UNIVERSITY OF LIVERPOOL

LEVERHULME TRUST

The Leverhulme Research Centre for Functional Materials Design

Geometric Perspectives on the Crystallization of Molecular Crystals

Crystallographic Symmetry Group Packings, Uniform Tessellations, and Molecular Frameworks

Miloslav Torda

diamond

Hartree Centre

Science & Technology Facilities Council

Imperial College London

ICNS

King Abdullah University of Science and Technology

University of Southampton

“There is nothing more in physical theories than symmetry groups except the mathematical construction which allows precisely to show that there is nothing more”§

Jean-Marie Souriau

§ F. Barbaresco, (2020). Jean-Marie Souriau’s symplectic model of statistical physics: seminal papers on Lie groups thermodynamics-Quod Erat demonstrandum. In Workshop on Joint Structures and Common Foundations of Statistical Physics, Information Geometry and Inference for Learning (pp. 12-50). Cham: Springer International Publishing.

Crystal Structure Prediction

- **Physical problem:** Predict the arrangement of molecules within a crystalline solid based only on the chemical composition of the target molecule from first-principles (i.e. thermodynamics, quantum mechanics)

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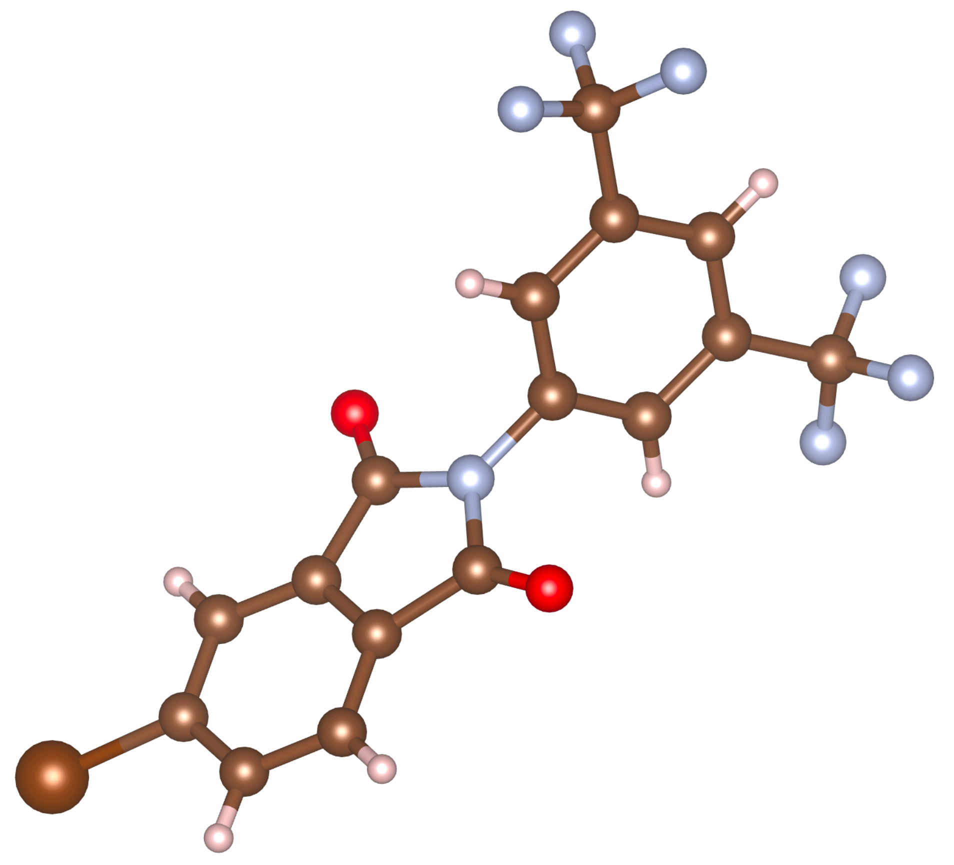

Chemical composition of the target molecule

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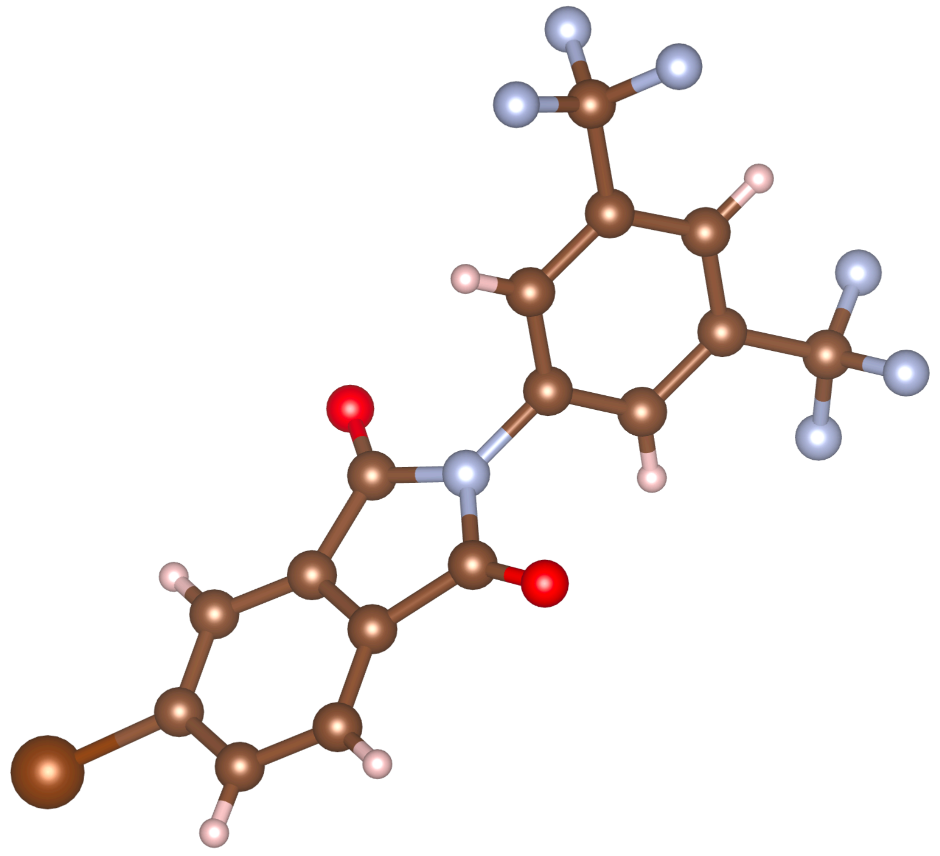

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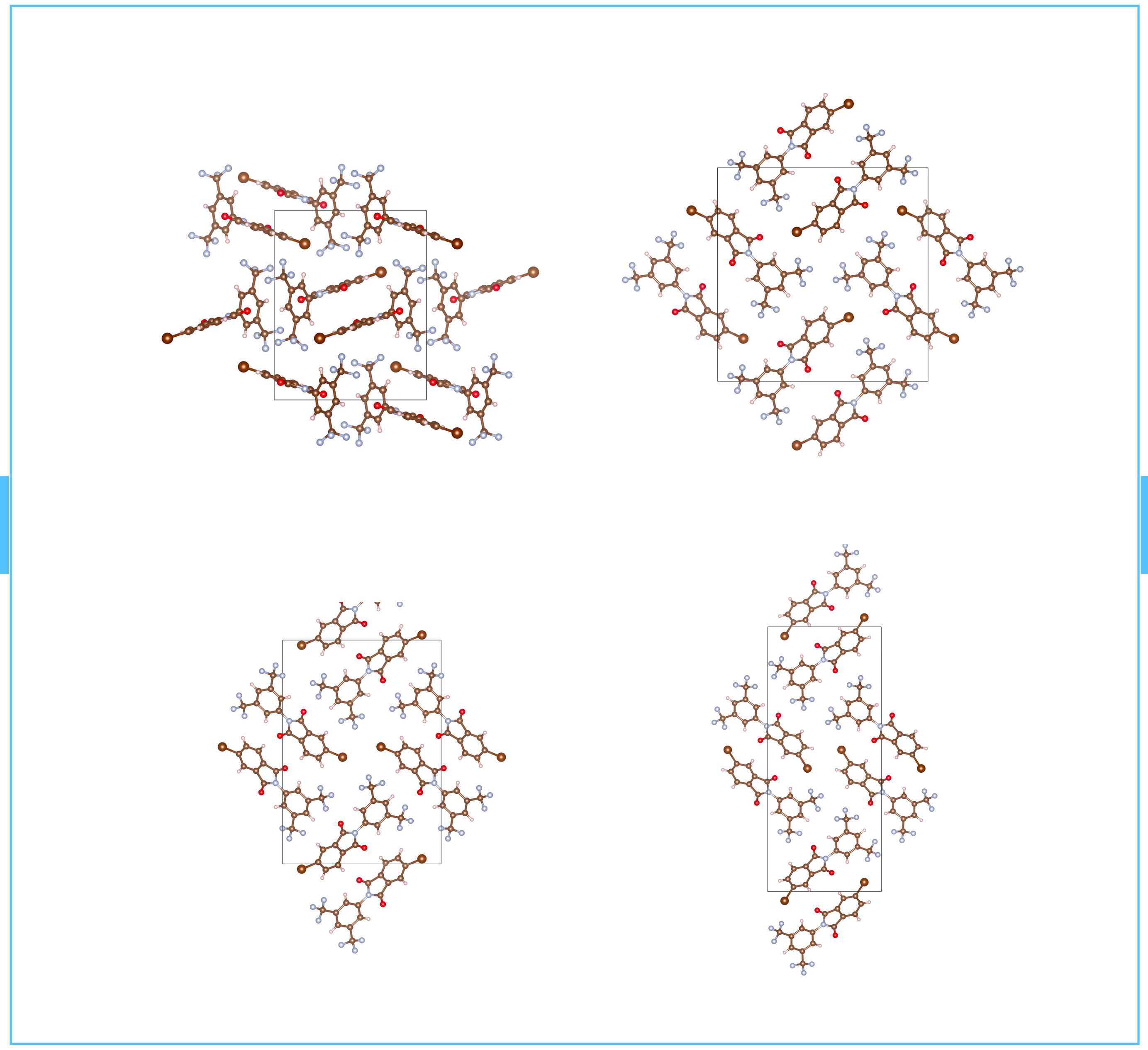

