UNIVERSITY OF LIVERPOOL

LEVERHULME TRUST

The Leverhulme Research Centre for Functional Materials Design

Symmetries of maximally dense plane group packings of regular convex polygons.

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diamond

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- M. Torda, J. Y. Goulermas, V. Kurlin and G. M. Day, *Densest plane group packings of regular polygons*, Physical Review E **106** (5), 054603 (2022).

Crystal Structure Prediction (CSP)
motivation

- An approach to accelerate Molecular CSP solvers:
  - Energy minimization $\rightarrow$ Geometric packing density maximization

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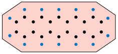

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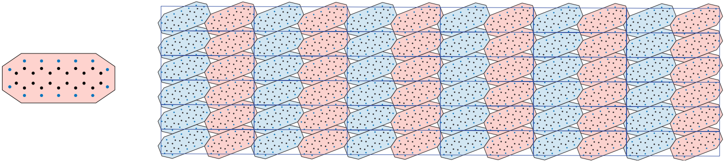

(Left) A geometric representation of pentacene as the convex hull of the atomic positions of the molecule with an offset given by hydrogen's van der Waals radius of 1.09Å. The dots symbolize atomic positions of (blue) hydrogen and (black) carbon. (Right) Visualization of the ETRPA output configuration of the densest $p2$-packing of the pentacene representation with density of 0.9533821 and resembles the configuration of single layer pentacene thin-film on graphite surface found in *W. Chen, H. Huang, A. Thye, and S. Wee, Molecular orientation transition of organic thin films on graphite: the effect of intermolecular electrostatic and interfacial dispersion forces, Chemical communications, (2008), pp. 4276–4278.*

Crystallographic Symmetry Group (CSG) packing

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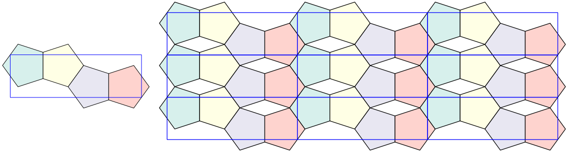
- CSG packing

$$\mathcal{K}_G = \bigcup_{g \in G} gK,$$

$$\operatorname{int}(g_i K) \cap \operatorname{int}(g_j K) = \emptyset, \quad \forall\, g_i,\ g_j \in G,\ \ g_i \neq g_j$$

  - G - CSG
  - K - Compact subset of $\mathbb{R}^n$



The 2D periodic structure with the *p2mg* plane group symmetry where K is a regular convex pentagon with the packing density of approximately 0.8541019. (Left) A single primitive cell. (Right) 9 primitive cells. The blue parallelogram denotes the primitive cell of the respective configuration. Colors represent symmetry operations modulo lattice translations.

CSG packing problem

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$$\mathcal{K}_{\max} = \underset{\mathcal{K}_G : G \in \mathcal{G}}{\operatorname{argmax}} \, \rho\left(\mathcal{K}_G\right), \; \mathcal{G} = \{H | H \cong G\}.$$

  - $\rho\left(\mathcal{K}_G\right) = \frac{N \mathrm{area}(K)}{\det(\mathbf{U})}$ - 2D packing density.
    - $\mathbf{U}$ - Unit cell.
    - N - number of symmetry operation modulo lattice translations.

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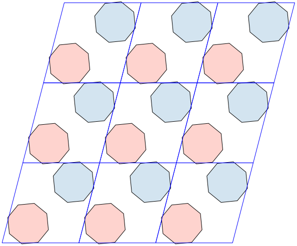

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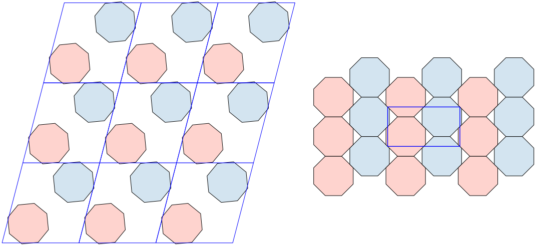

CSG packings where $\mathcal{G}$ of type $p2$ and K is a regular octagon. (Left) packing with density $\rho(\mathcal{K}_{p2}) \approxeq 0.413705$ and (right) optimal packing with density $\rho(\mathcal{K}_{p2}) = \frac{4+4\sqrt{2}}{5+4\sqrt{2}} \approxeq 0.90616$ [1]. The blue parallelogram denotes the primitive cell of the respective configuration. Colors represent symmetry operations modulo lattice translations.

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Entropic Trust Region Packing Algorithm (ETRPA)

- Stochastic relaxation: $\tilde{\boldsymbol{\theta}} = \operatorname{argmax}_{\boldsymbol{\theta}\in\boldsymbol{\Theta}} \int_{\mathbf{x}\in\mathcal{X}} \mathbf{F}(\mathbf{x}) dP(\boldsymbol{\theta})$, $dP(\boldsymbol{\theta}) \in S$.

