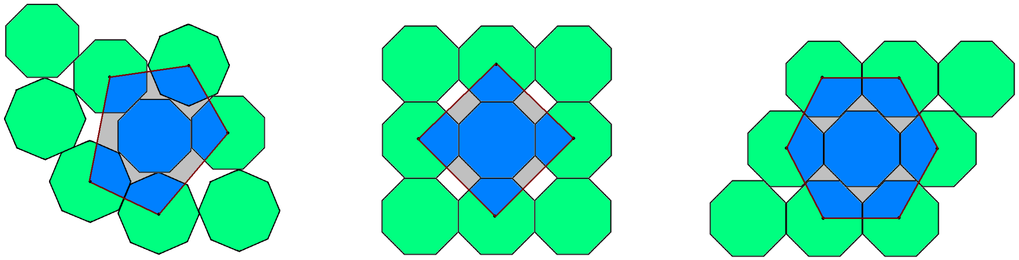

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**where $v_{sphere}$ is the volume of the largest sphere that can be inscribed in the nonspherical particle.**

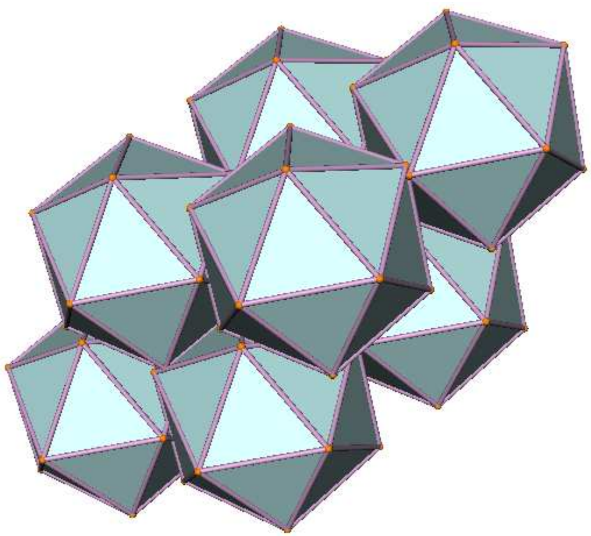
- **These considerations lead to the following conjecture:**

*The densest packings of the centrally symmetric Platonic and Archimedean solids are given by their corresponding optimal lattice packings.*

**S. Torquato and Y. Jiao, Nature 2009; PRE 2009; PRE**

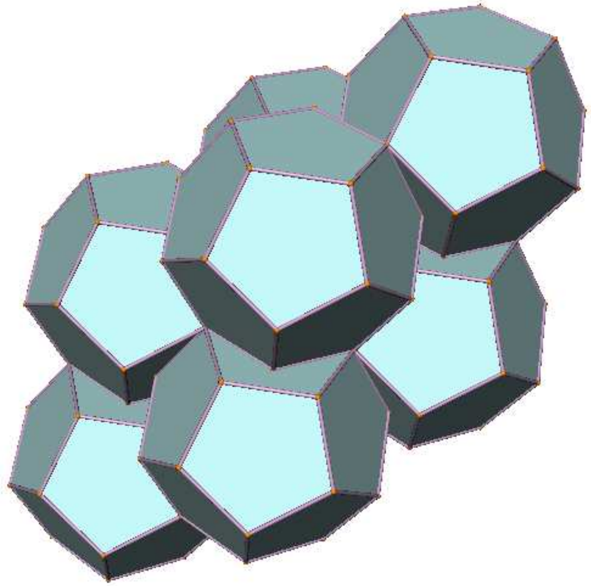
# Dense Packings of Icosahedra, Dodecahedra & Octahedra

- **ASC scheme with many particles per cell yield densest lattice packings for centrally Platonic solids!**