Force Field Based Structure Generation and filtering

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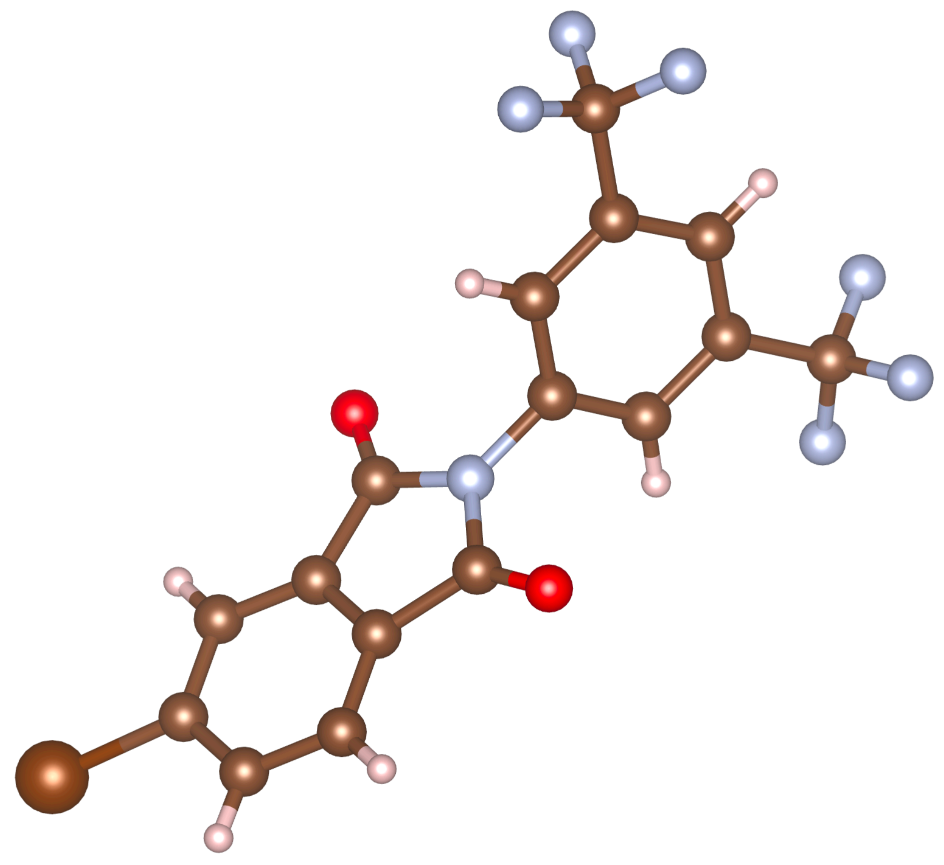

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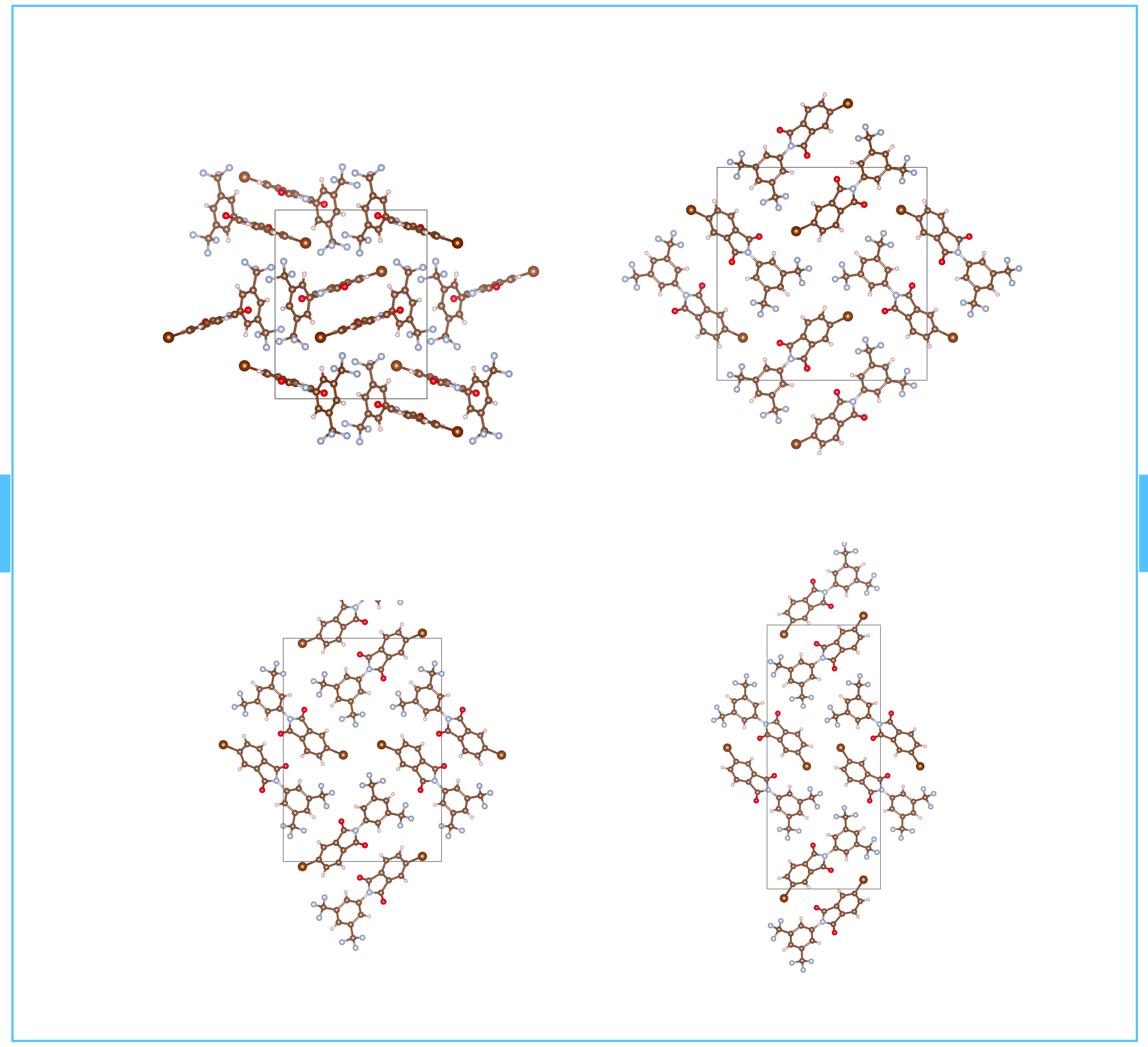

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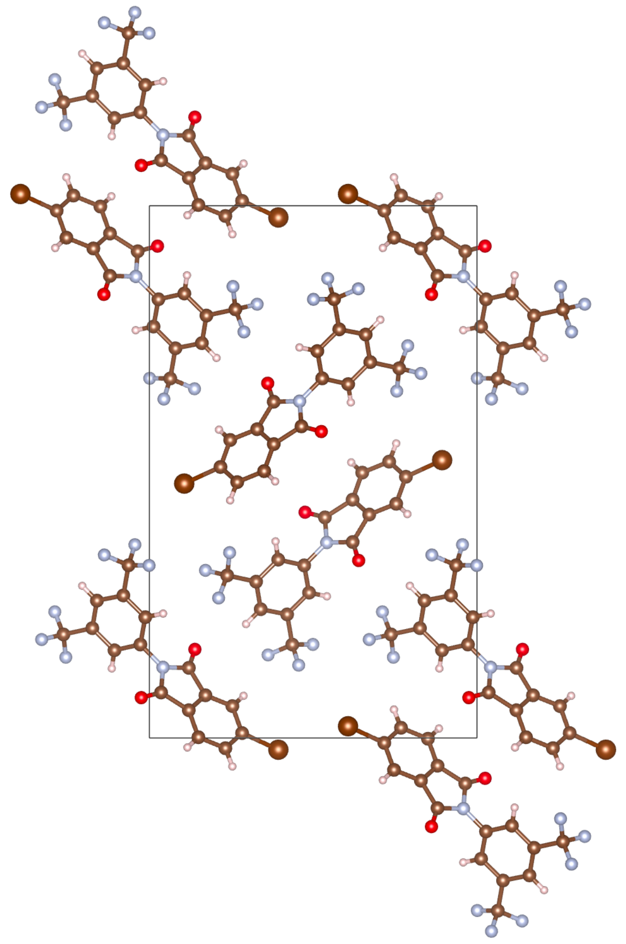

High-Accuracy DFT Geometry Refinement
and Final Structure Assessment

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Table 7
Summary of CPU core hours reported per target molecule for each group where predictions were attempted.

Group	XXVII	XXVIII	XXIX	XXX	XXXI	XXXII	XXXIII	Total	Processors
1			652,495		840,000	1,597,000	412,000	3,501,495	AMD EPYC 7742 / Intel Xeon E5-2620, E5-2650 v4, Gold 6248, E5-2695
3			1,600,000		1,500,000	3,600,000		6,700,000	Intel Xeon X5650, E5-2650 v3, Silver 4214R, Platinum 8174
5	768,766		33,000	2,900,000	510,563	846,698	228,957	5,287,984	Intel Skylake 2.0 GHz
6	8,120	1,350	1,310	9,800	1,470	2,900	4,980	29,930	Various computers, CPU times standardized to 2.66 GHz Intel Quad 9400
8	3,200	10			4,000		1,840	9,050	Intel Xeon 2650
10	772,500	1,242,500	1,146,588	644,927	381,672	644,927	612,500	5,445,614	Intel Xeon Platinum 8124M
11			643,882					643,882	Intel Xeon E5-2683 v4
12			20,000	80,000	20,000			120,000	Intel Xeon Gold 6132
13			350	1,500			500	2,350	Intel Xeon E5450
16	1,700,000		2,128,000		630,000			4,458,000	AMD EPYC 7742 / Intel Platinum 8280 Nvidia RTX 3090, GTX 1080, GTX 1080ti / Tesla V100S
17	95,819							95,819	Intel Xeon Gold 6154
18			1,050	36,864	632	1,561		40,107	Intel Xeon Gold 6230R
19	30,000		40,000	1,250,000	140,000	400,000	60,000	1,920,000	Intel Xeon Haswell E5-2666 v3
20	1,022,976	283,538	755,712	1,769,472	1,028,064	3,935,232	728,064	9,523,058	Intel Xeon E5-2650 v4
21	333,586		92,890	580,436	1,889,649		477,210	3,373,771	Intel Xeon Gold 6154, 6132, FUJITSU A64FX
22	20,000	2,000	15,000	180,000	20,000	25,000	25,000	287,000	Intel Xeon Gold 6230
23			10,000					10,000	Intel Xeon Scalable Processors / Apple M1
24	450,290	89,666	76,541	100,000	49,177	244,520	123,427	1,133,621	Intel Xeon E5-2650v3, L5630 & E5-2660v4 mixed clusters
25	55,150	29,691	4,784		6,476	76,161	34,648	206,910	Intel Xeon Gold 6248, Platinum 8168
26					28,332			28,332	Intel Xeon Gold
27	1,280,566	60,457	242,424	213,722		1,663,940	150,650	3,611,759	Intel Xeon Platinum, Gold-6132, Xeon E5-2695 v3
28	1,600		1,500	7,680	1,500	1,500	1,500	15,280	Intel Xeon E5-2697 A v4

Group 20 generated correct structures for all target compounds§

§ Hunnisett, L. M., Nyman, J., Francia, N., Abraham, N. S., Adjiman, C. S., Aitipamula, S., ... & Zeng, Q. (2024). The seventh blind test of crystal structure prediction: structure generation methods. *Structural Science*, *80*(6).