[1] **Further information on ETRPA**: M. Torda, J. Y. Goulermas, R. Púček and V. Kurlin, *Entropic trust region for densest crystallographic symmetry group packings*, arXiv:2202.11959. To appear in SIAM Journal on Scientific Computing.

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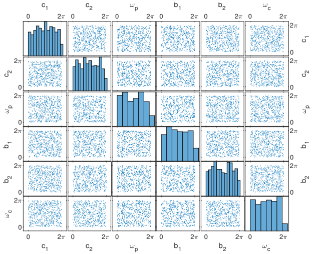

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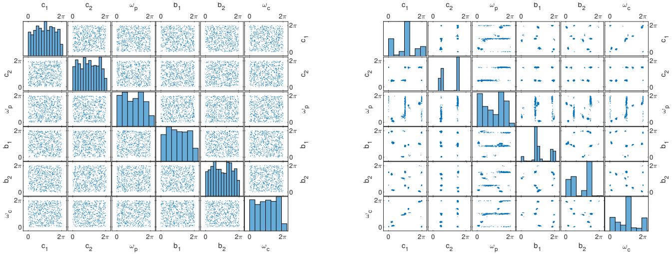

600 realizations of the Extended Multivariate von Mises distribution defined on an T^6 from a single run of the ETRPA. (Left) Initial distribution and (Right) output distribution[1].

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Symmetries of maximally dense plane group packings of regular polygons

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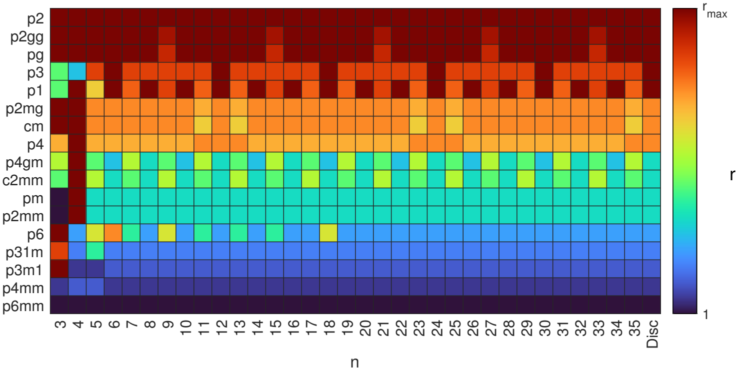
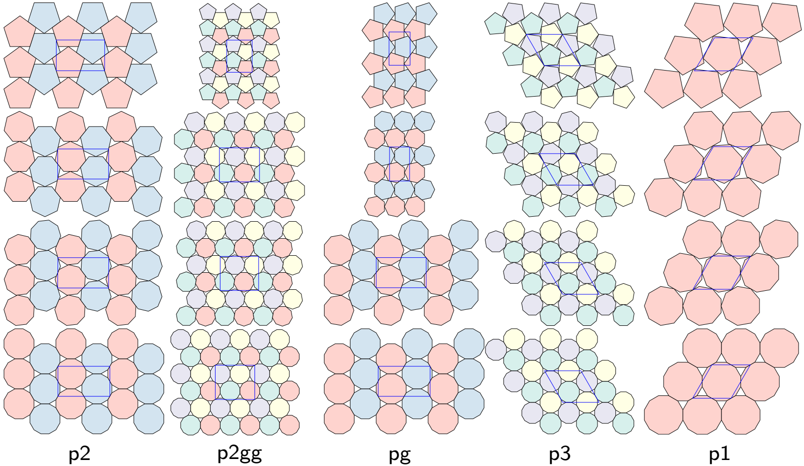


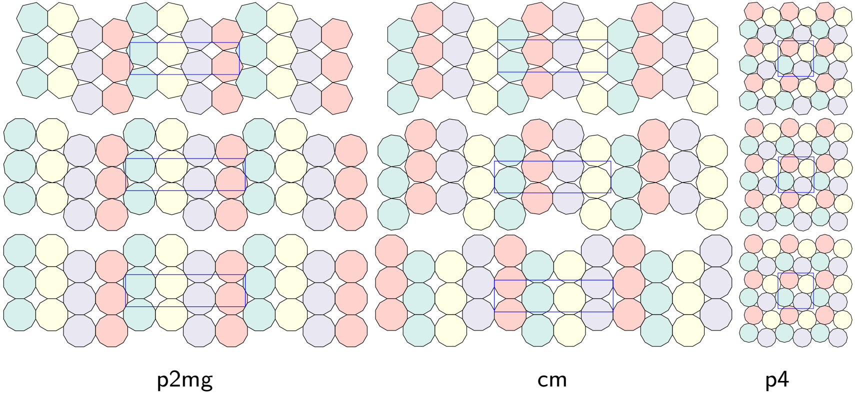
The colored rank table. For every $n = 3, \ldots, 35$ plane groups are ranked according to densities of the densest packing attained in each plane group, and a color is assigned based on rank r ranging from one to r_{max}.

