Density of Binary Disc Packings

Thomas Fernique
CNRS & Univ. Paris 13

Sphere packings

Sphere packing: interior disjoint unit spheres.
Density: limsup of the proportion of $B(0, r)$ covered.
Questions: maximum density? densest packings?

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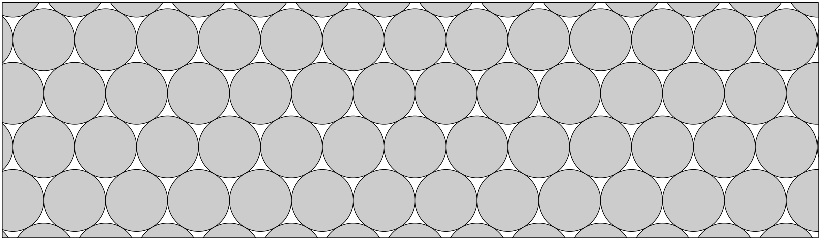
Theorem (Toth, 1943)

The maximum density of sphere packings in $\mathbb{R}^2$ *is* $\frac{\pi}{2\sqrt{3}} \approx 0.9069$.



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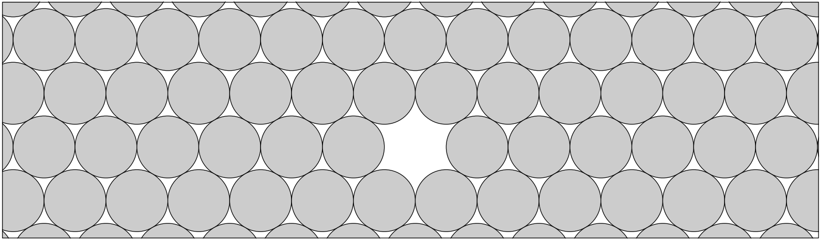

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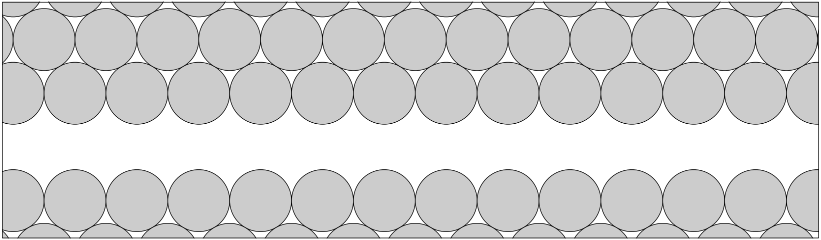

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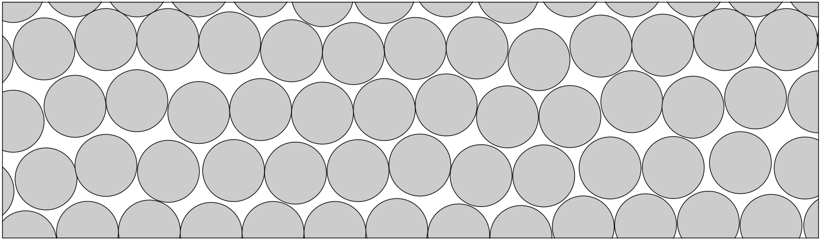

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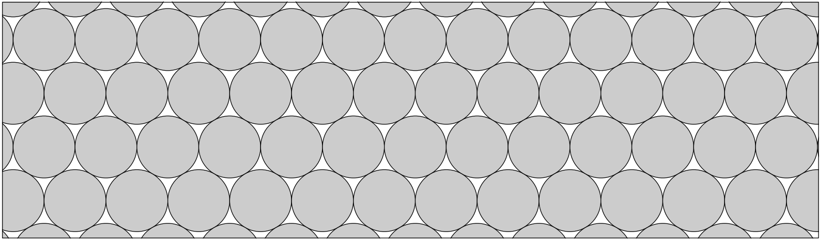

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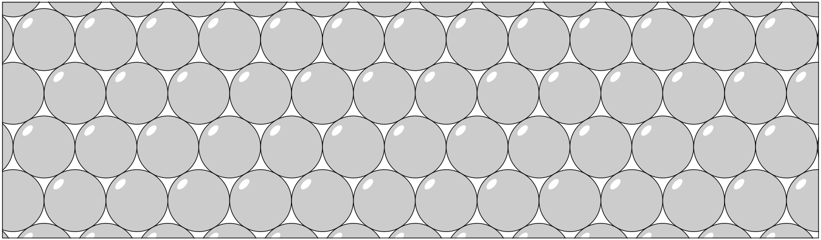
Theorem (Hales, 1998)

The maximum density of sphere packings in $\mathbb{R}^3$ is $\frac{\pi}{3\sqrt{2}} \approx 0.7404$.



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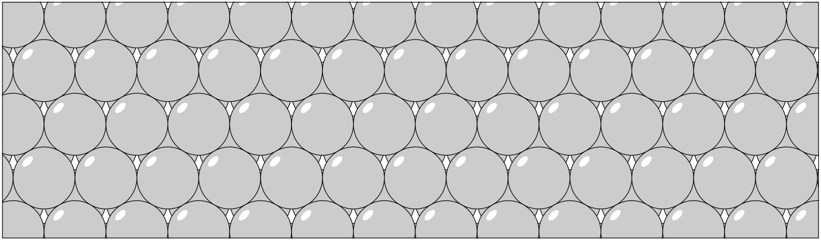

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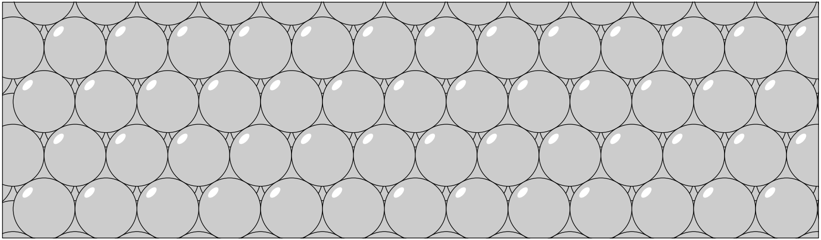

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Theorem (Vyazovska, 2017)

The maximum density of sphere packings in $\mathbb{R}^8$ is $\frac{\pi^4}{384} \approx 0.2536$.

It is reached for spheres centered on the E_8 lattice.

Sphere packings

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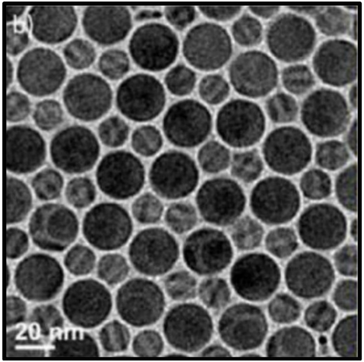
Theorem (Vyazovska *et al., 2017)*

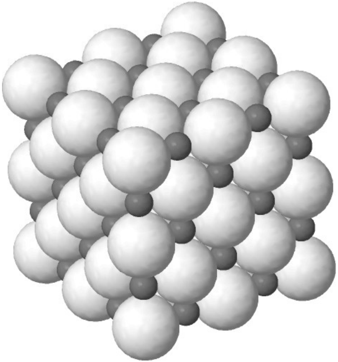
The maximum density of sphere packings in $\mathbb{R}^{24}$ *is* $\frac{\pi^{12}}{12!} \approx 0.0019$.