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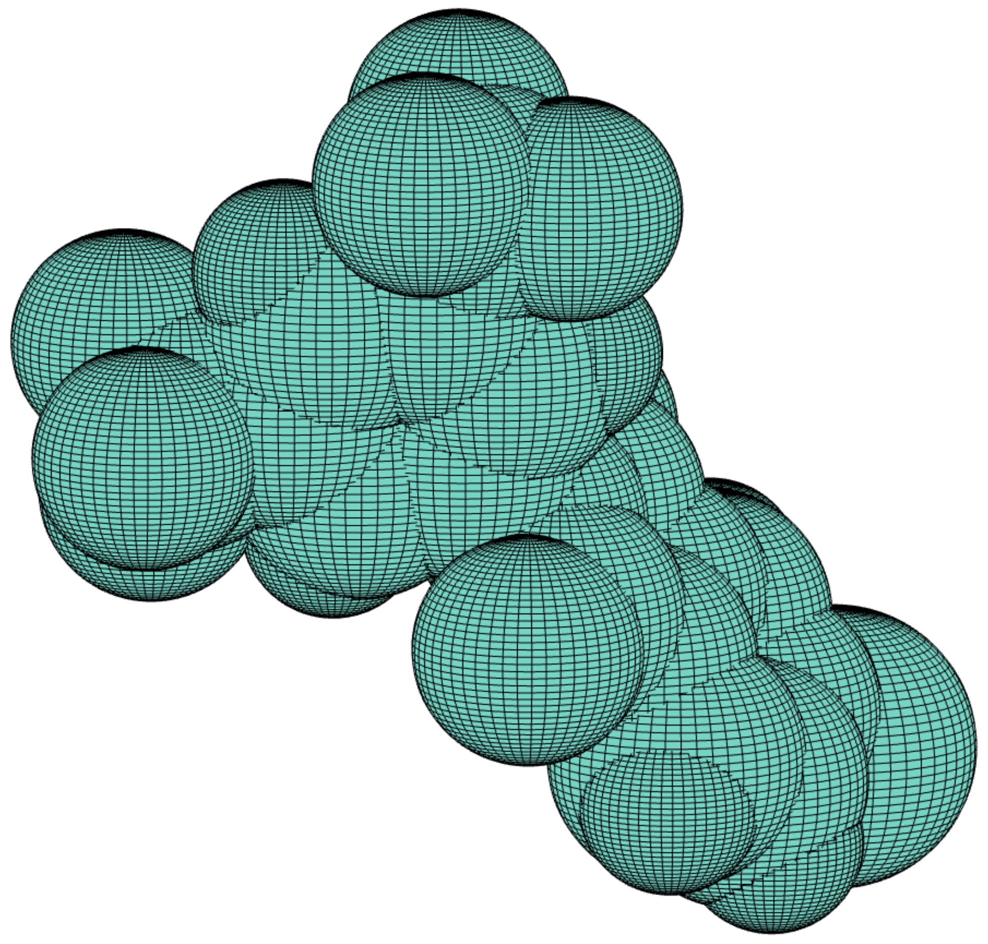
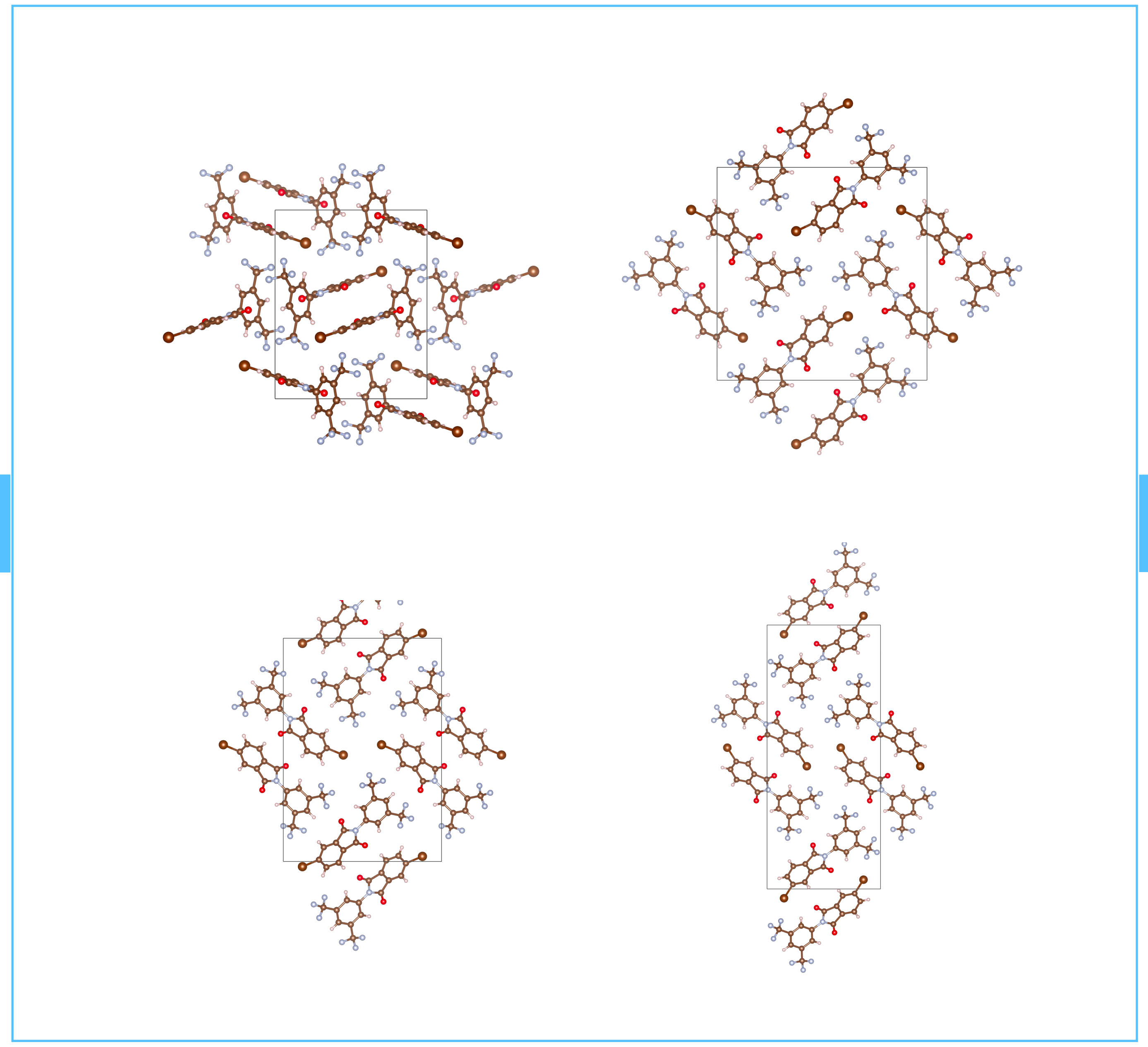
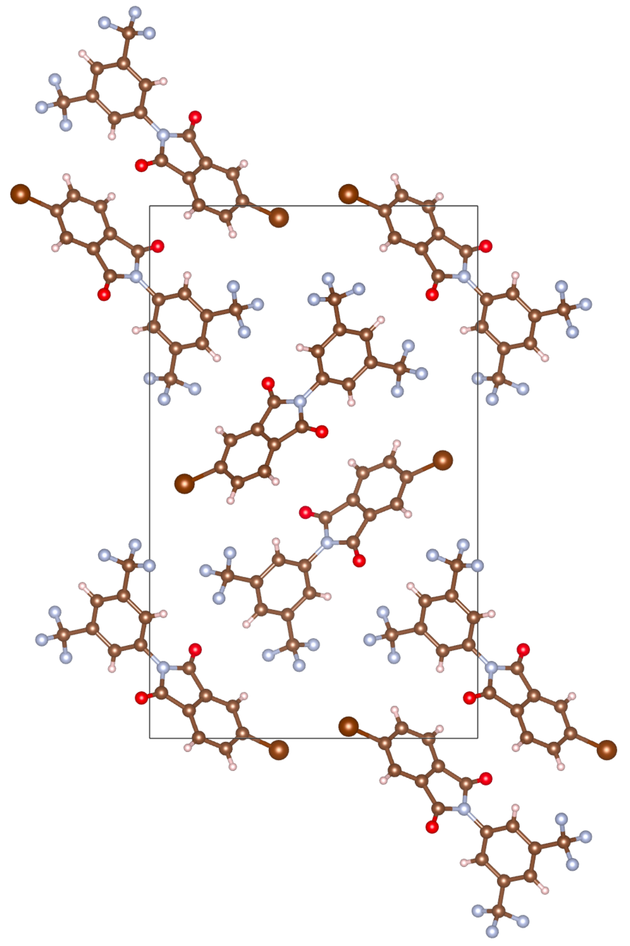