Densest p2, pg, p2gg, p3, and p1 packings



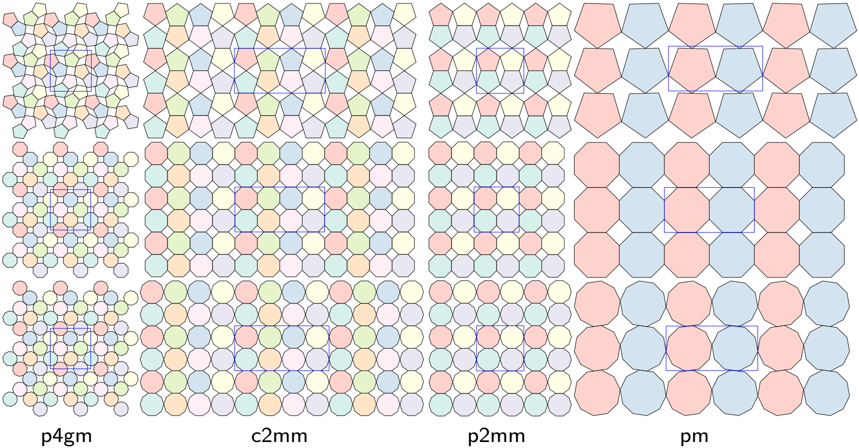
Densest configurations of (from top to bottom) **pentagon**, **heptagon**, **enneagon**, and **dodecagon** in plane groups $p2$, $p2gg$, pg, $p3$, and $p1$ with the following densities: **pentagon** in $p2/p2gg/pg \approxeq 0.92131$, $p3 \approxeq 0.87048$ and $p1 \approxeq 0.81725$; **heptagon** in $p2/p2gg/pg \approxeq 0.89269$, $p3 \approxeq 0.88085$ and $p1 \approxeq 0.86019$; **enneagon** in $p2 \approxeq 0.90103$, $p2gg \approxeq 0.89989$, $pg \approxeq 0.89860$ and $p3/p1 \approxeq 0.88773$; **dodecagon** in $p2/p2gg/pg/p3/p1 \approxeq 0.92820$. The blue parallelogram denotes the primitive cell of the respective configuration. Colors represent symmetry operations modulo lattice translations.

Densest p2mg, cm, and p4 packings



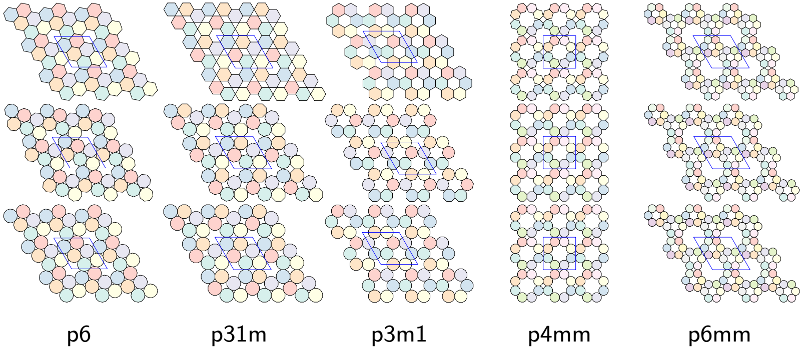
Densest configurations of (top) **heptagon**, (middle) **endecagon**, and (bottom) **dodecagon** in plane groups *p2mg*, *cm*, and *p4* with the following densities: **heptagon** in $p2mg/cm \approxeq 0.84226$ and $p4 \approxeq 0.84219$; **endecagon** in $p2mg \approxeq 0.83116$, $cm \approxeq 0.82795$ and $p4 \approxeq 0.83780$; **dodecagon** in $p2mg/cm/p4 \approxeq 0.86156$. The blue parallelogram denotes the primitive cell of the respective configuration. Colors represent symmetry operations modulo lattice translations.

Densest p4gm, c2mm, pm, and p2mm packings



Densest configurations of (top) **pentagon**, (middle) **octagon**, and (bottom) **decagon** in plane groups *p4gm*, *c2mm*, *p2mm* and *pm* with the following densities: **pentagon** in *p4gm* $\approxeq$ 0.71119, *c2mm* $\approxeq$ 0.71714 and *p2mm*/*pm* $\approxeq$ 0.69098; **octagon** in *p4gm*/*c2mm*/*p2mm*/*pm* $\approxeq$ 0.82842; **decagon** in *p4gm* $\approxeq$ 0.77205 and *c2mm*/*p2mm*/*pm* $\approxeq$ 0.77254. The blue parallelogram denotes the primitive cell of the respective configuration. Colors represent symmetry operations modulo lattice translations.