It is reached for spheres centered on the Leech lattice.

Unequal sphere packings

The density becomes parametrized by the ratios of sphere sizes.
Natural problem in materials science!





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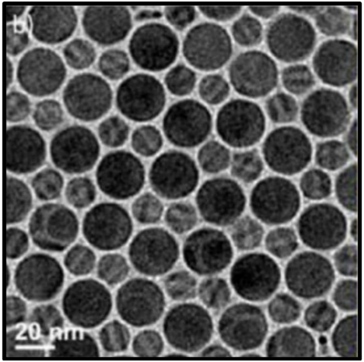
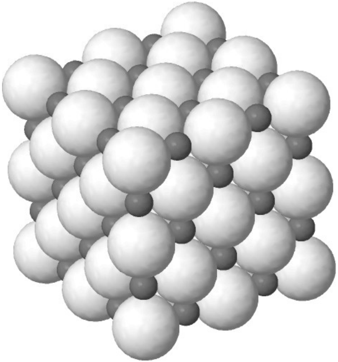
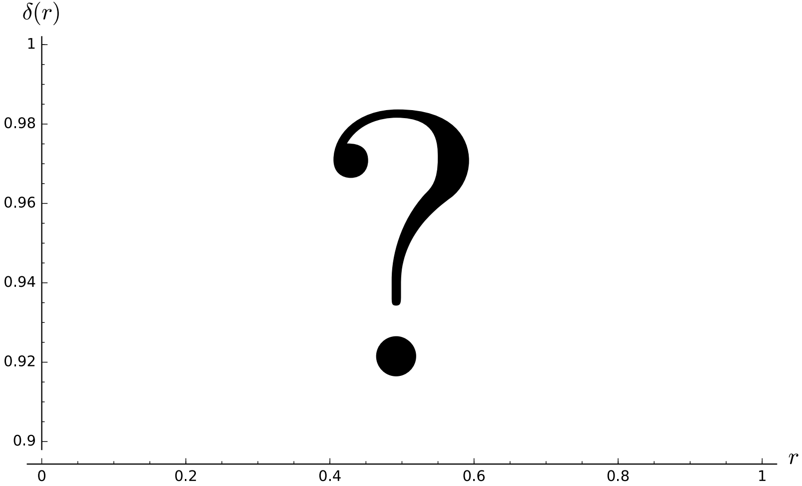




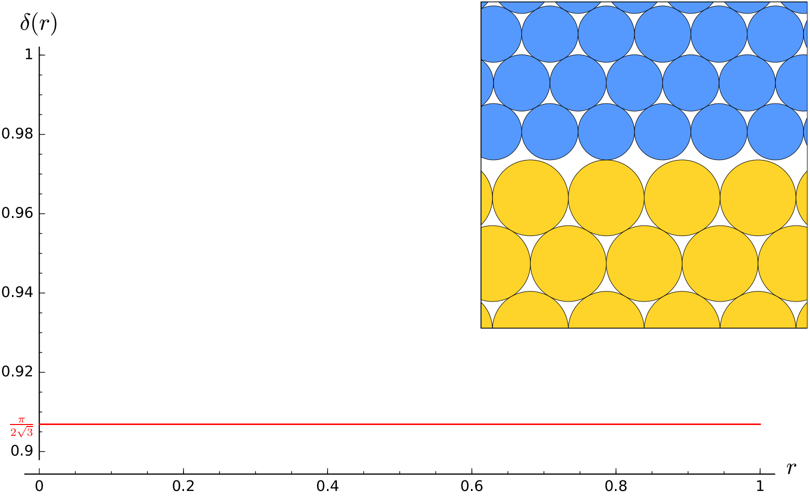
Simplest non-trivial case: two discs in $\mathbb{R}^2$, *i.e.*, binary disc packings.

Density of binary disc packings



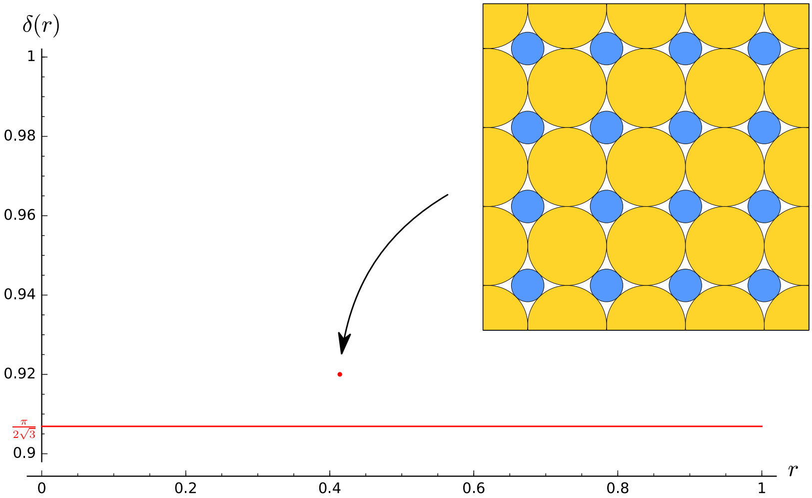
The maximum density is a function $\delta(r)$ of the ratio $r \in (0, 1)$.

Lower bounds



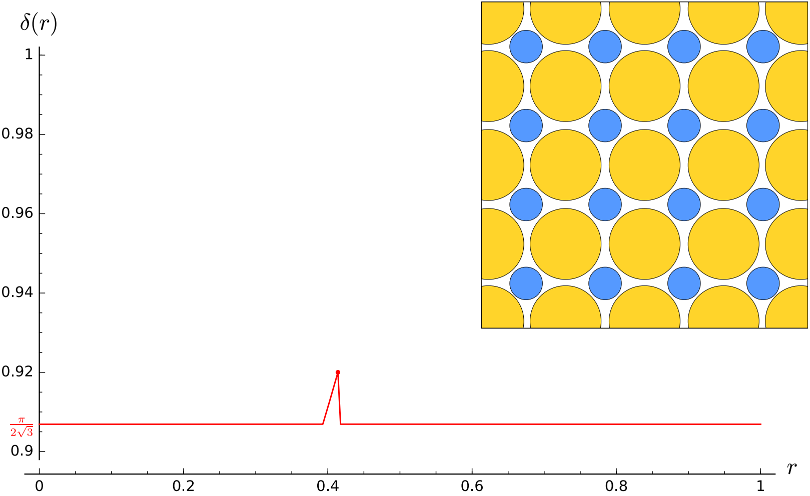
The hexagonal compact packing yields a uniform lower bound.