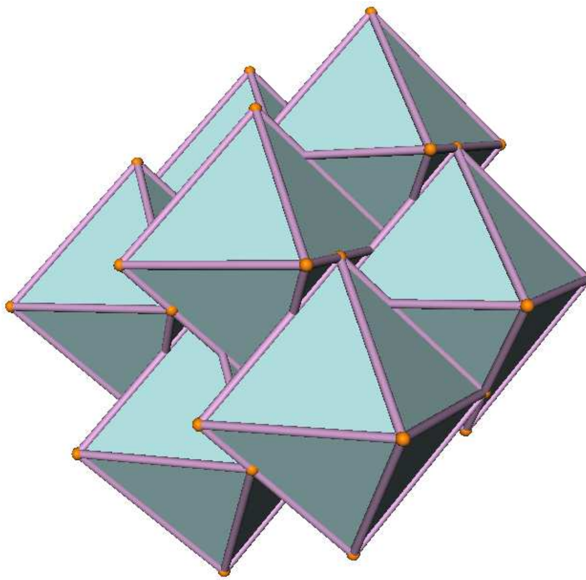
**Icosahedra**

$\phi = 0.836$



**Dodecahedra**

$\phi = 0.904$



**Octahedra**

$\phi = 0.947$

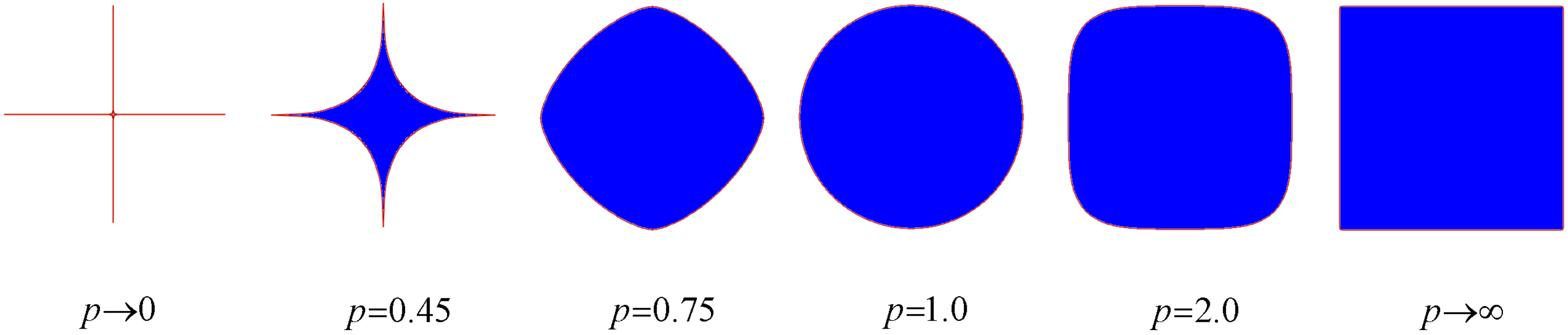
- **Later showed octahedron packing leads to uncountably infinite number of tessellations by octahedra and tetrahedra (Conway, Jiao & Torquato 2010).**

# Superballs

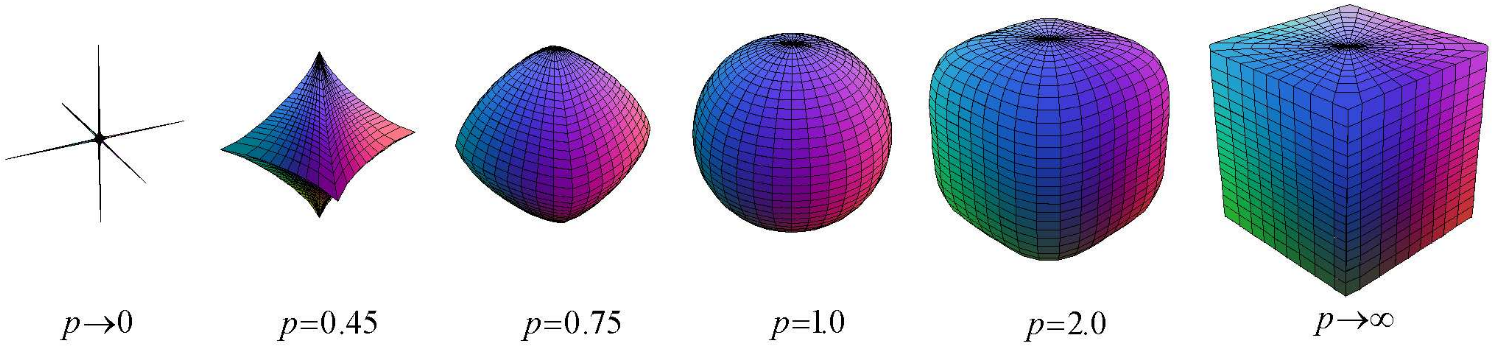
**A $d$-dimensional superball is a centrally symmetric body in $\mathbb{R}^d$ occupying**

$$|x_1|^{2p} + |x_2|^{2p} + \cdots + |x_n|^{2p} \leq 1 \qquad (p\text{: deformation parameter})$$