Densest p6, p31m, p3m1, p4mm, and p6mm packings

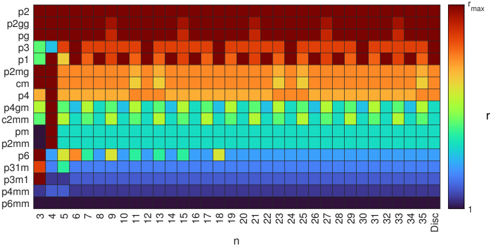


Densest configurations of (from top to bottom) **hexagon**, **octagon**, and **dodecagon** in plane groups $p6$, $p31m$, $p3m1$, $p4mm$, and $p6mm$ with the following densities: **hexagon** in $p6 \approxeq 0.85714$, $p31m \approxeq 0.71999$, $p3m1 \approxeq 0.66666$, $p4mm \approxeq 0.52148$ and $p6mm \approxeq 0.47999$; **octagon** in $p6 \approxeq 0.76438$, $p31m \approxeq 0.71565$, $p3m1 \approxeq 0.57980$, $p4mm \approxeq 0.56854$ and $p6mm \approxeq 0.48235$; **dodecagon** in $p6 \approxeq 0.79560$, $p31m \approxeq 0.74613$, $p3m1 \approxeq 0.61880$, $p4mm \approxeq 0.53589$ and $p6mm \approxeq 0.49742$. The blue parallelogram denotes the primitive cell of the respective configuration. Colors represent symmetry operations modulo lattice translations.

Plane group packing conjectures

Conjecture 1

Densities of the densest p2, pg, and p2gg packings are equal for all, but centrally nonsymmetric n-gons with three-fold rotational symmetry and $n \geq 9$, densities of the denses p2, pg, p2gg, and p1 packings are equal for all centrally symmetric n-gons, and densities of the densest p2, pg, p2gg, p1, and p3 packings are equal for all n-gons containing a six-fold rotational symmetry.

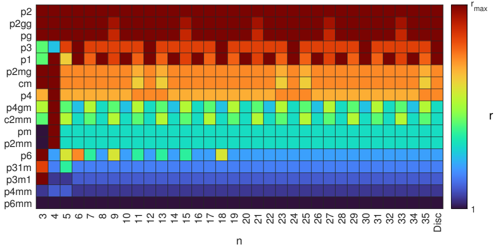


The colored rank table. For every $n = 3, \ldots, 35$ plane groups are ranked according to densities of the densest packing attained in each plane group, and a color is assigned based on rank r ranging from one to r_{max}.

Plane group packing conjectures

Conjecture 2

Densities of the densest p2mg and cm packings are equal for all but n-gons with a $12k-1$ and $12k+1$ rotational symmetry where $k \in \mathbb{N}$ and densities of densest p2mg, cm, and p4 packings are equal for all n-gons containing a 12-fold rotational symmetry.



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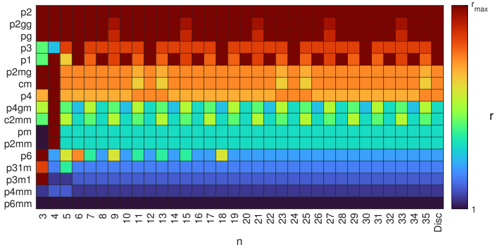
Plane group packing conjectures

Conjecture 3

Densities of the densest pm and p2mm packings are equal for all n-gons, densities of the densest c2mm, pm and p2mm packings are equal for all centrally symmetric n-gons, and densities of the densest p4gm, c2mm, pm, and p2mm packings are equal for all n-gons containing a four-fold rotational symmetry.



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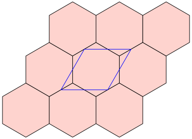
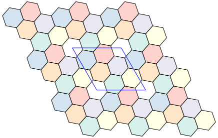
Relationships between $p2/p2gg/pg/p3/p1$, $p6$, $p3m1$, $p31m$ and $p6mm$ packing densities of a hexagon

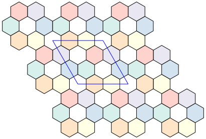
- $\rho\left(\mathcal{K}_{p2/p2gg/pg/p3/p1_{\max}}\right) = \frac{7}{6}\rho\left(\mathcal{K}_{p6_{\max}}\right) = \frac{3}{2}\rho\left(\mathcal{K}_{p3m1_{\max}}\right)$



p1



p6



p3m1

Relationships between $p2/p2gg/pg/p3/p1$, $p6$, $p3m1$, $p31m$ and $p6mm$ packing densities of a hexagon

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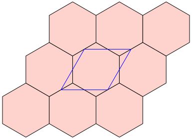
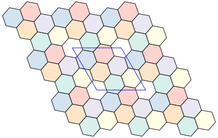
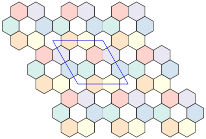
  $\rho\left(\mathcal{K}_{p31m_{\max}}\right) = \frac{3}{2}\rho\left(\mathcal{K}_{p6mm_{\max}}\right)$