Lower bounds



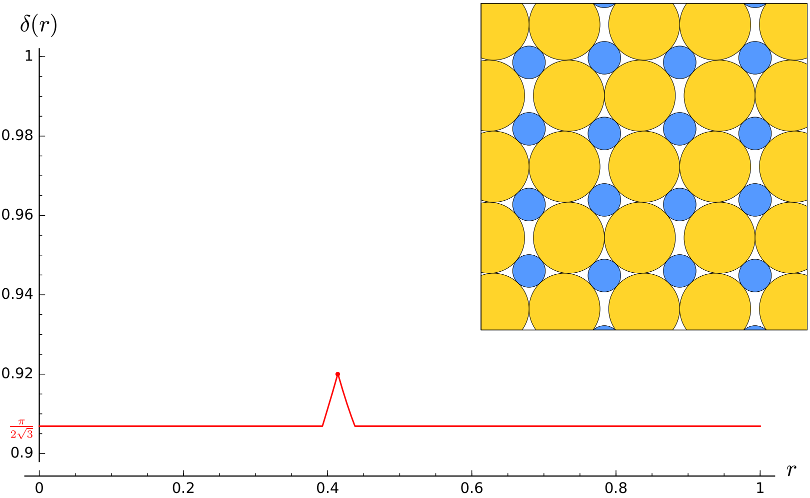
Any given packing yields a lower bound for a specific r.

Lower bounds



It can be extended over a neighborhood of r (more or less cleverly).

Lower bounds



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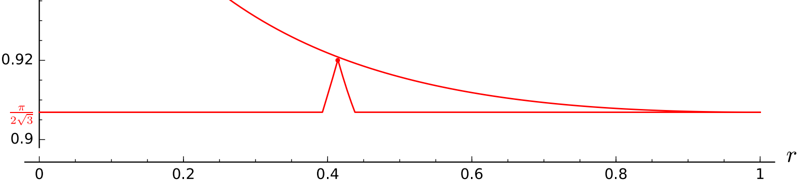
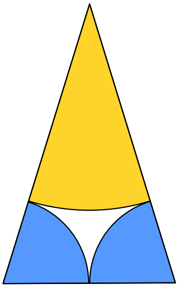
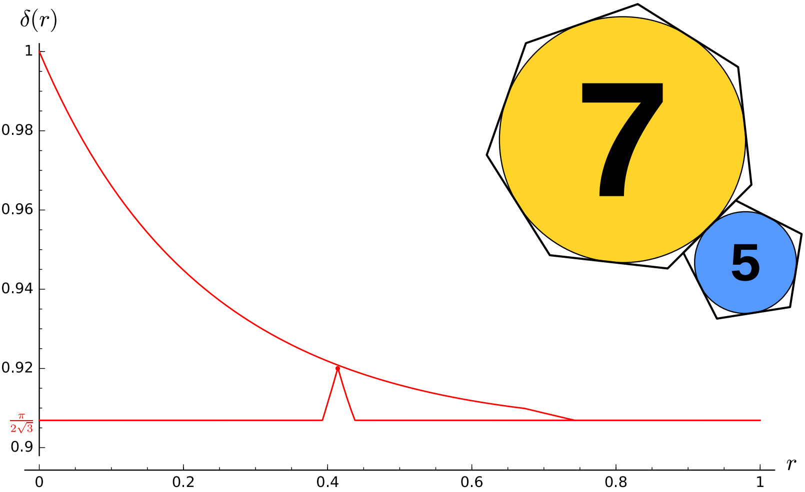
Upper bounds





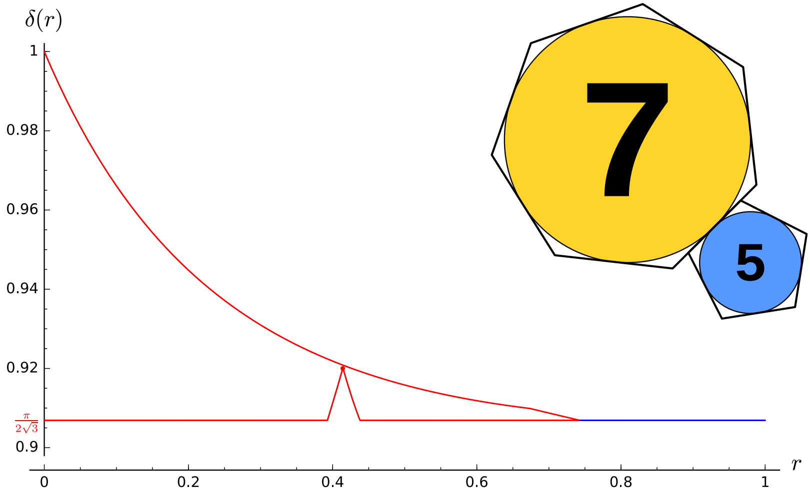
First upper bound by Florian in 1960.

Upper bounds



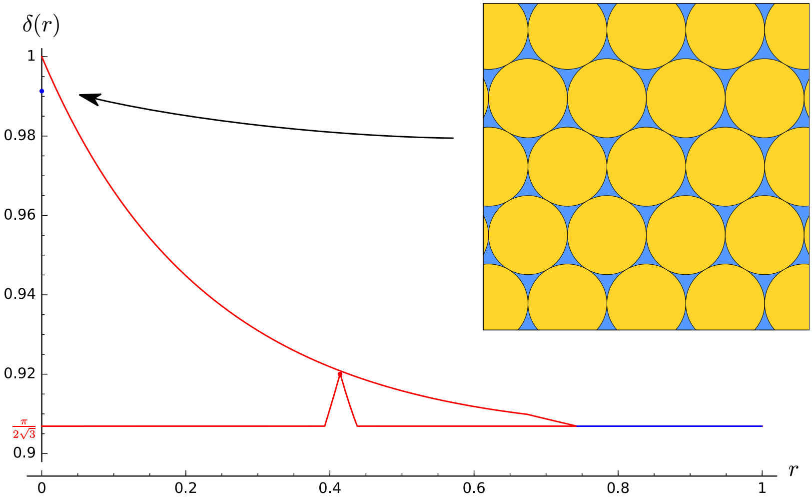
First upper bound by Florian in 1960. Improved by Blind in 1969.