Geometric Representation of a Molecule



Geometric-Inductive-Biased Structure Generation



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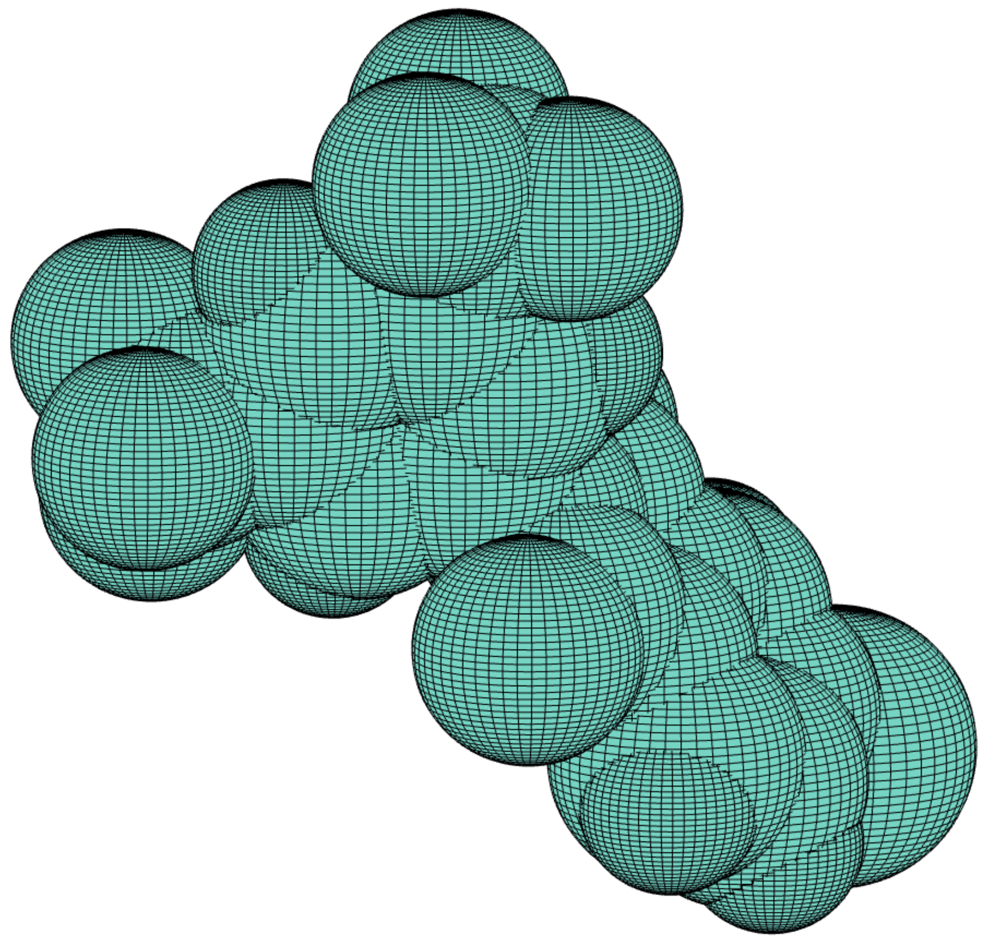

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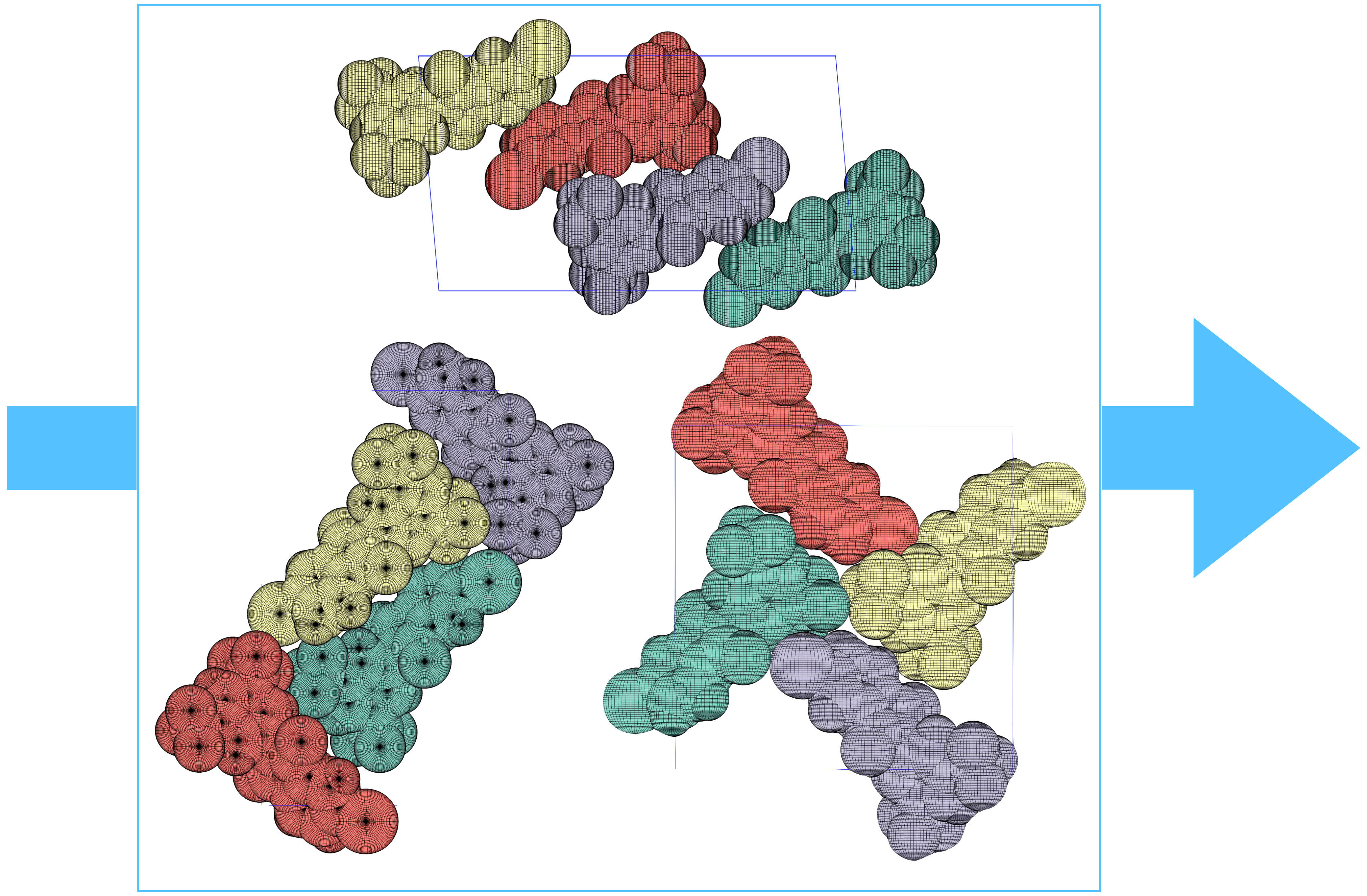
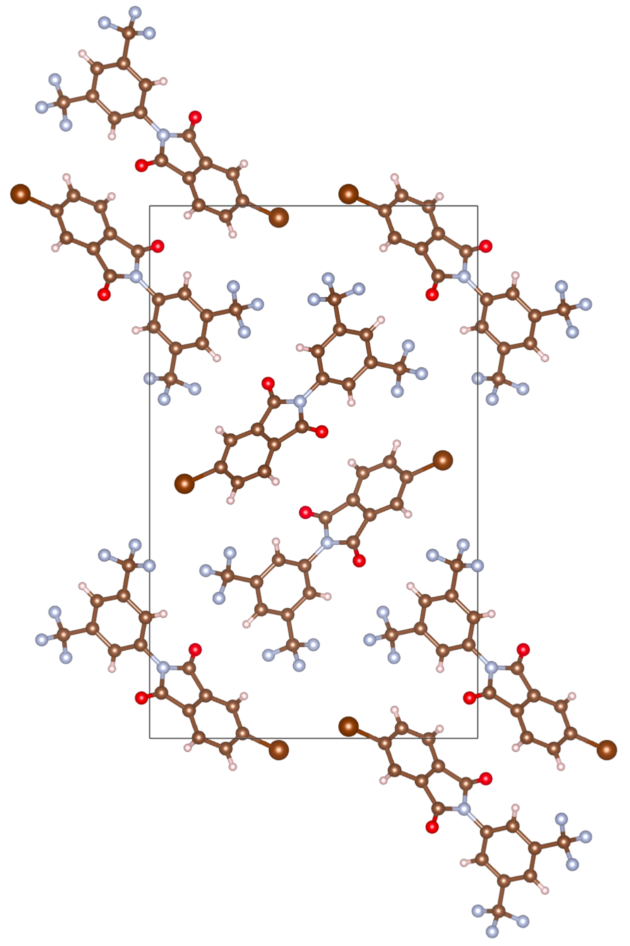


Force Field Based Structure Generation and filtering



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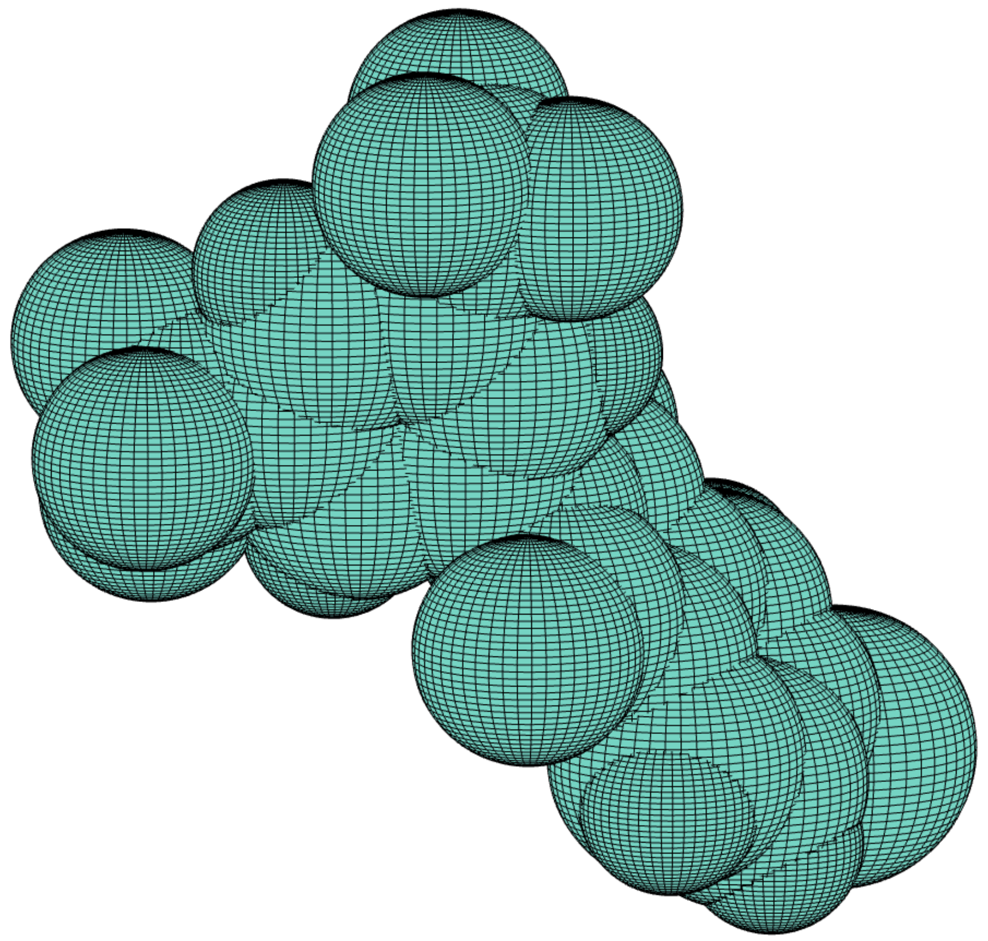