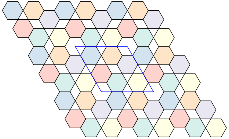
p1



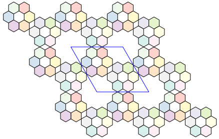
p6



p3m1



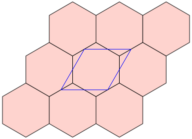
p31m

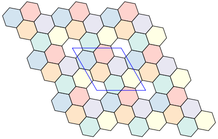


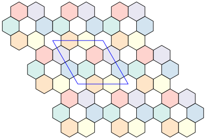
p6mm

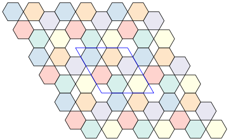
Relationships between $p2/p2gg/pg/p3/p1$, $p6$, $p3m1$, $p31m$ and $p6mm$ packing densities of a hexagon

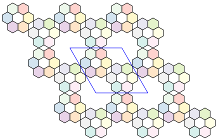
- $\rho\left(\mathcal{K}_{p2/p2gg/pg/p3/p1_{\max}}\right) = \frac{7}{6}\rho\left(\mathcal{K}_{p6_{\max}}\right) = \frac{3}{2}\rho\left(\mathcal{K}_{p3m1_{\max}}\right)$
  $\rho\left(\mathcal{K}_{p31m_{\max}}\right) = \frac{3}{2}\rho\left(\mathcal{K}_{p6mm_{\max}}\right)$
- Numerically, these relationships approximately hold for all n -gons with 6-fold rotational symmetry.


p1


p6

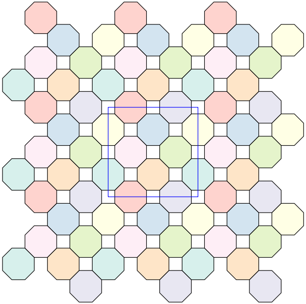

p3m1


p31m

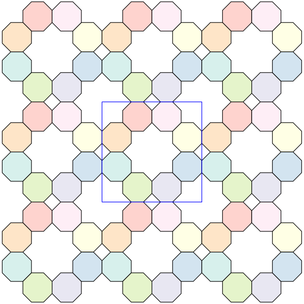

p6mm

Relationships between $p4mg/c2mm/pm/p2mm$ and $p4mm$ packing densities of an octagon

- $\rho\left(\mathcal{K}_{p4mg/c2mm/pm/p2mm_{\mathsf{max}}}\right) = \frac{3+2\sqrt{2}}{4}\rho\left(\mathcal{K}_{p4mm_{\mathsf{max}}}\right)$



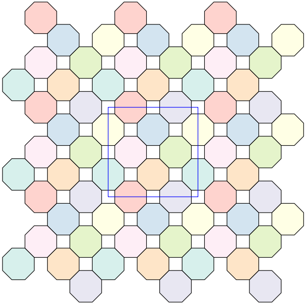
p4gm



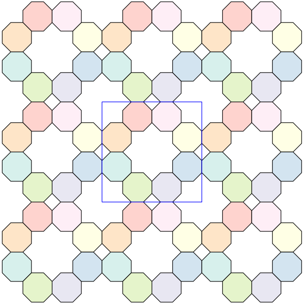
p4mm

Relationships between $p4mg/c2mm/pm/p2mm$ and $p4mm$ packing densities of an octagon

- $\rho\left(\mathcal{K}_{p4mg/c2mm/pm/p2mm_{\max}}\right) = \frac{3+2\sqrt{2}}{4}\rho\left(\mathcal{K}_{p4mm_{\max}}\right)$
- Numerically, these relationships approximately hold for all n -gons with 8-fold rotational symmetry.



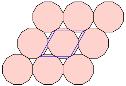
p4gm



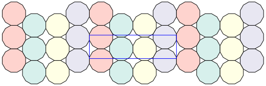
p4mm

Relationships between $p2/p2gg/pg/p3/p1$, $p2mg/cm/p4$, $p4mg/c2mm/pm/p2mm$ and $p31m$ packing densities of a dodecagon

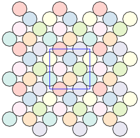
- $\rho\left(\mathcal{K}_{p2/p2gg/pg/p3/p1_{\text{max}}}\right) = \frac{3+2\sqrt{3}}{6}\rho\left(\mathcal{K}_{p2mg/cm/p4_{\text{max}}}\right) = = \frac{2\sqrt{3}}{3}\rho\left(\mathcal{K}_{p4mg/c2mm/pm/p2mm_{\text{max}}}\right) = \frac{2+\sqrt{3}}{3}\rho\left(\mathcal{K}_{p31m_{\text{max}}}\right)$



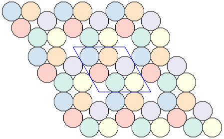
p1



cm



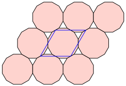
p4gm



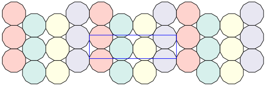
p31m

Relationships between $p2/p2gg/pg/p3/p1$, $p2mg/cm/p4$, $p4mg/c2mm/pm/p2mm$ and $p31m$ packing densities of a dodecagon

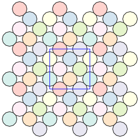
- $\rho\left(\mathcal{K}_{p2/p2gg/pg/p3/p1_{\text{max}}}\right) = \frac{3+2\sqrt{3}}{6}\rho\left(\mathcal{K}_{p2mg/cm/p4_{\text{max}}}\right) =$
  $= \frac{2\sqrt{3}}{3}\rho\left(\mathcal{K}_{p4mg/c2mm/pm/p2mm_{\text{max}}}\right) = \frac{2+\sqrt{3}}{3}\rho\left(\mathcal{K}_{p31m_{\text{max}}}\right)$
- Numerically, these relationships approximately hold for all n -gons with 12-fold rotational symmetry.