Tight bounds



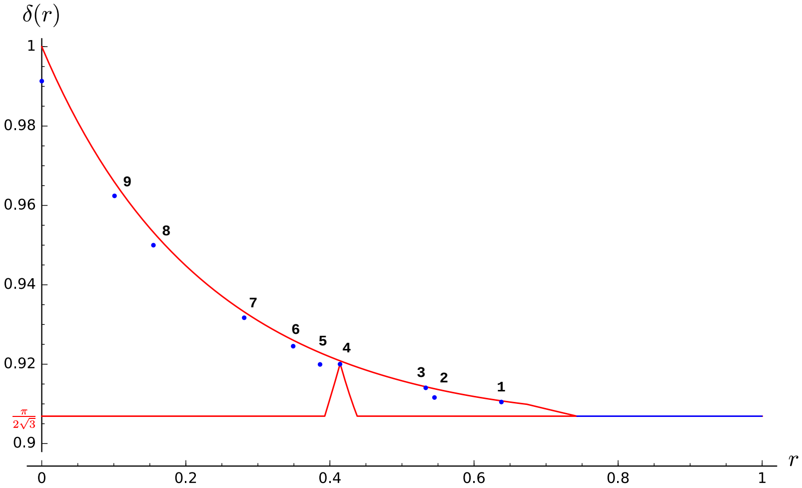
Blind's bound is tight for $r \geq \sqrt{\frac{7\tan(\pi/7)-6\tan(\pi/6)}{6\tan(\pi/6)-5\tan(\pi/5)}} \approx 0.743$

Tight bounds



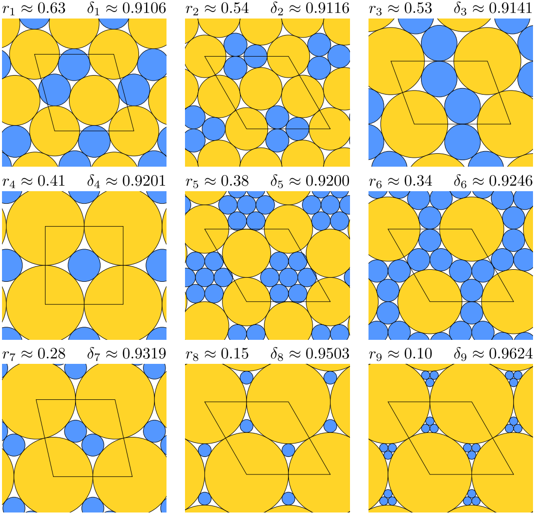
On the other side: $\lim_{r \to 0} \delta(r) = \frac{\pi}{2\sqrt{3}} + \left(1 - \frac{\pi}{2\sqrt{3}}\right) \frac{\pi}{2\sqrt{3}} \simeq 0.9913$

Tight bounds



The exact maximum density is also known for 9 "magic" ratios!

Compact packings

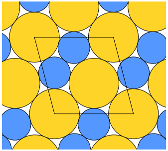


Theorem (Heppes'00, Heppes'03, Kennedy'04, Bédaride-F.'20)

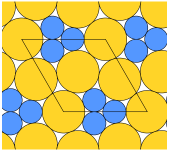
These periodic binary disc packings have maximum density.

Compact packings

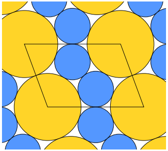
$r_1 \approx 0.63 \quad \delta_1 \approx 0.9106$



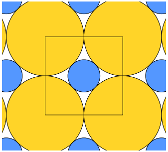
$r_2 \approx 0.54 \quad \delta_2 \approx 0.9116$



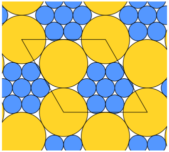
$r_3 \approx 0.53 \quad \delta_3 \approx 0.9141$



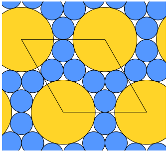
$r_4 \approx 0.41 \quad \delta_4 \approx 0.9201$



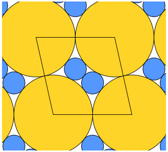
$r_5 \approx 0.38 \quad \delta_5 \approx 0.9200$



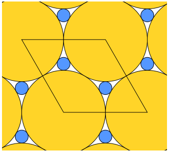
$r_6 \approx 0.34 \quad \delta_6 \approx 0.9246$



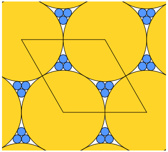
$r_7 \approx 0.28 \quad \delta_7 \approx 0.9319$



$r_8 \approx 0.15 \quad \delta_8 \approx 0.9503$



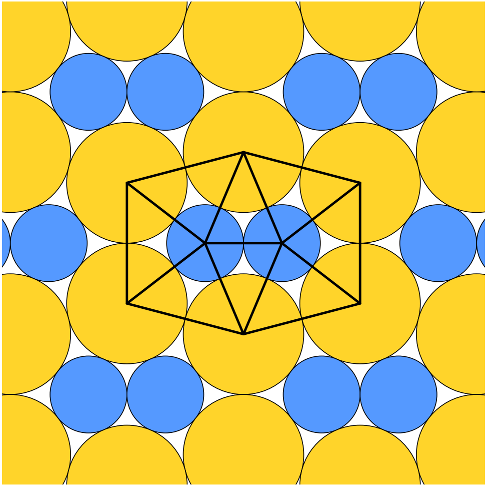
$r_9 \approx 0.10 \quad \delta_9 \approx 0.9624$



Theorem (Kennedy, 2006)

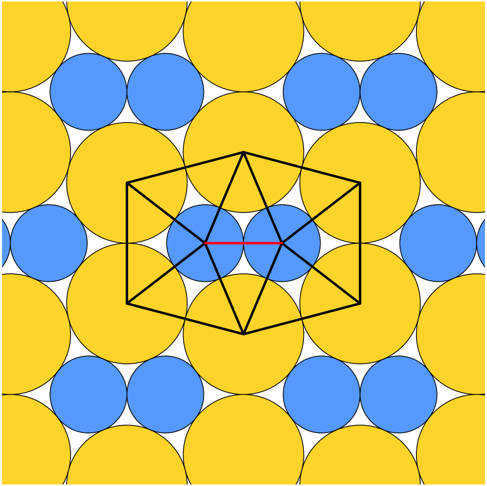
The ratios are those that allow for a triangulated contact graph.

Flipping and flowing



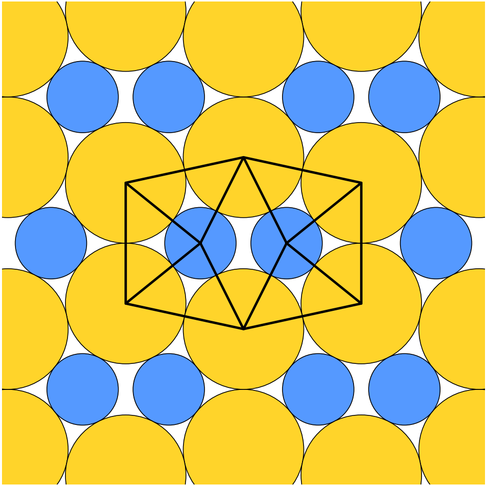
The disc ratio of a compact packing is determined by the contacts.

Flipping and flowing



Allowing some discs to separate may give a degree of freedom. . .