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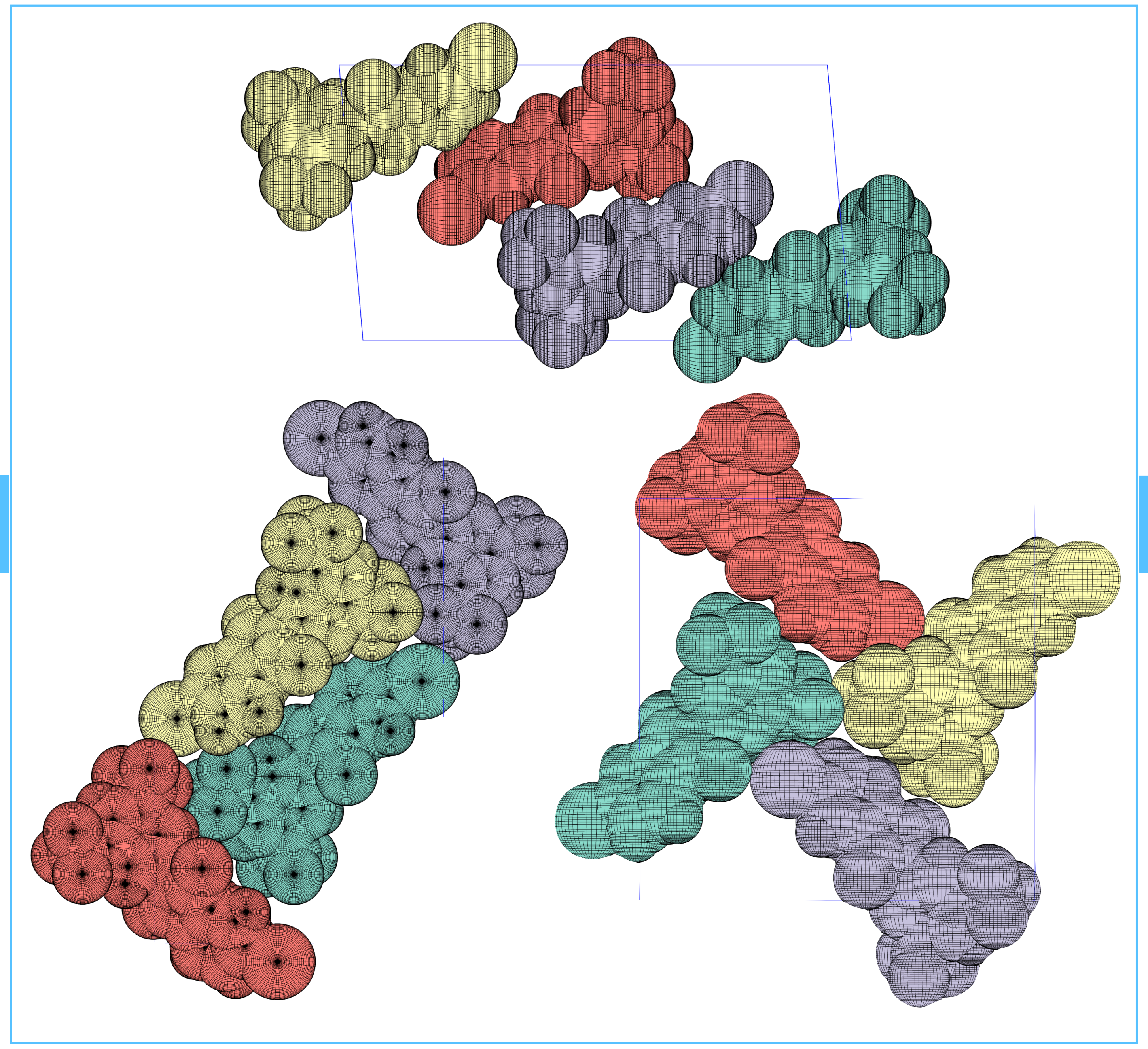

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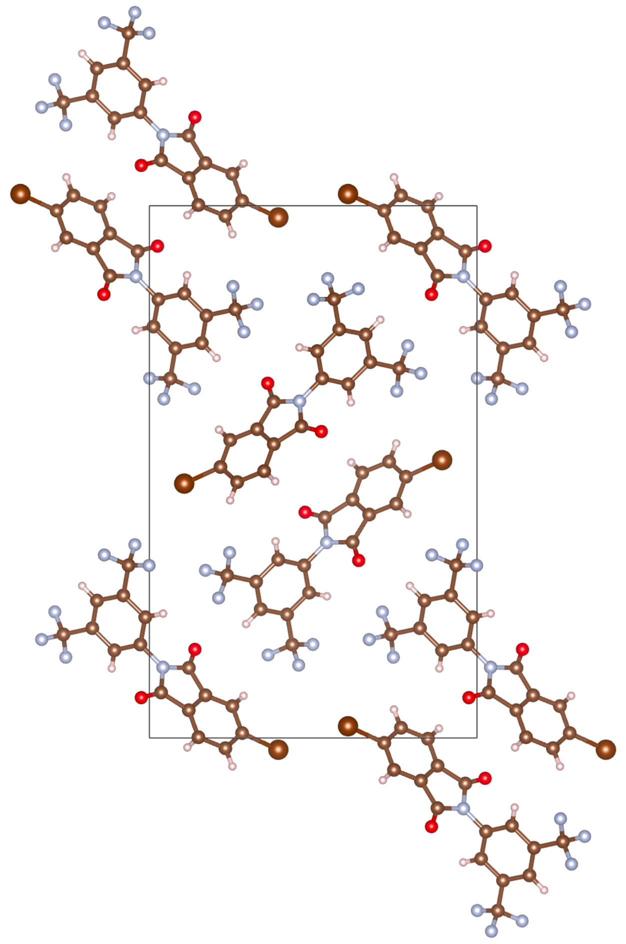

High-Accuracy DFT Geometry Refinement
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L. Lewis, H. Y. Huang, V. T. Tran, S. Lehner, R. Kueng, and J. Preskill. (2024). Improved machine learning algorithm for predicting ground state properties. Nature Communications, 15(1), 895.

N. Galanakis and M. E. Tuckerman (2024). Rapid prediction of molecular crystal structures using simple topological and physical descriptors. Nature Communications, 15(1), 9757.

The Crystallization Conjecture

- **Statement.** In suitable boundary conditions, the energy ground states of interacting particles form periodic configurations in the thermodynamic limit.

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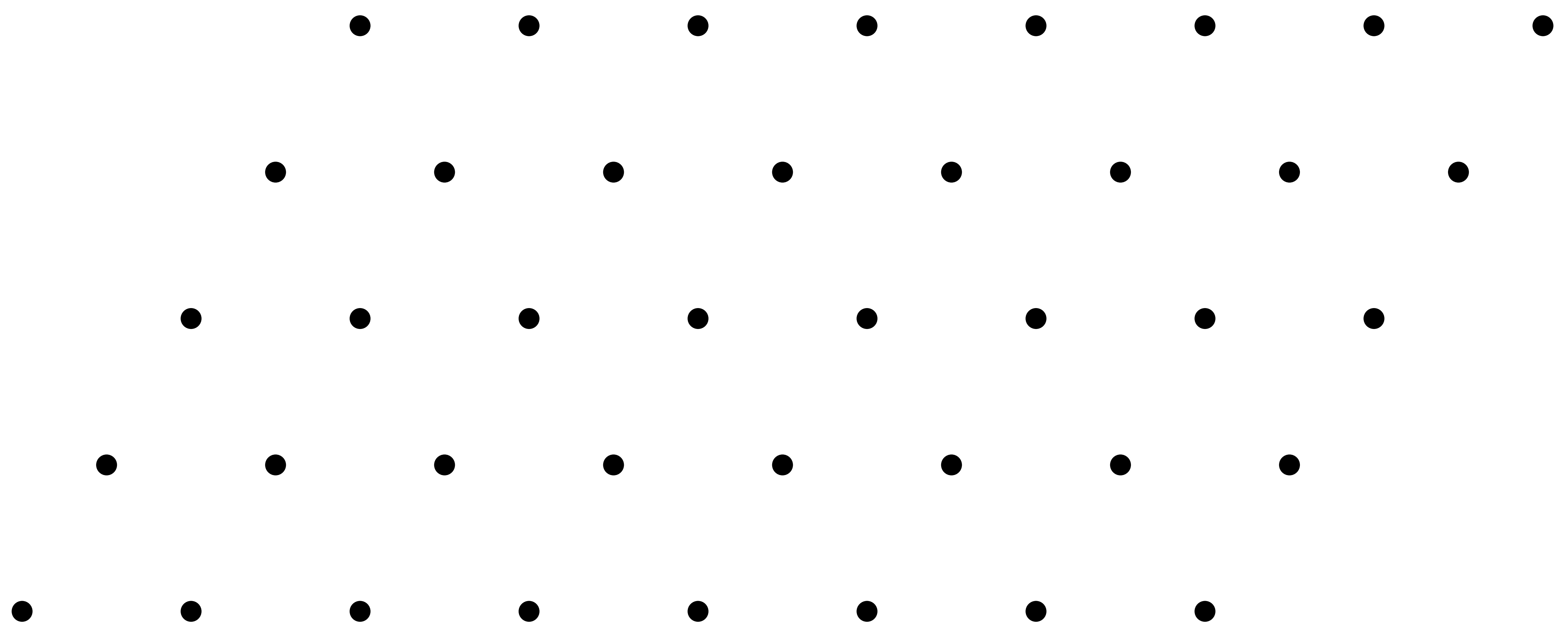
- **Ground state energy per particle.** $$\lim_{|\mathcal{I}|\to\infty} \frac{1}{|\mathcal{I}|} \min \sum_{\substack{(i,j)\in\mathcal{I}\\ i\neq j}} \left[\left(\frac{1}{r_{(i,j)}}\right)^{12} - \left(\frac{1}{r_{(i,j)}}\right)^{6}\right] \qquad \begin{matrix} r_{(i,j)} = \|x_i - x_j\| \\ x_* \in \mathbb{R}^2 \end{matrix}$$