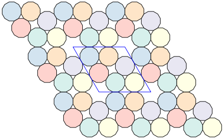
p1



cm



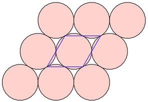
p4gm

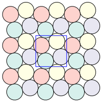


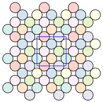
p31m

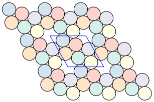
Relationships between $p2/p2gg/pg/p3/p1$, $p2mg/cm/p4$, $p4mg/c2mm/pm/p2mm$ and $p31m$ packing densities of a 24-gon

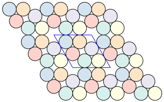
- $\rho\left(\mathcal{K}_{p2/p2gg/pg/p3/p1_{\text{max}}}\right) = \frac{3+2\sqrt{3}}{6}\rho\left(\mathcal{K}_{p2mg/cm/p4_{\text{max}}}\right) =$
  $= \frac{2\sqrt{3}}{3}\rho\left(\mathcal{K}_{p4mg/c2mm/pm/p2mm_{\text{max}}}\right) = \frac{7}{6}\rho\left(\mathcal{K}_{p6_{\text{max}}}\right) =$
  $= \frac{2+\sqrt{3}}{3}\rho\left(\mathcal{K}_{p31m_{\text{max}}}\right) = \frac{3}{2}\rho\left(\mathcal{K}_{p3m1_{\text{max}}}\right) = \frac{3\sqrt{3}+2\sqrt{6}}{6}\rho\left(\mathcal{K}_{p4mm_{\text{max}}}\right) =$
  $= \frac{2+\sqrt{3}}{2}\rho\left(\mathcal{K}_{p6mm_{\text{max}}}\right)$

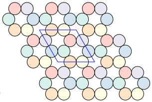

p1

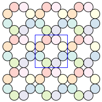

p4

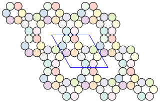

p4gm


p6


p31m

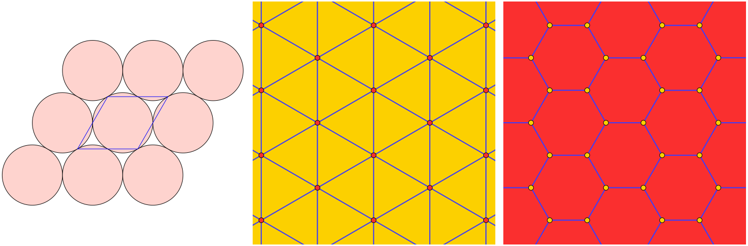

p3m1


p4mm


p6mm

$p2/p2gg/pg/p3/p1$ packing of a disc

- $\rho\left(\mathcal{K}_{p2/p2gg/pg/p3/p1_{\max}}\right) = \frac{\sqrt{3}}{6}\pi = 0.9068996\ldots$
  - **Optimal lattice packing**
    - Lagrange, J. L. (1773). *Recherches d'arithmétique.* Nouveaux Mémoires de l'Académie de Berlin.
    - Gauss, C. F. (1840). *Untersuchungen über die Eigenschaften der positiven ternären quadratischen Formen von Ludwig August Seeber.* J. reine angew. Math, 20(312-320), 3.

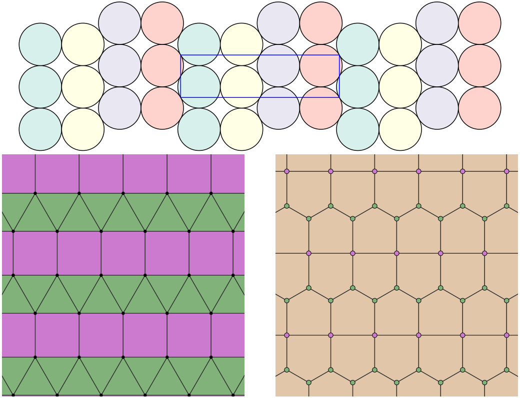


(**Left**) $p1$ packing of a disc, (**middle**) the corresponding 3^6 regular tiling, and (**right**) its dual tiling[1].

[1] List of Euclidean uniform tilings. (2023, April 2). In Wikipedia. https://en.wikipedia.org/wiki/List_of_Euclidean_uniform_tilings.