## Superdisks



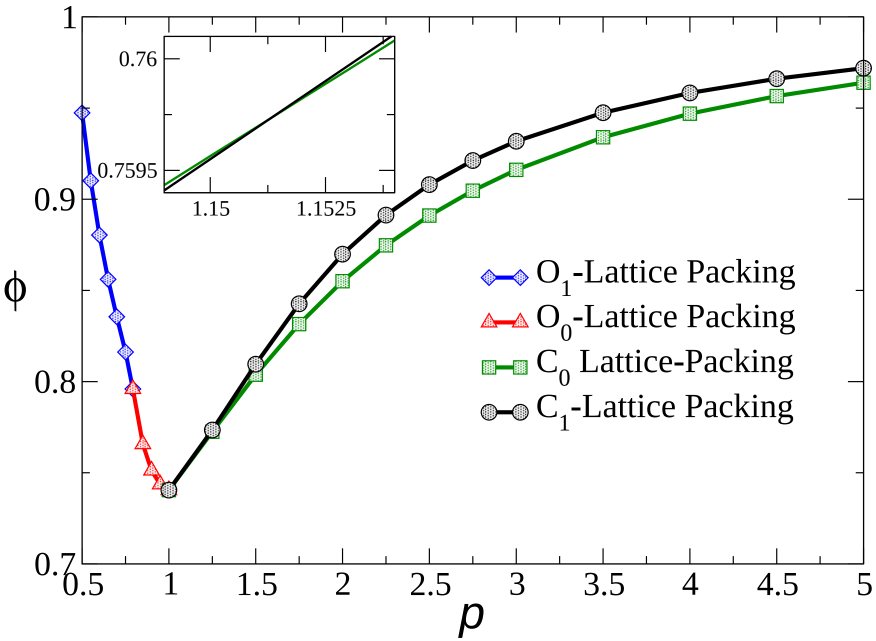

## Superballs

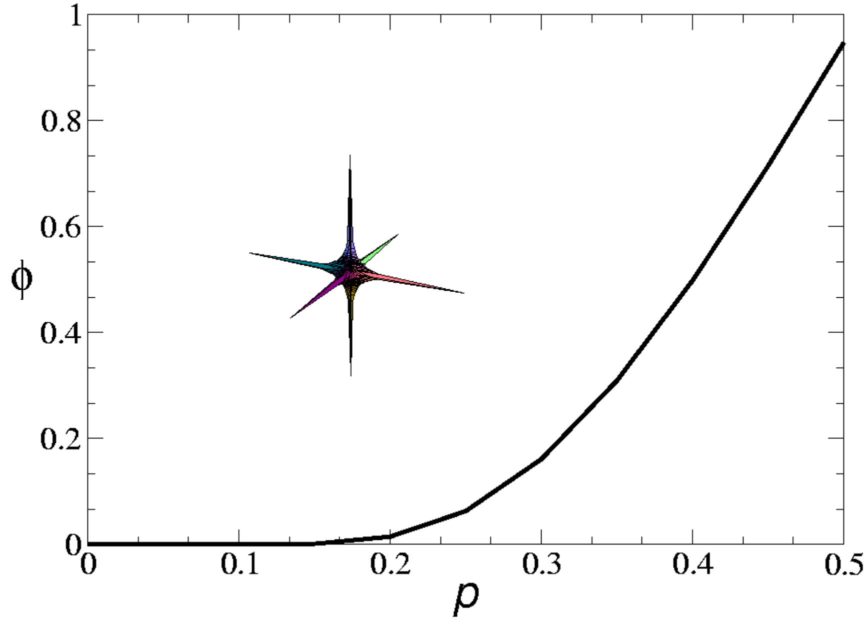



- **Densest packings are lattices and behave quite differently from ellipsoid packings! Jiao, Stillinger & Torquato, PRL (2008); PRE (2009)**

# Maximally Dense Superball Packings

**Jiao, Stillinger & Torquato, PRE (2009)**




- **Maximally dense packings are certain families of lattices for $p \geq 1/2$. Densest ellipsoid packings are non-lattices.**
- **Maximal density is nonanalytic at the "sphere" point ($p = 1$) (in contrast to ellipsoids) and increases dramatically as $p$ moves away from unity.**
- **Rich phase behavior depending on $p$ (Batten, Stillinger & Torquato 2010; Ni et al. 2012).**

# Another Organizing Principle

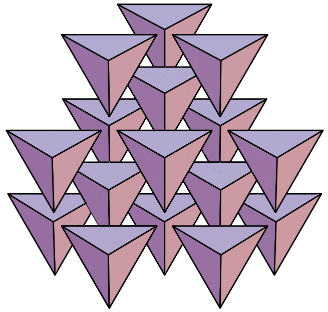
- **Conjecture 2:**

  *The optimal packing of any convex, congruent polyhedron without central symmetry is generally not a (Bravais) lattice packing.*

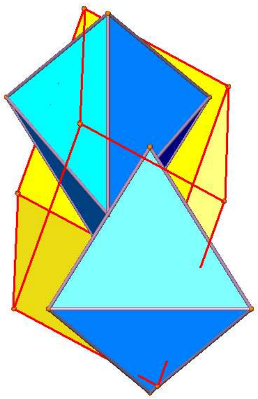
  **S. Torquato and Y. Jiao, Nature 2009; PRE 2009; PRE 2010.**

# Tetrahedron Packings

- **Regular tetrahedra cannot tile space.**
- **Densest lattice packing (Hoylman, 1970):** $\phi = 18/49 = 0.3673\ldots$

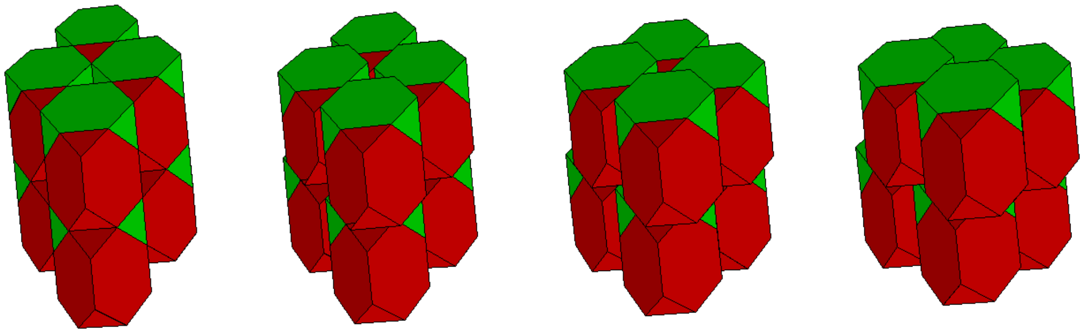


- **Densest packing must be a non-lattice (Conway & Torquato, 2006). Constructed a 20-particle packing with** $\phi \approx 0.72$
- **MRJ isostatic packings of tetrahedral dice (Chaikin et al., 2007):** $\phi \approx 0.74$
- **Many subsequent studies improved on this density with complicated fundamental cells (Chen, 2008; Torquato & Jiao, 2009; Haji-Akbari et. al. 2009).**
- **Recently, 3 different groups (Kallus et al. 2010; Torquato and Jiao 2010; and Chen et al. 2010) have found 4-particle packings with** $\phi \approx 0.86$**.**