Flipping and flowing



. . . that can be used to vary continuously the ratio. . .

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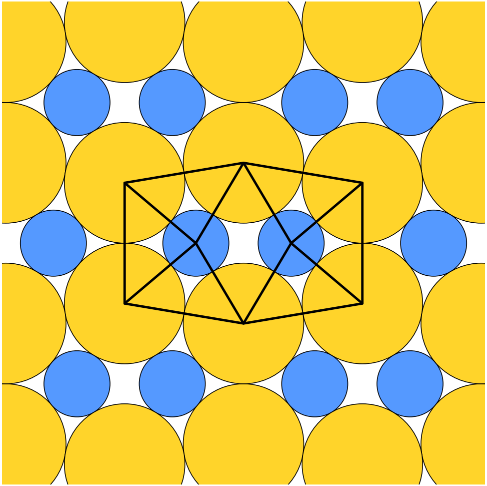

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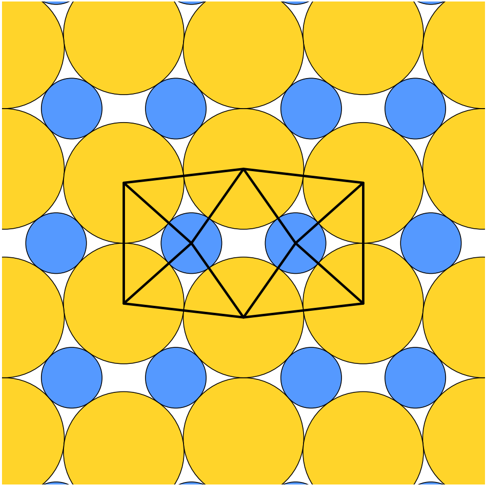

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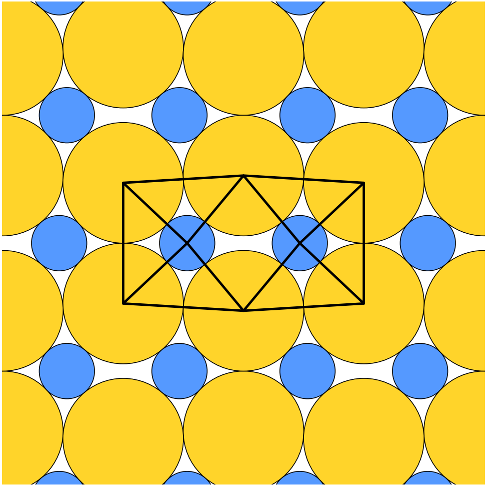

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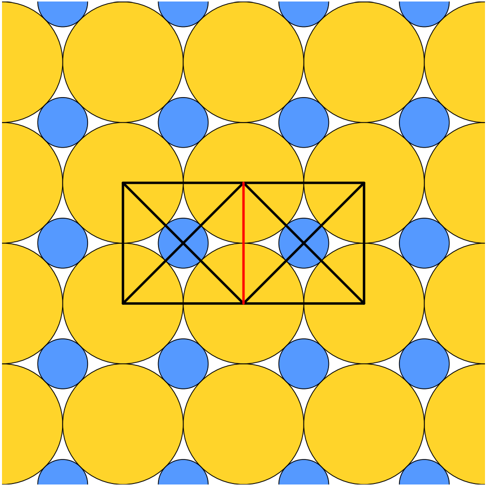
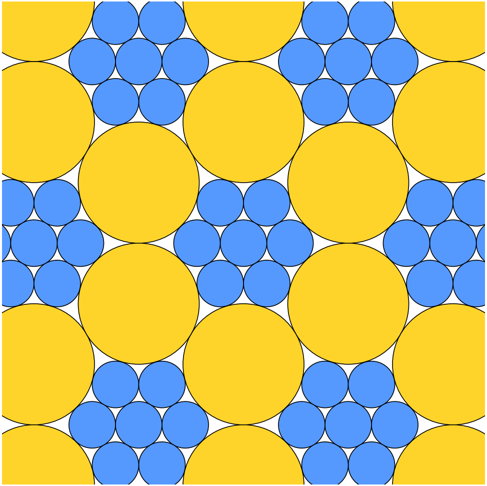


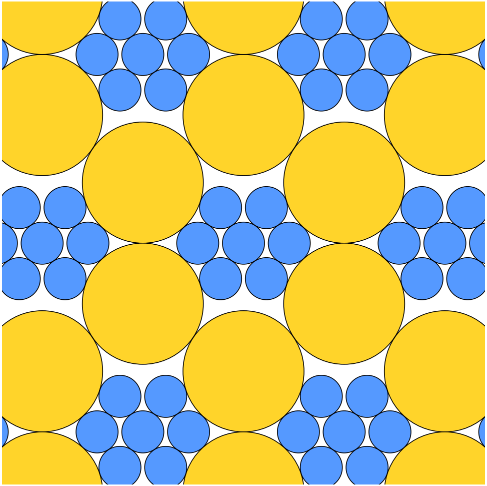
...until it is blocked by new contacts.

Flipping and flowing



Some cases may be tricky: how many (which) contacts to keep?

Flipping and flowing



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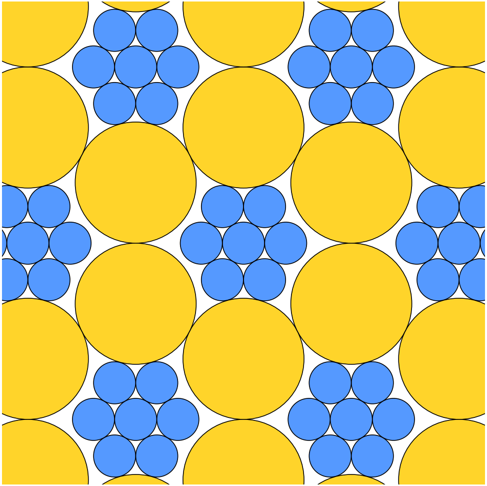

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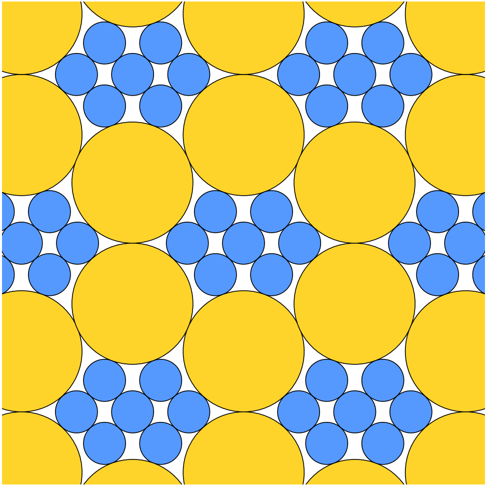