$p2mg/cm/p4$ packing of a disc

- $\rho\left(\mathcal{K}_{p2mg/cm/p4_{\text{max}}}\right) = \left(2-\sqrt{3}\right)\pi = 0.8417872\ldots$



(**Top**) *p*2*mg* packing of a disc, (**bottom left**) the corresponding $3^3.4^2$ semiregular tiling, and (**bottom right**) its dual tiling[1].

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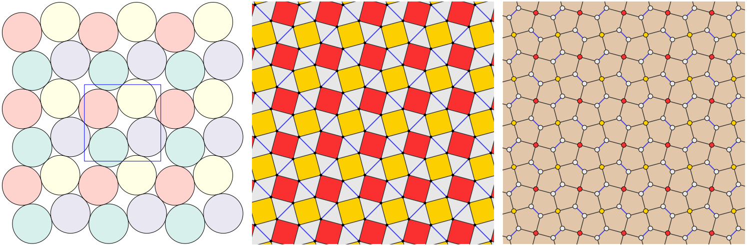
[1] List of Euclidean uniform tilings. (2023, April 2). In Wikipedia. https://en.wikipedia.org/wiki/List_of_Euclidean_uniform_tilings.

$p2mg/cm/p4$ packing of a disc

- $\rho\left(\mathcal{K}_{p2mg/cm/p4_{\mathrm{max}}}\right) = \left(2-\sqrt{3}\right)\pi = 0.8417872\ldots$

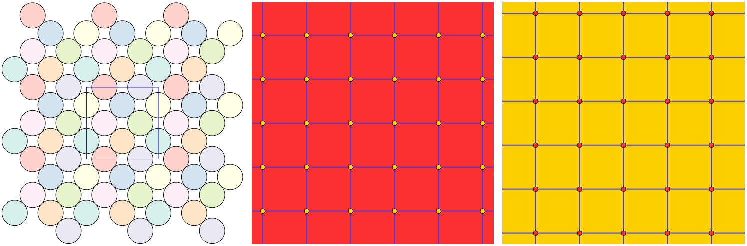


(**Left**) $p4$ packing of a disc, (**middle**) the corresponding $3^2.4.3.4$ semiregular tiling, and (**right**) its dual tiling[1].

[1] List of Euclidean uniform tilings. (2023, April 2). In Wikipedia. https://en.wikipedia.org/wiki/List_of_Euclidean_uniform_tilings.

p4mg/*c2mm*/*pm*/*p2mm* packing of a disc

- $\rho\left(\mathcal{K}_{p4mg/c2mm/pm/p2mm_{\max}}\right) = \frac{\pi}{4} = 0.7853981\ldots$

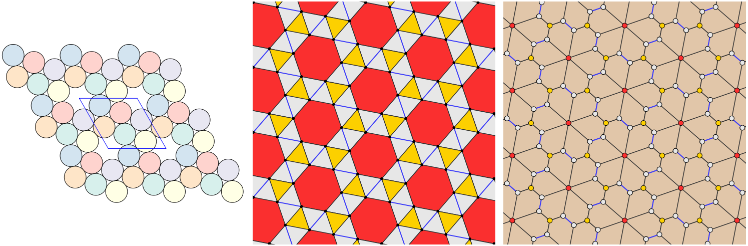


(**Left**) *p4mg* packing of a disc, (**middle**) the corresponding 4^4 semiregular tiling, and (**right**) its dual tiling[1] (self-dual).

[1] List of Euclidean uniform tilings. (2023, April 2). In Wikipedia. https://en.wikipedia.org/wiki/List_of_Euclidean_uniform_tilings.

$p6$ packing of a disc

- $\rho\left(\mathcal{K}_{p6_{\text{max}}}\right) = \frac{\sqrt{3}}{7}\pi = 0.7773425\ldots$

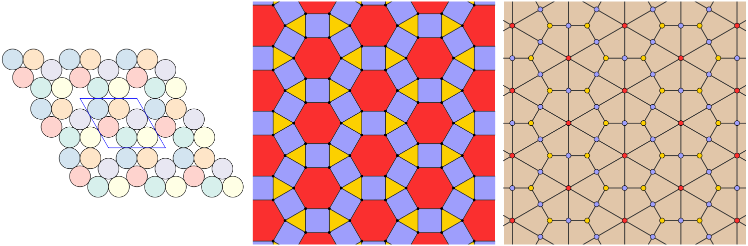


(**Left**) $p6$ packing of a disc, (**middle**) the corresponding $3^4.6$ semiregular tiling, and (**right**) its dual tiling[1] (self-dual).

[1] List of Euclidean uniform tilings. (2023, April 2). In Wikipedia. https://en.wikipedia.org/wiki/List_of_Euclidean_uniform_tilings.