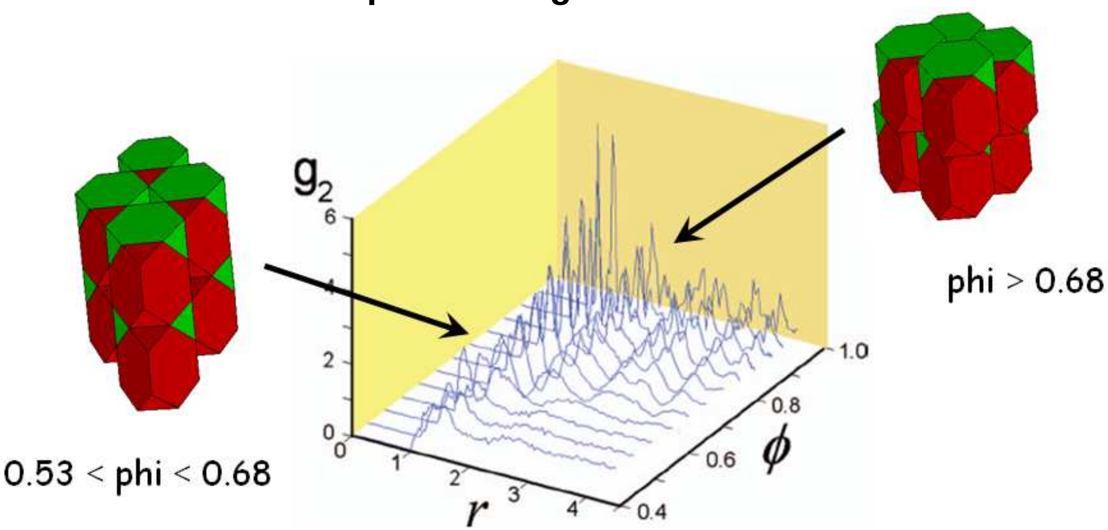


# Packings of Truncated Tetrahedra

- **The Archimedean truncated tetrahedron cannot tile space.**
- **Densest lattice packing (Betke & Henk, 2000):** $\phi = 207/304 = 0.680\ldots$
- **A dense non-lattice packing with a two-particle (dimer) basis was constructed by Conway and Torquato (2006) with** $\phi = 23/24 = 0.958\ldots$**.**



- **Derived analytically packing that nearly fills space:** $\phi = 207/208 = 0.995\ldots$**. Can be obtained by continuously deforming the Conway-Torquato packing. It has small tetrahedral holes and is a new tessellation of space with truncated tetrahedra and tetrahedra (Jiao & Torquato, 2011).**
- **Two-stage melting process: optimal packing is stable at high densities and the Conway-Torquato packing is stable at lower densities upon melting.**



# Another Organizing Principle

- **Conjecture 3:**

  *Optimal packings of congruent, centrally symmetric particles that do not possesses three equivalent principle axes generally cannot be a Bravais lattice.*