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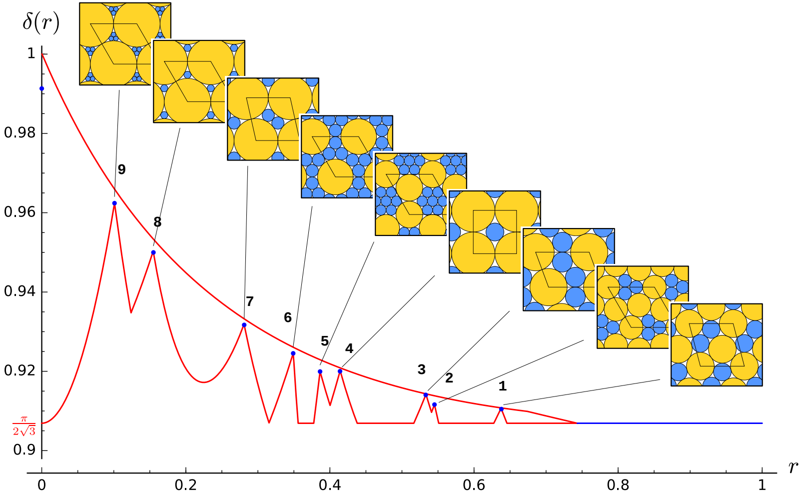
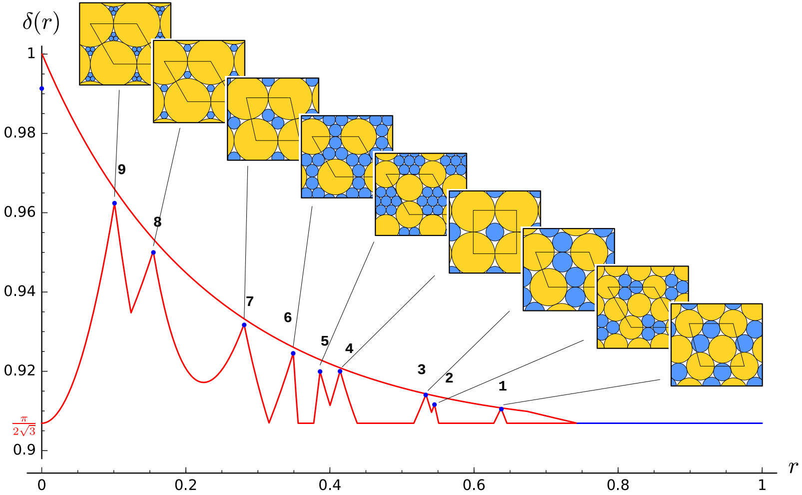
Lower bounds reloaded



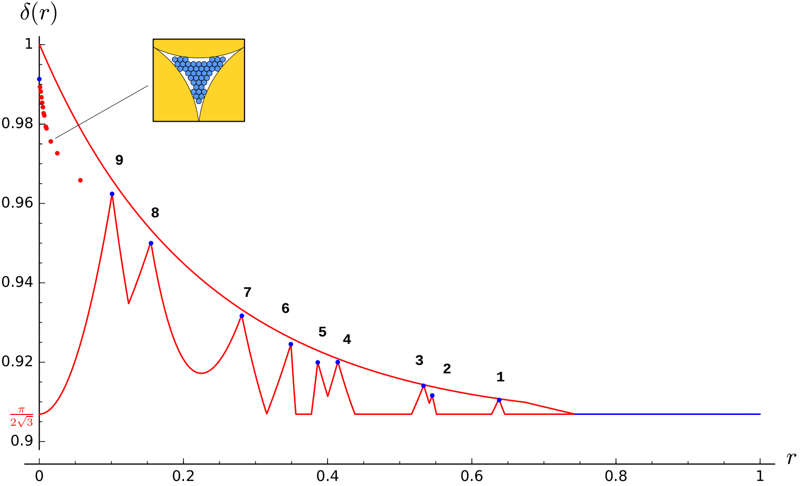
Flipping and flowing greatly improves the lower bound.

Lower bounds reloaded



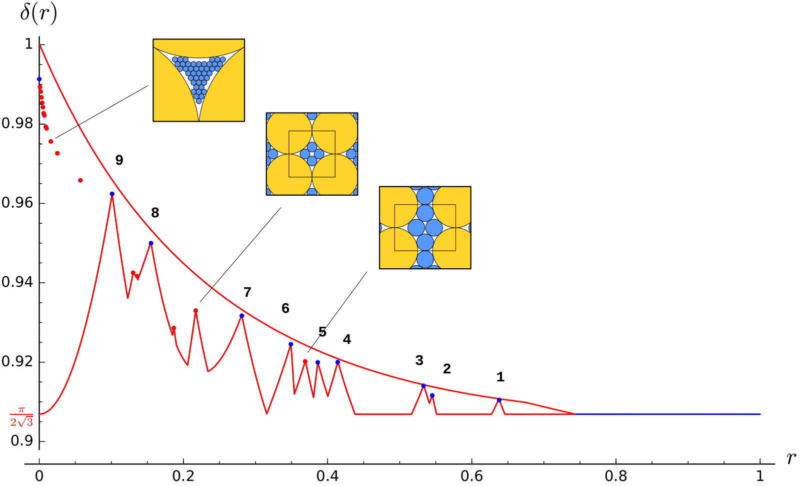
Flipping and flowing greatly improves the lower bound. Is it tight?

Other dense packings



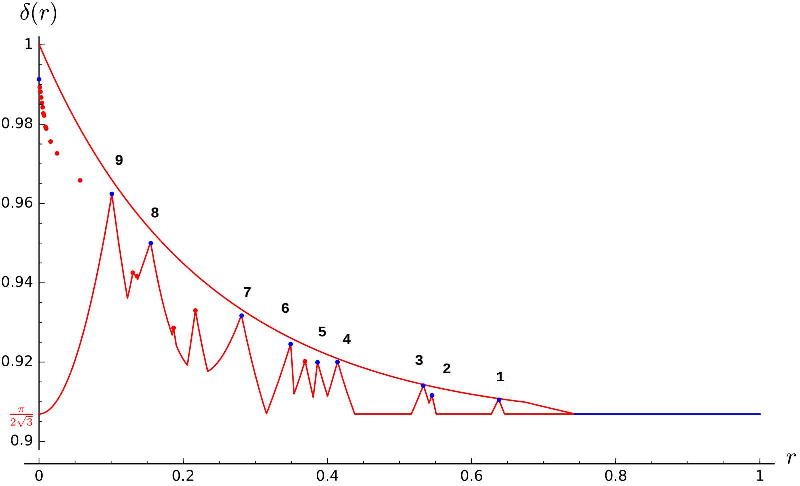
For small ratio, there are many dense packings.