$p31m$ packing of a disc

- $\rho\left(\mathcal{K}_{p31m_{\max}}\right) = \frac{2\sqrt{3}-3}{2}\pi = 0.7290091\ldots$

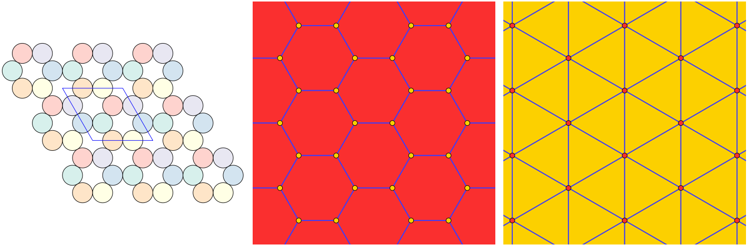


(**Left**) $p31m$ packing of a disc, (**middle**) the corresponding 3.4.6.4 semiregular tiling, and (**right**) its dual tiling[1].

[1] List of Euclidean uniform tilings. (2023, April 2). In Wikipedia. https://en.wikipedia.org/wiki/List_of_Euclidean_uniform_tilings

$p3m1$ packing of a disc

- $\rho\left(\mathcal{K}_{p3m1_{\max}}\right) = \frac{\sqrt{3}}{9}\pi = 0.6045997\ldots$

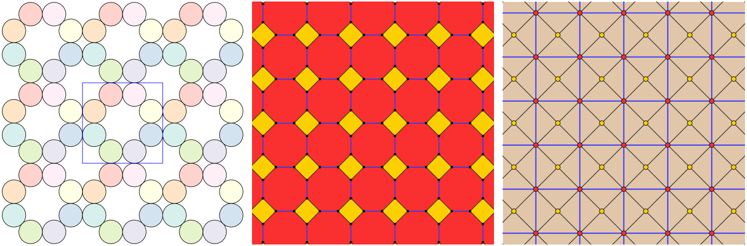


(**Left**) $p31m$ packing of a disc, (**middle**) the corresponding 6^3 regular tiling, and (**right**) its dual tiling[1].

[1] List of Euclidean uniform tilings. (2023, April 2). In Wikipedia. https://en.wikipedia.org/wiki/List_of_Euclidean_uniform_tilings.

$p4mm$ packing of a disc

- $\rho\left(\mathcal{K}_{p4mm_{\max}}\right) = \left(3 - 2\sqrt{2}\right)\pi = 0.5390120\ldots$

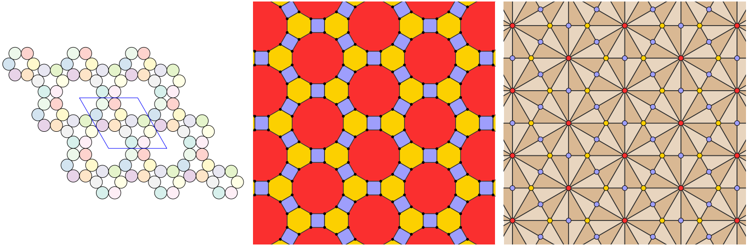


(**Left**) $p4mm$ packing of a disc, (**middle**) the corresponding 4.8^2 semiregular tiling, and (**right**) its dual tiling[1].

[1] List of Euclidean uniform tilings. (2023, April 2). In Wikipedia. https://en.wikipedia.org/wiki/List_of_Euclidean_uniform_tilings.

p6mm packing of a disc

- $\rho\left(\mathcal{K}_{p6mm_{\text{max}}}\right) = \frac{2\sqrt{3}-3}{3}\pi = 0.4860060\ldots$



(**Left**) *p6mm* packing of a disc, (**middle**) the corresponding 4.6.12 semiregular tiling, and (**right**) its dual tiling[1].

[1] List of Euclidean uniform tilings. (2023, April 2). In Wikipedia. https://en.wikipedia.org/wiki/List_of_Euclidean_uniform_tilings.

Table 2-2. DENSITIES OF PLANE ARRANGEMENTS OF CIRCLES

PACKING (TESSELLATION)	DENSITY
$\{3,6\}$	$\pi/\sqrt{12} = 0.9069$
$\{4,4\}$	$\pi/4 = 0.7854$
$\{6,3\}$	$\pi/\sqrt{27} = 0.6046$
$3^3.4^2$	$\pi/(\sqrt{3}+2) = 0.8418$
$3^2.4.3.4$	$\pi/(\sqrt{3}+2) = 0.8418$
$3.6.3.6$	$3\pi/(8\sqrt{3}) = 0.6802$
$3^4.6$	$3\pi/(7\sqrt{3}) = 0.7773$
3.12^2	$3\pi/(12+7\sqrt{3}) = 0.3906$
4.8^2	$\pi/(3+\sqrt{8}) = 0.5390$
$3.4.6.4$	$3\pi/(4\sqrt{3}+6) = 0.7290$
$4.6.12$	$\pi/(3+2\sqrt{3}) = 0.4860$

Williams, R. (1979). Circle packings, plane tessellations, and networks. *The Geometrical Foundation of Natural Structure: A Source Book of Design*, 34-47.

THANK YOU