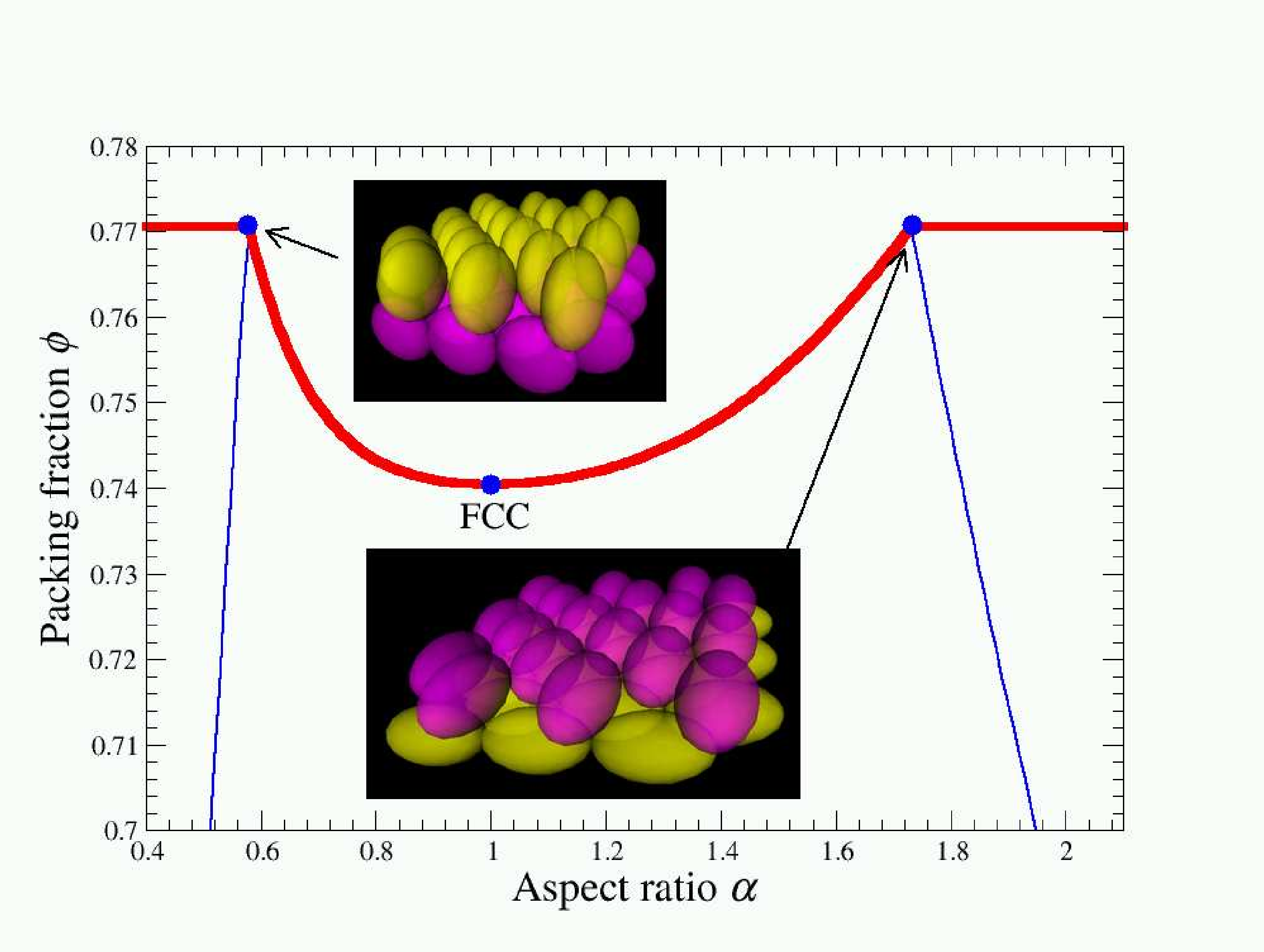
  **S. Torquato and Y. Jiao, Nature 2009; PRE 2009; PRE 2010.**

# Maximally Dense Ellipsoidal Packings

- **Densest known packings are non-Bravais lattices.**

  **Donev, Stillinger, Chaikin and Torquato, PRL, 2004.**

- **With relatively small asphericity, can achieve $\phi = 0.7707$.**



# Densest Known Packings of Some Convex Particles

**Table 1:** Densest Known Packings of Some Convex Particles

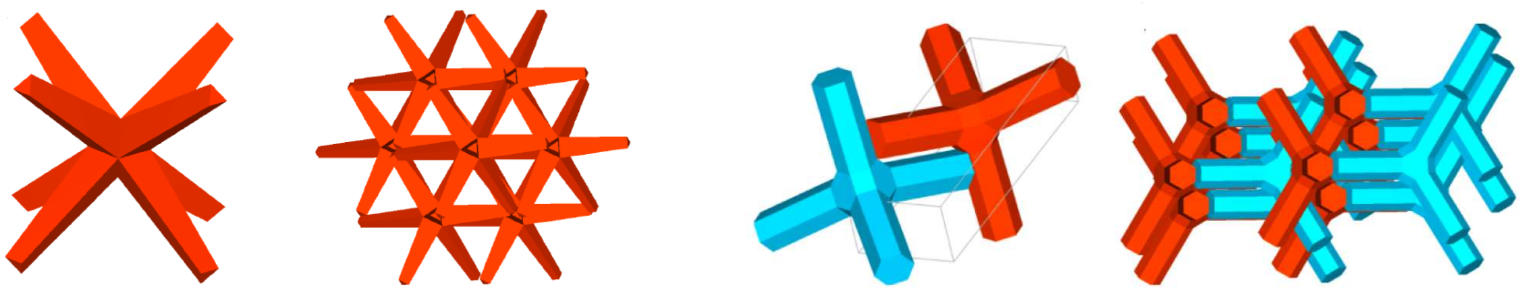
| Particle | Packing Density | Central Symmetry | Equivalent Axis | Structure |
|---|---|---|---|---|
| Sphere | 0.740 | Y | Y | Bravais Lattice |
| Ellipsoid | 0.740 - 0.770 | Y | N | Periodic, 2-particle basis |
| Superball | 0.740 - 1 | Y | Y | Bravais Lattice |
| Tetrahedron | 0.856 | N | Y | Periodic, 4-particle basis |
| Icosahedron | 0.836 | Y | Y | Bravais Lattice |
| Dodecahedron | 0.904 | Y | Y | Bravais Lattice |
| Octahedron | 0.945 | Y | Y | Bravais Lattice |
| Trun. Tetrah. | 0.995 | N | Y | Periodic, 2-particle basis |
| Cube | 1 | Y | Y | Bravais Lattice |

# Generalizations of the Organizing Principles to Concave Particles

**Torquato and Jiao, PRE, 2010.**

- **Generalization of Conjecture 1:**
  *Dense packings of centrally symmetric concave, congruent polyhedra with three equivalent axes are given by their corresponding densest lattice packings, providing a tight density lower bound that may be optimal.*

- **Generalization of Conjecture 2:**
  *Dense packings of concave, congruent polyhedra without central symmetry are composed of centrally symmetric compound units of the polyhedra with the inversion-symmetric points lying on the densest lattice associated with the compound units, providing a tight density lower bound that may be optimal.*