Other dense packings



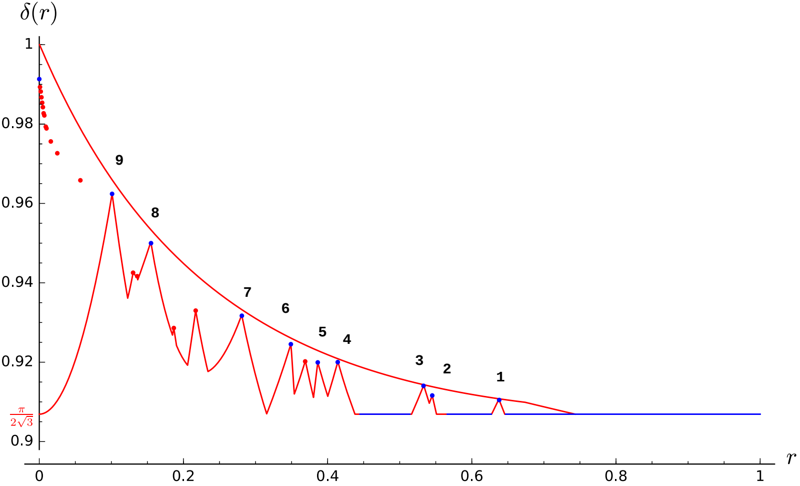
But they seem to become more sparse as the ratio grows.

Phase separation



Can we at least do better than the hexagonal compact packing?

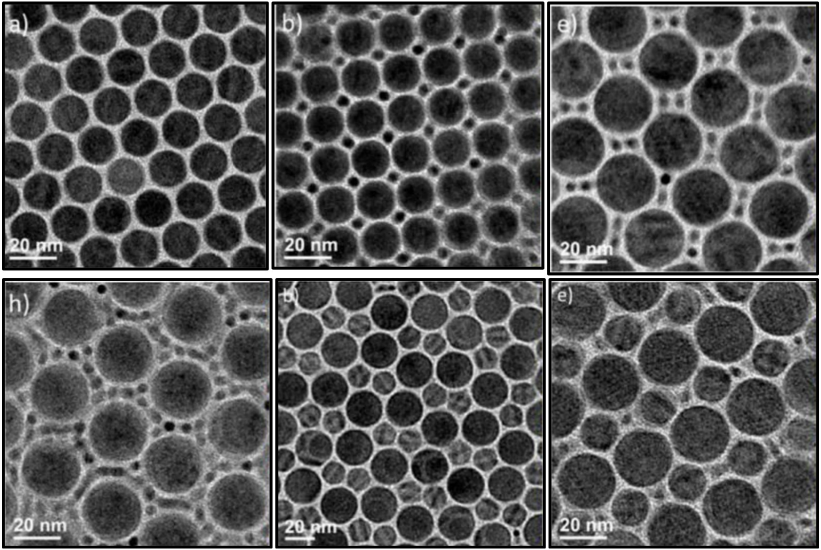
Phase separation



Theorem (F., to be improved)

For $r \in [0.445, 0.514] \cup [0.566, 0.627] \cup [0.647, 1)$, $\delta(r) = \frac{\pi}{2\sqrt{3}}$.

Back to materials science



T. Paik, B. Diroll, C. Kagan, Ch. Murray J. Am. Chem. Soc. **137**, 2015.
Binary and ternary superlattices self-assembled from colloidal nanodisks and nanorods.

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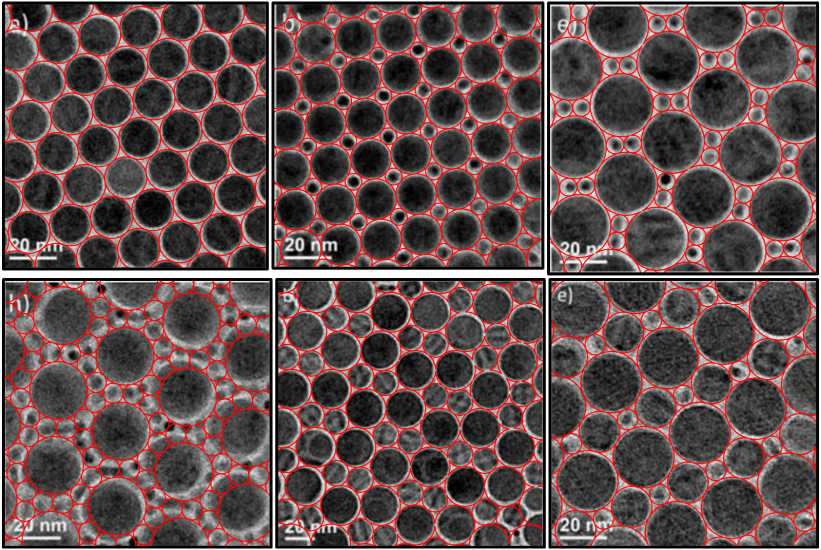

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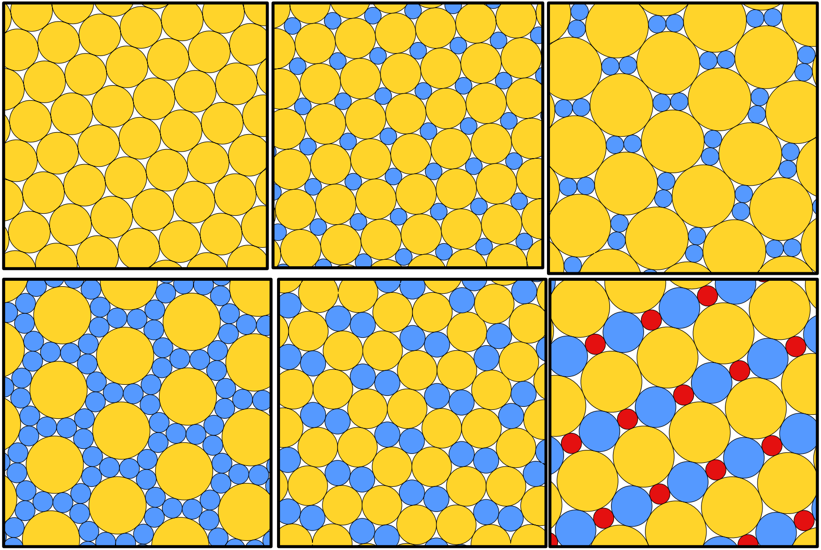