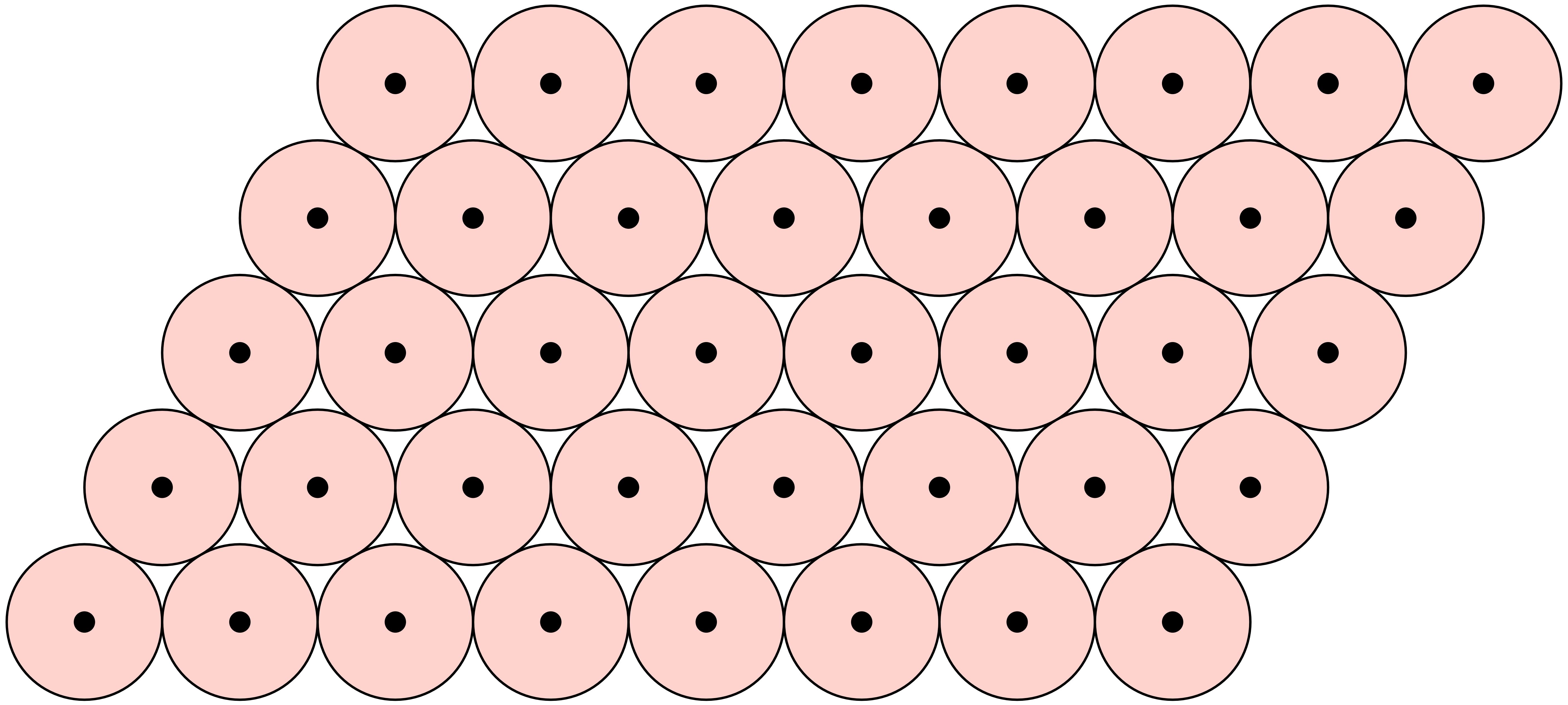
Ground state configuration of a mono-atomic Lennard-Jones system at zero temperature[1].

1 F. Theil, A Proof of Crystallization in Two Dimensions, Communications in Mathematical Physics, 262 (2006), pp. 209–236.

The Crystallization Conjecture

- **Statement:** In suitable boundary conditions, the energy ground states of interacting particles form periodic configurations in the thermodynamic limit.

- **Ground state energy per particle:** $$\lim_{|\mathcal{J}|\to\infty} \frac{1}{|\mathcal{J}|} \min \sum_{\substack{(i,j)\in\mathcal{J} \\ i\neq j}} \left[\left(\frac{1}{r_{(i,j)}}\right)^{12} - \left(\frac{1}{r_{(i,j)}}\right)^{6} \right] \qquad r_{(i,j)} = \|x_i - x_j\|^2, \quad x_* \in \mathbb{R}^2$$



Densest circle packing with a density of $\frac{\sqrt{3}}{6}\pi$.

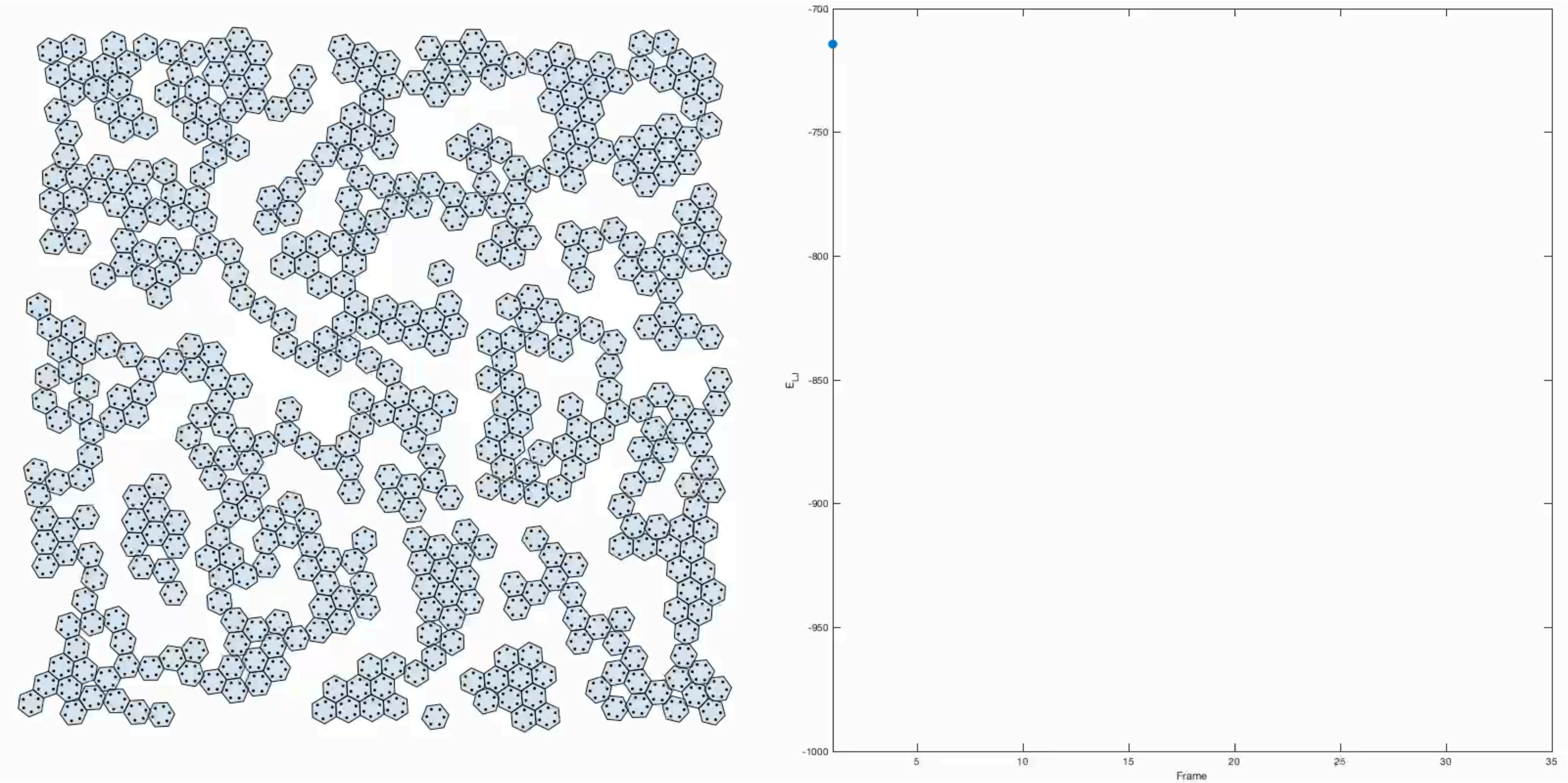
Lagrange, J. L. (1773). Recherches d’arithmétique. Nouveaux Mémoires de l’Académie de Berlin.

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.

Crystallization of Molecular Crystals

A system of 500 model molecules in a square box - 6 atoms each.

$$E_{LJ} = \sum_{\substack{\{I,J\} \\ I\cap J=0}} \frac{1}{2} \sum_{i\in I} \sum_{j\in J} \left[\left(\frac{1}{r_{(i,j)}}\right)^{12} - \left(\frac{1}{r_{(i,j)}}\right)^{6} \right]$$



Crystallization of Molecular Crystals

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Each frame is an output of a Sequential Quadratic Programming run

- Random initial configuration
- Boundaries are reduced after each iteration

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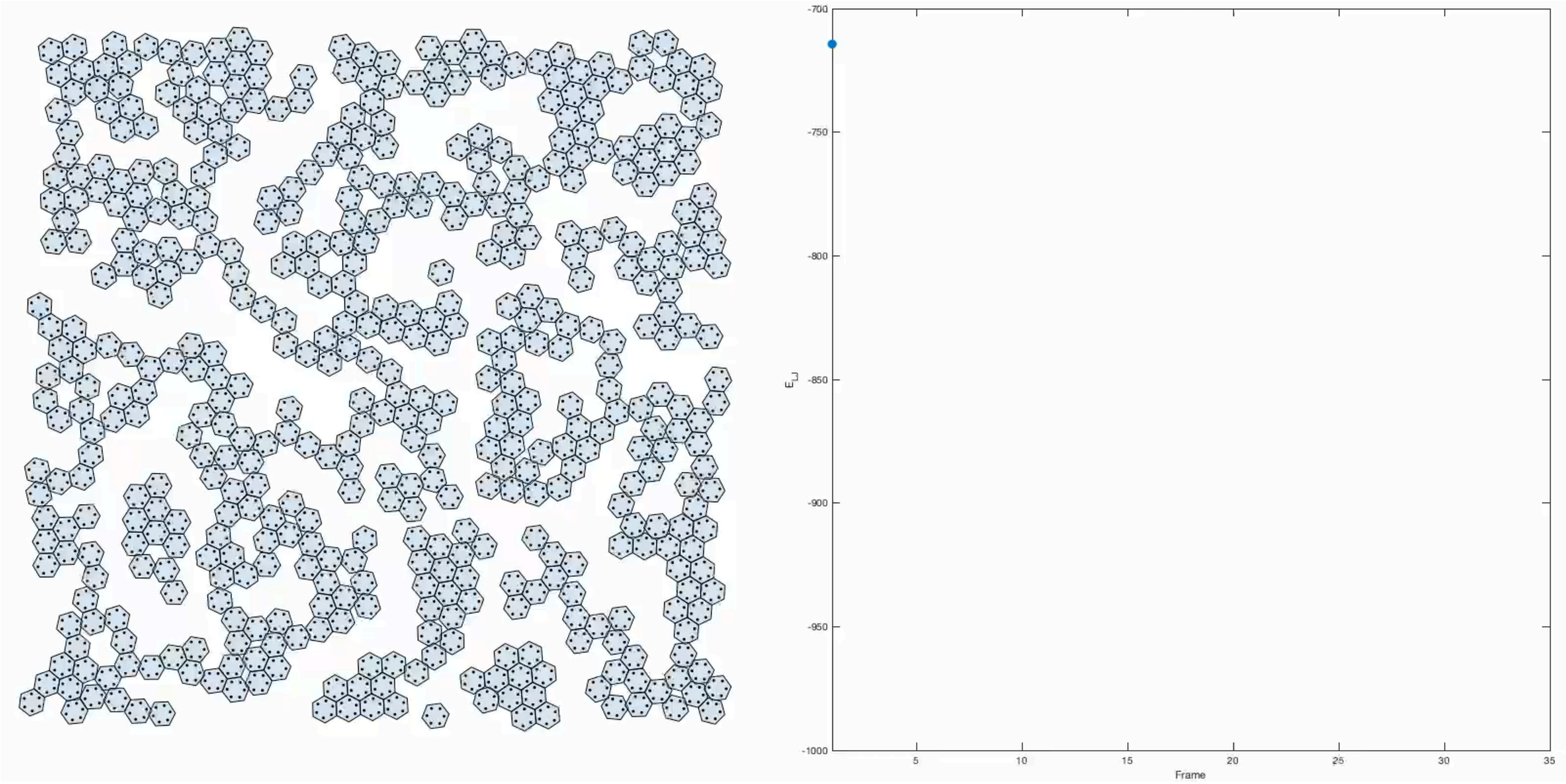