**(a)** **(b)**

**Figure 1:** **(a) Centrally symmetric concave octapod and the associated optimal Bravais-lattice packing. (b) Concave tetrapods without center symmetry forming a centrally symmetric dimer, which then pack on a Bravais lattice [de Graaf et al, Phys. Rev. Lett. 107, 155501 (2011)].**

# Nonspherical Particles and Rotational Degrees of Freedom

- **Isostatic (Isoconstrained): Total number of contacts (constraints) equals total number of degrees of freedom. Conventionally, thought to be associated minimal number of constraints for rigidity and random (generic) packings.**

$$Z = 2f$$

**Z: average no. of contacts/particle; f: degrees of freedom/particle** $f = 2$ **for disks,** $f = 3$ **for ellipses,** $f = 3$ **for spheres,** $f = 5$ **for spheroids, and** $f = 6$ **for general ellipsoids.**

- **Hypostatic:**

$$Z \leq 2f$$

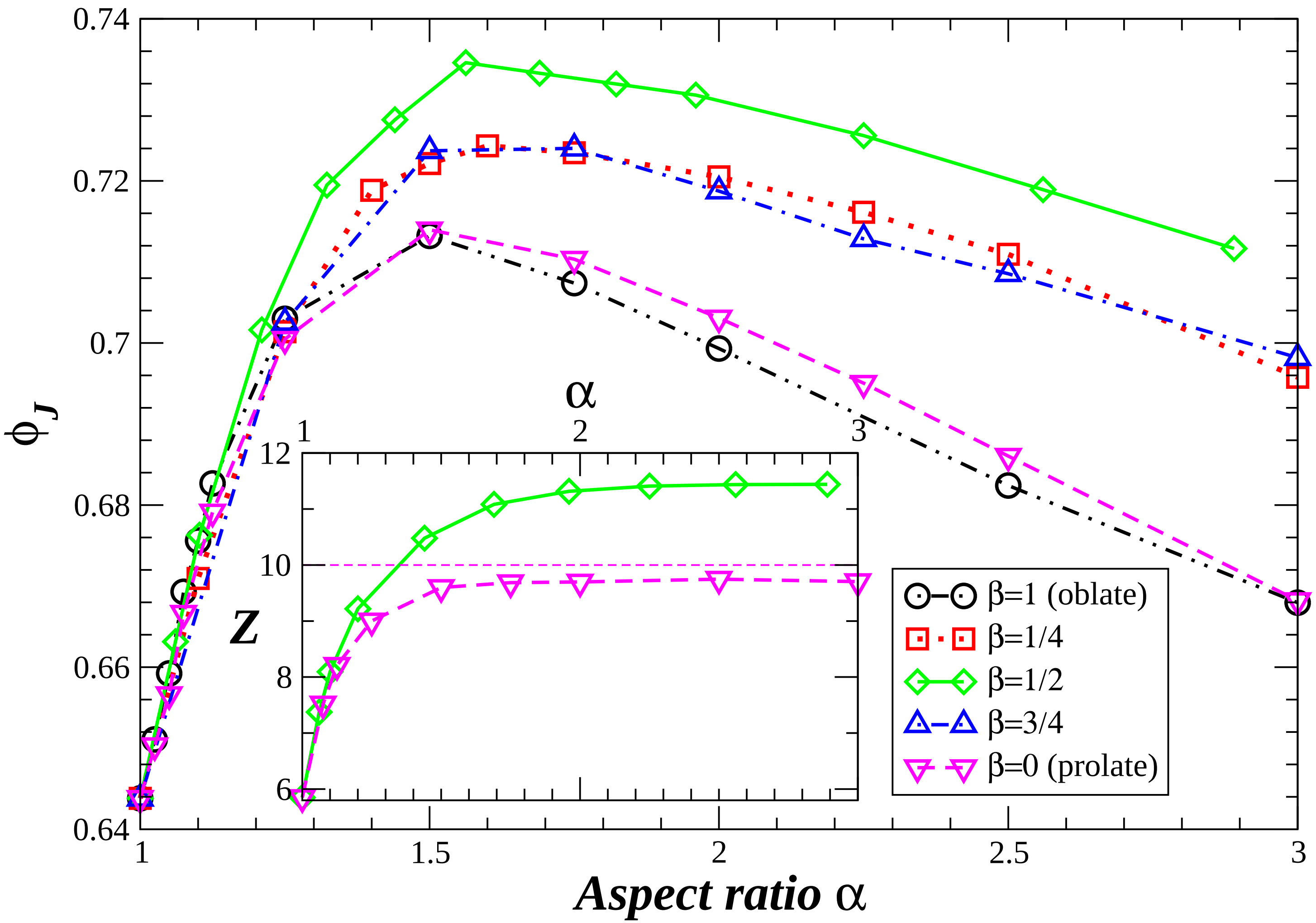
**Conventionally thought to be unstable.**