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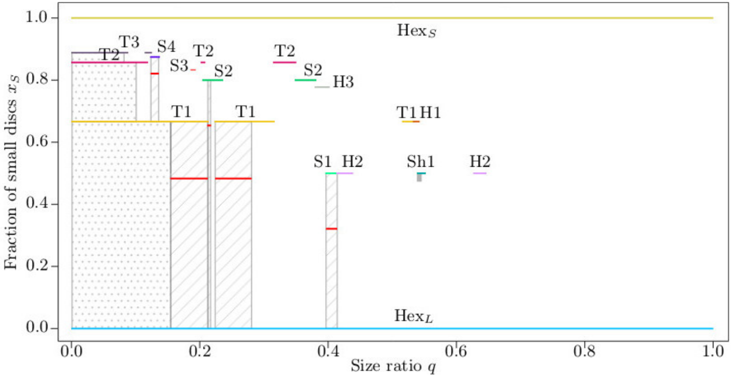
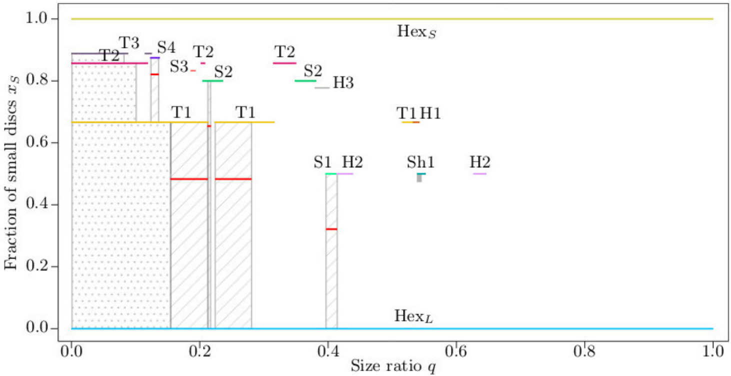
Phase diagram



E. Fayen, A. Jagannathan, G. Foffi, F. Smallenburg J. Chem. Phys. **152**, 2020.
Infinite-pressure phase diagram of binary mixtures of (non)additive hard disks.

Phase diagram

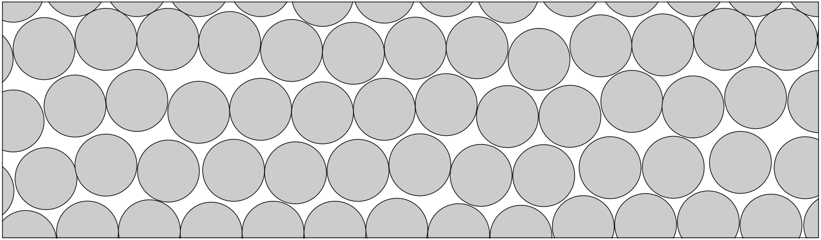


E. Fayen, A. Jagannathan, G. Foffi, F. Smallenburg J. Chem. Phys. **152**, 2020.
Infinite-pressure phase diagram of binary mixtures of (non)additive hard disks.

- Based on intensive Monte-Carlo simulations;
- The concept of "phase" needs to be formalized.

Equivalent disc packings

There is always infinitely many packings with the same density.



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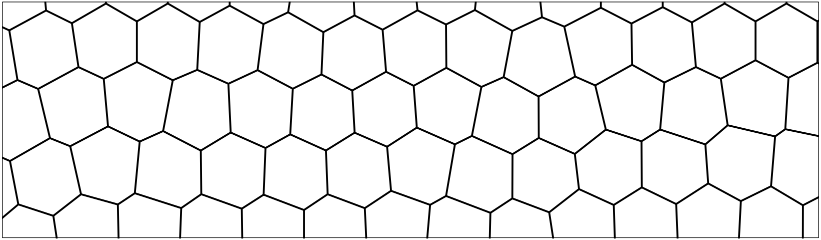

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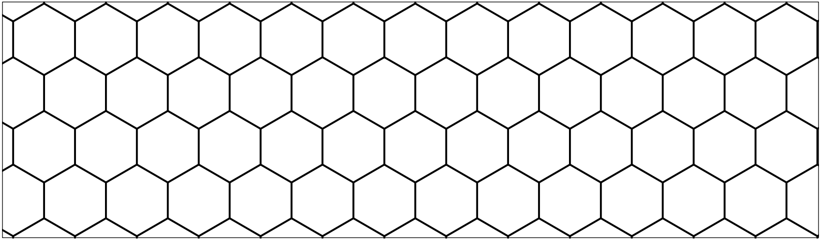

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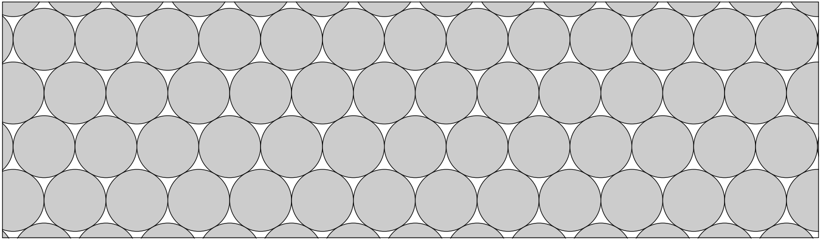

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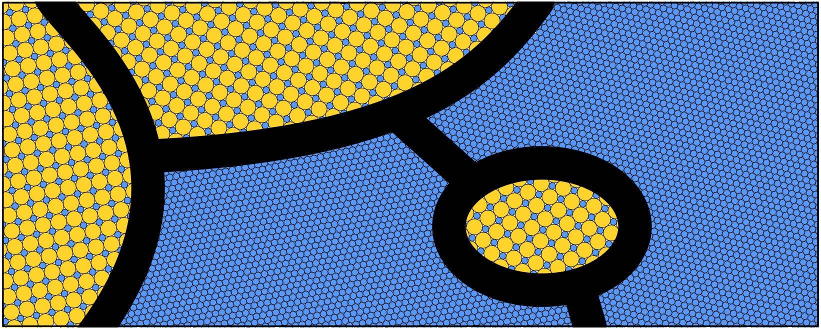
Playing with stoichiometry for $r = \sqrt{2} - 1$



Theorem (F. 2020)

The densest disc packings with a proportion x of large discs are:

- twinnings *of two periodic packings for* $x \leq 0.5$*;*

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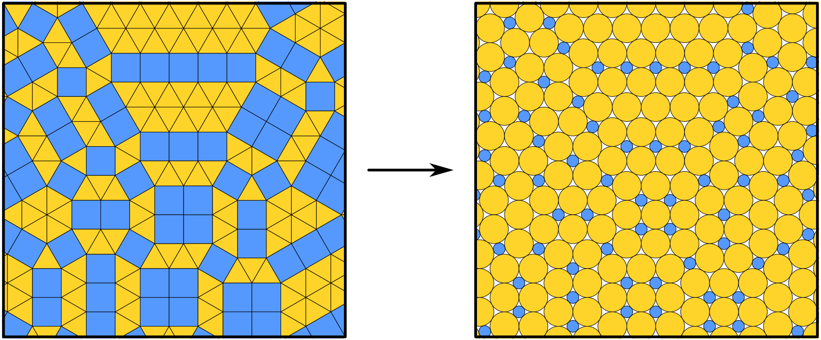

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- *recodings of* square-triangle tilings *for $x \geq 0.5$.*

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The overall density is bounded by checking inequalities over a **compact** set of triangles using **computer interval arithmetic**.