Model of the Potential Energy of Interaction Between Molecules§

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5. For the $u_{(i,j)}$, we may adopt various analytical expressions of the type of 6-exp or 6:n potentials with arbitrary parameters which must be determined by experiment.

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Crystallographic Symmetry Groups §

Definition. Let E_n be the n-dimensional Euclidean group and $T_n \subseteq E_n$ the translational symmetry group. An n-dimensional Crystallographic Symmetry Group G is a discrete subgroup of isometries of E_n such that $L_n = G \cap T_n$ is a lattice group.

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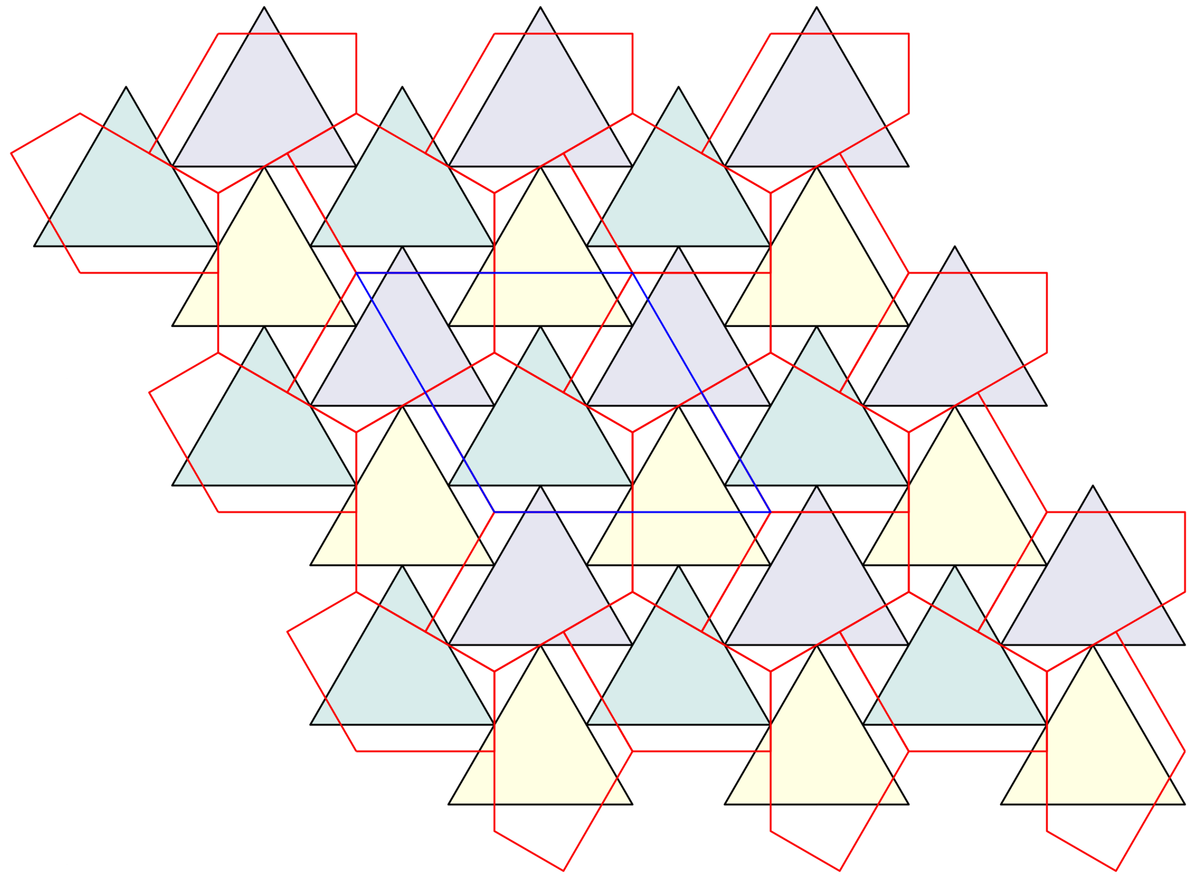
Wallpaper Groups ($n = 2$)

$p3$ (Hermann-Mauguin Notation)



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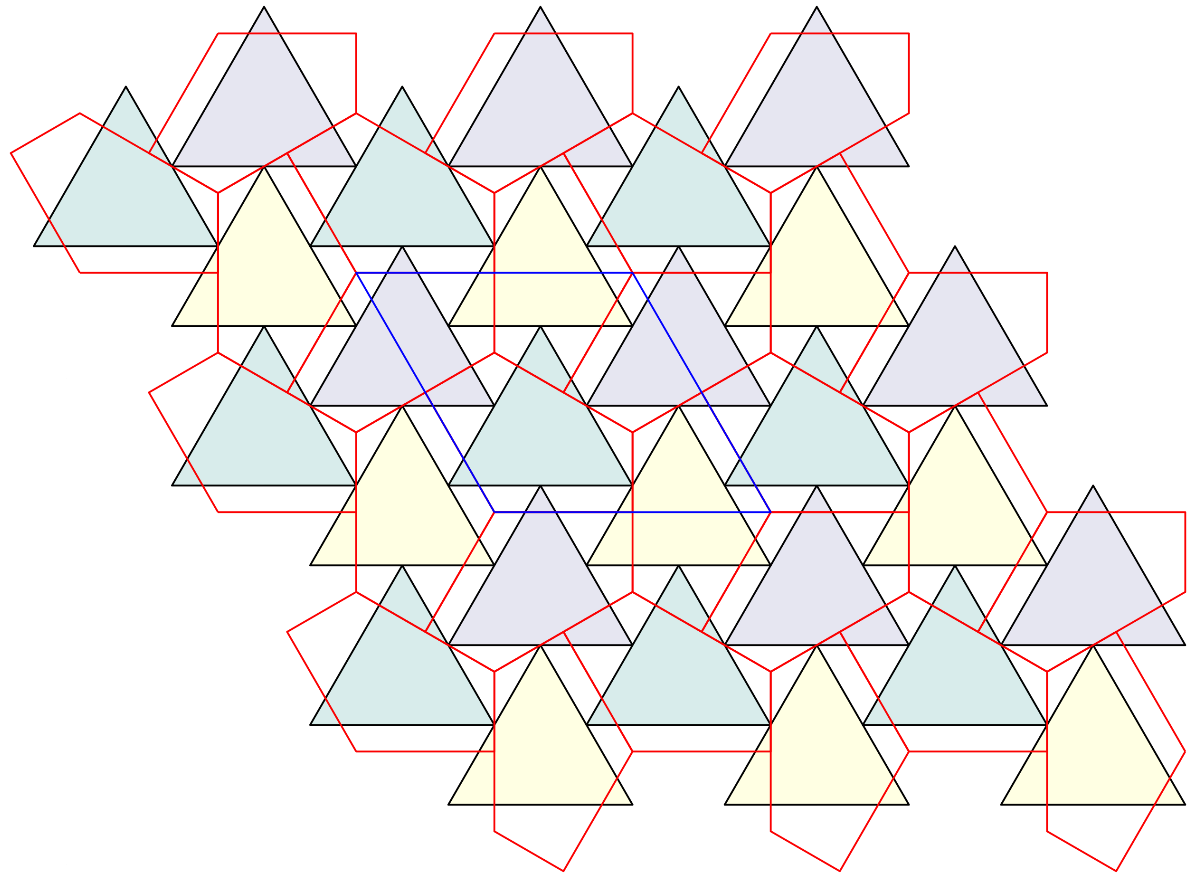
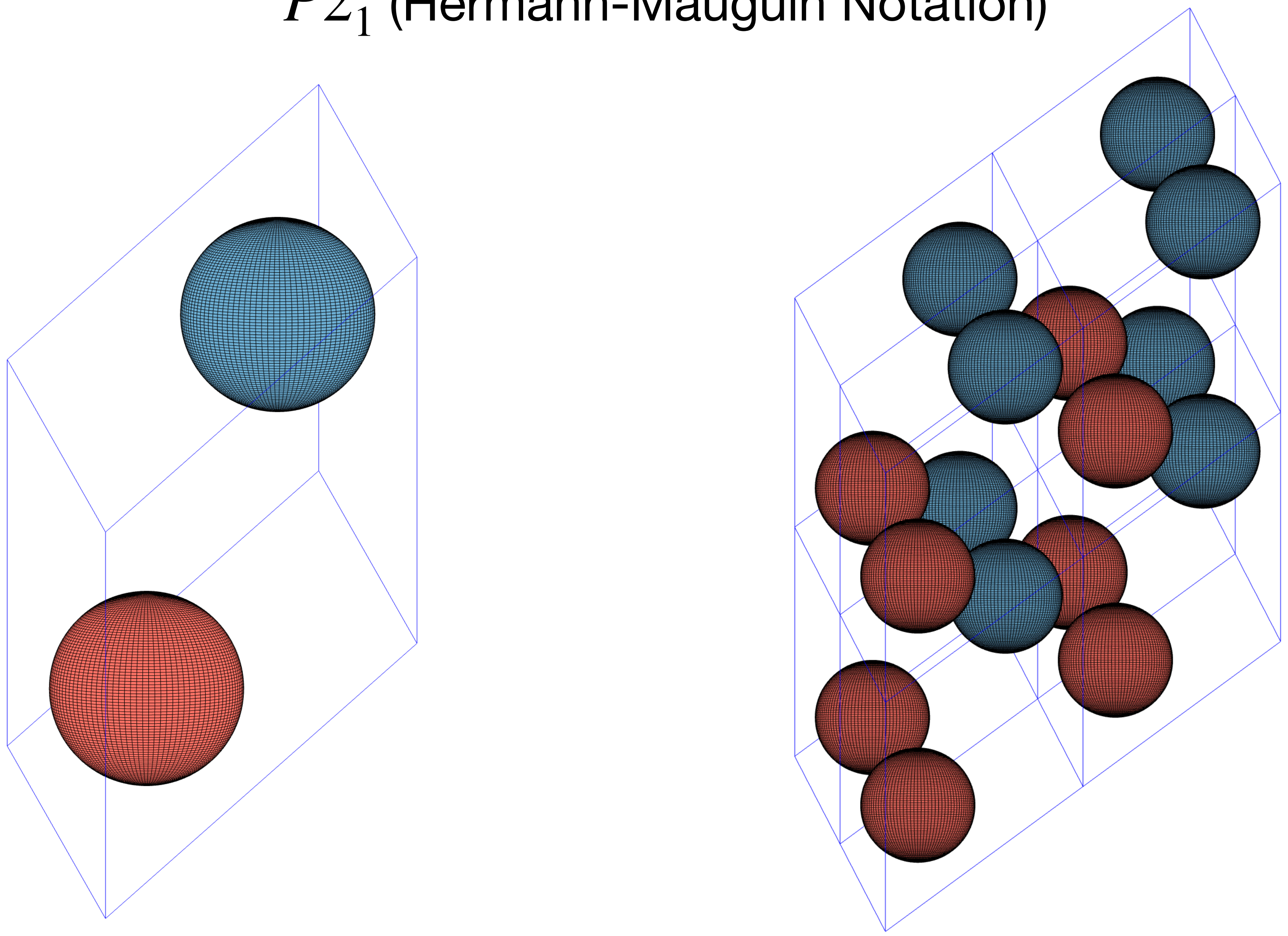