- **Hyperstatic:**

$$Z \geq 2f$$

**True of ordered packings.**

# MRJ Ellipsoidal Packings

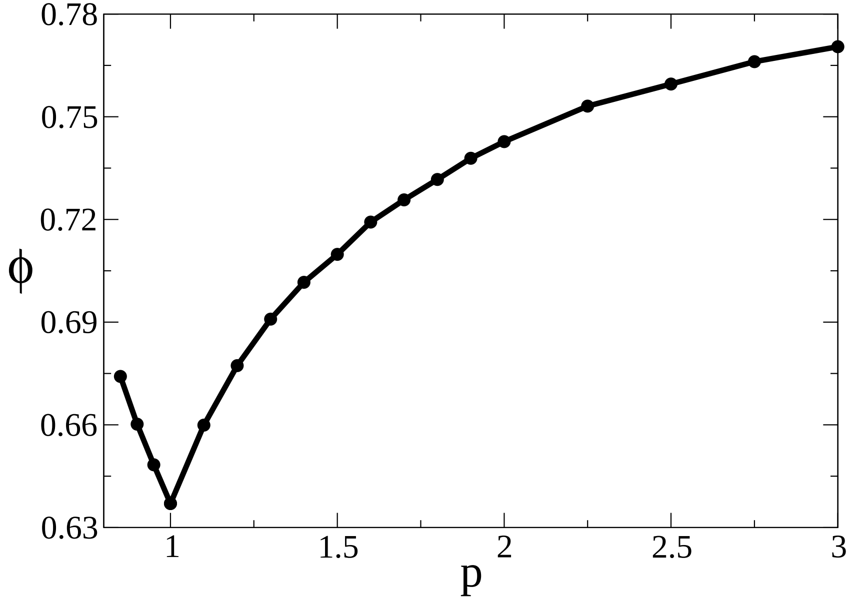


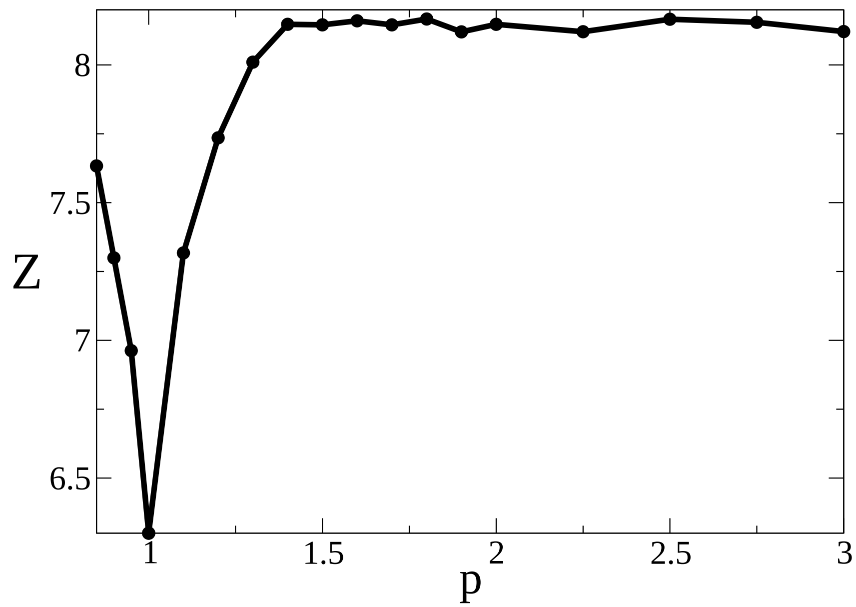

- **There is a competition between translational & rotational jamming.**
- **Rotational degrees of freedom lead to improved density (over spheres) and allows for correlated contacts, which leads to MRJ hypostatic jammed packings.**

**Donev, Connelly, Stillinger & Torquato, PRE (2007)**

# MRJ Superball Packings

**Jiao, Stillinger & Torquato (2009)**



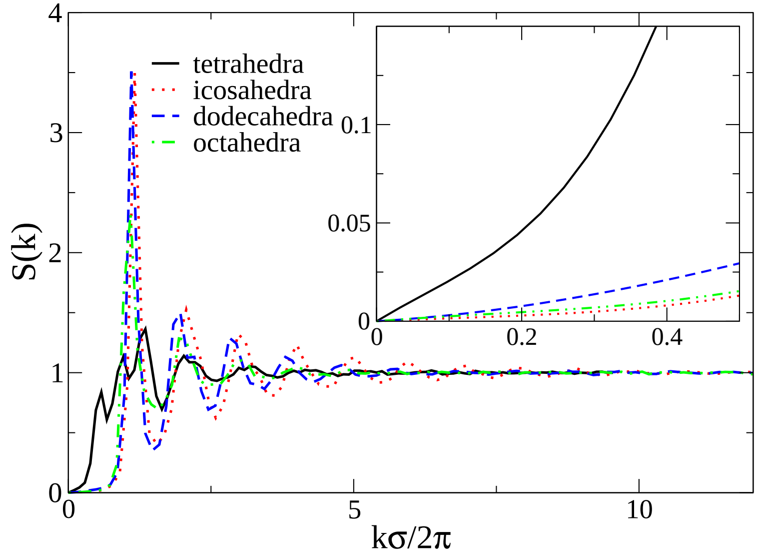




- **Packing density increases monotonically as $p$ deviates from 1.**
- **Disordered superball packings are always hypostatic and do not come close to the isostatic contact number as asphericity increases!**
- **Isostatic disordered superball packings are difficult to construct; they require $Z = 12$, which is associated with crystal packings.**

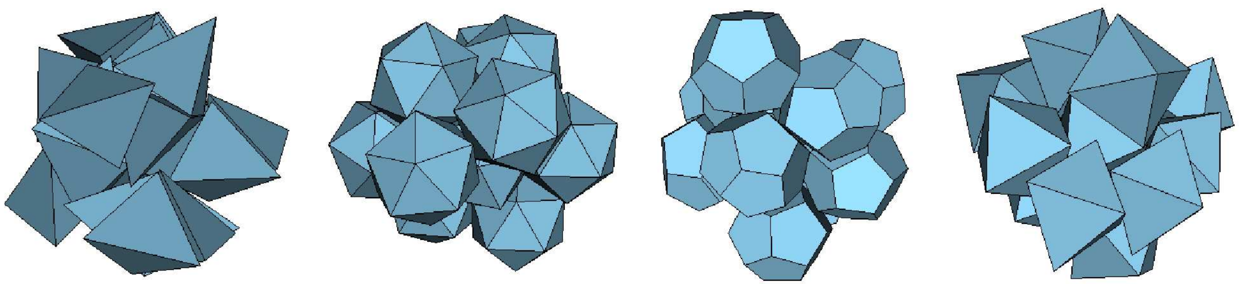
# MRJ Packings of Nontiling Platonic Solids

Jiao & Torquato, PRE (2011)

- **Hyperuniform with quasi-long-rang (QLR) pair correlations ($1/r^4$) and isostatic.**




**(a)**



**(b)**

**Figure 2:** **(a) Structure factor $S(k)$ of the MRJ packings of the nontiling Platonic solids. The inset shows that $S(k)$ is linear in $k$ for small $k$ values. (b) Local contacting configurations: from left to right, tetrahedra, icosahedra, dodecahedra, and octahedra.**

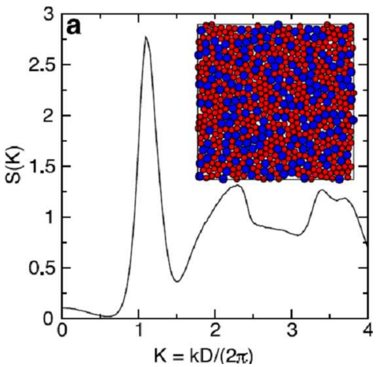
# MRJ Packings of Nontiling Platonic Solids

**Table 2:** **Characteristics of MRJ packings of hard particles with different shapes.**

| Particle Shape | Isostatic | Hyperuniform QLR | MRJ Packing Fraction |
|---|---|---|---|
| Sphere | Yes | Yes | **0.642** |
| Ellipsoid | No (hypostatic) | Yes | $0.642 - 0.720$ |
| Superball | No (hypostatic) | Yes | $0.642 - 0.674$ |
| Superellipsoid | No (hypostatic) | Yes | $0.642 - 0.758$ |
| Octahedron | Yes | Yes | $0.697$ |
| Icosahedron | Yes | Yes | $0.707$ |
| Dodecahedron | Yes | Yes | $0.716$ |
| Tetrahedron | Yes | Yes | $0.763$ |

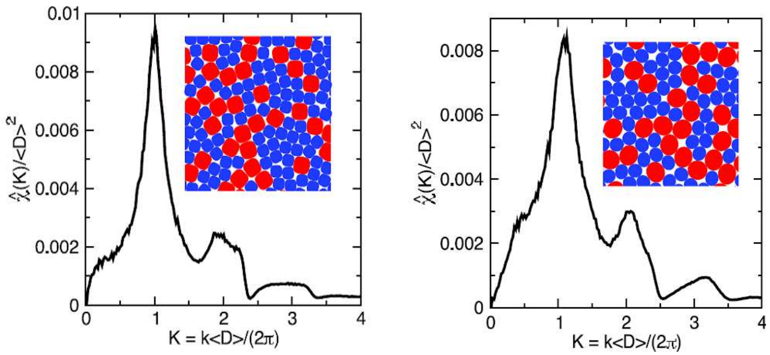
# Generalization of Hyperuniformity to Polydisperse Systems

- **Structure factor of the MRJ packing of polydisperse particles does not vanish at $k = 0$ (Kurita & Weeks, PRE 2010; Berthier et al., PRL 2011; Zachary, Jiao, & Torquato, PRL 2011).**




- **Introduced a more general notion of hyperuniformity involving local-volume-fraction fluctuations and associated spectral function $\tilde{\chi}(k)$ for general two-phase media (packings or not) (Zachary & Torquato, J. Stat. Mech. 2009).**

- **We have shown that MRJ packings of hard-particles are hyperuniform with QLR correlations (i.e., $\tilde{\chi}(k) \rightarrow 0$ as $k \rightarrow 0$), regardless of the particle shapes or relative sizes (Zachary, Jiao & Torquato, PRL 2011; PRE 2011).**



# CONCLUSIONS

- **Non-spherical particles are not created equal! Changing the shape of a particle can dramatically alter its packing attributes.**
- **We now have some organizing principles for both maximally dense and MRJ packings of nonspherical particles.**
- **Tunability capability via particle shape could be used to tailor many-particle systems (e.g., colloids and granular media) to have designed crystal, liquid and glassy states.**

**Collaborators**

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