Space Groups ($n = 3$)

$P2_1$ (Hermann-Mauguin Notation)



Point Group $K \cong G/L_n$

§ W. Miller, Symmetry Groups and Their Applications, Academic Press, 1973.

Case of The Pairwise Potential $\phi_{(i,j)} = u_{(i,j)}$ ($\phi^{\text{electrostatic}}_{(i,j)} = 0$).

- Experimental analysis of symmetries of the densest packings of 34 regular polygons[1]

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

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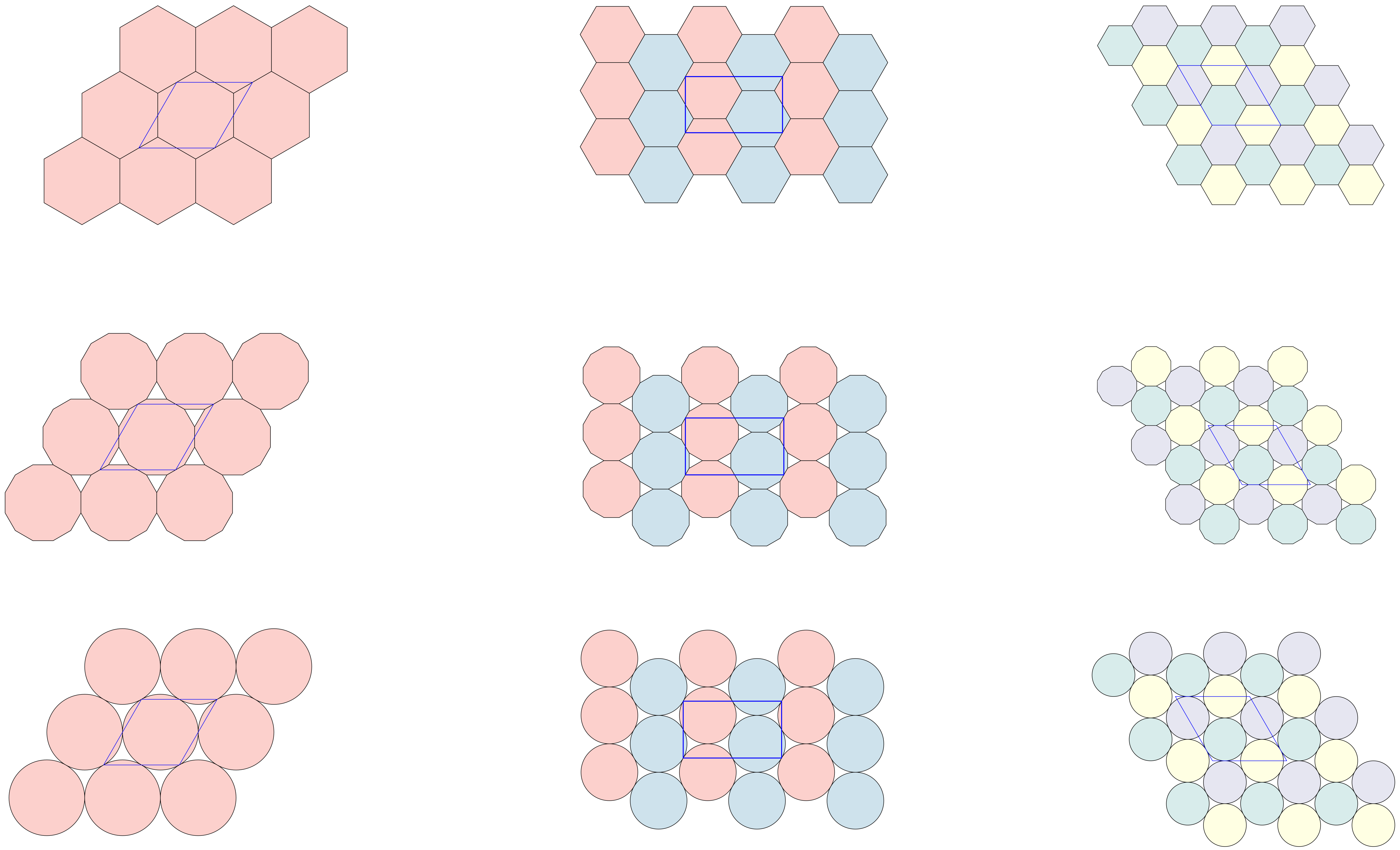
$p1$ $p2$ $p3$

Hexagon

Dodecagon

Disc[2]



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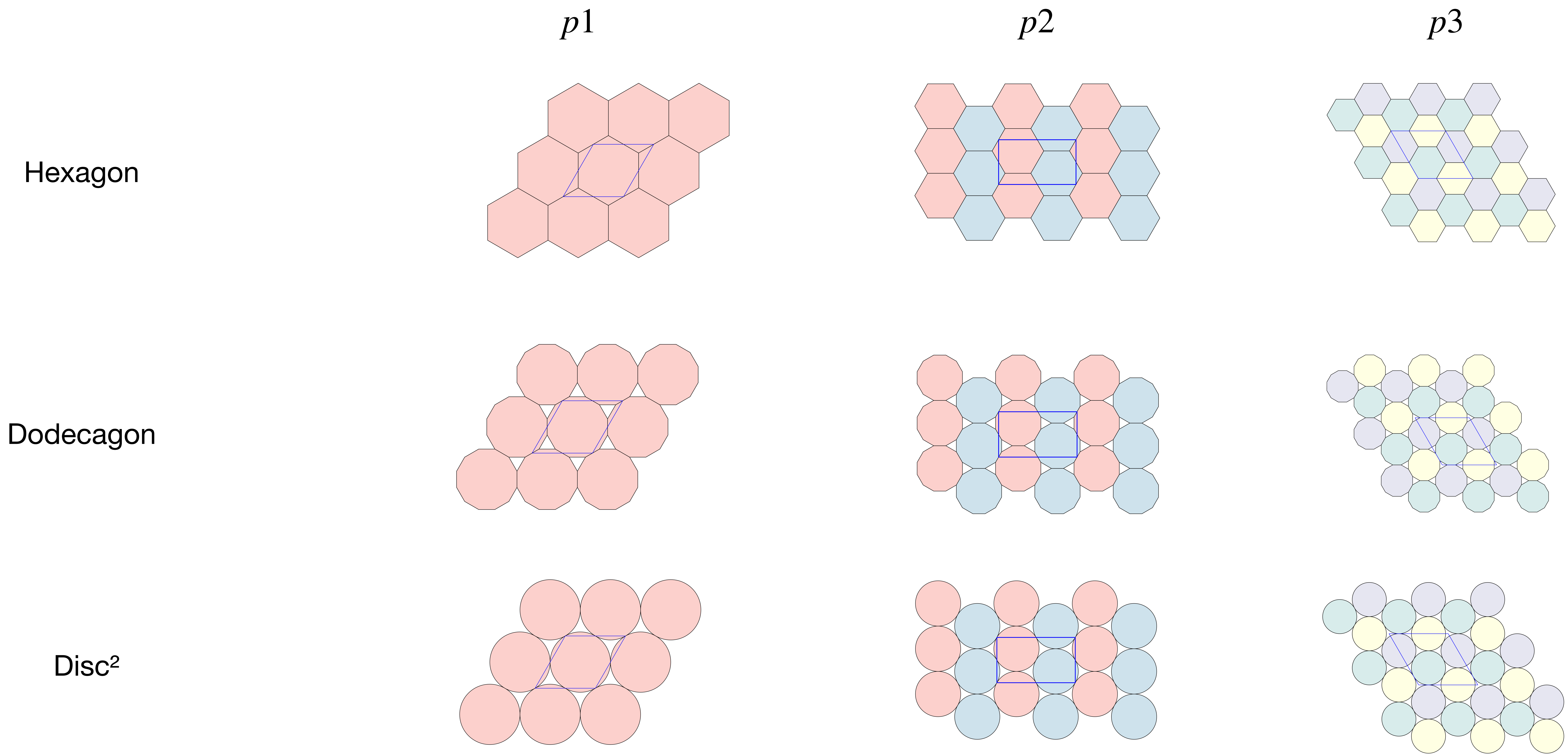
Case of The Pairwise Potential $\phi_{(i,j)} = u_{(i,j)}$ ($\phi^{\text{electrostatic}}_{(i,j)} = 0$).

- Experimental analysis of symmetries of the densest packings of 34 regular polygons[1]
- **Observation.** Symmetries of the densest packing of a disc coincide with the symmetries of the densest packings of regular polygons with six-fold rotational symmetries.



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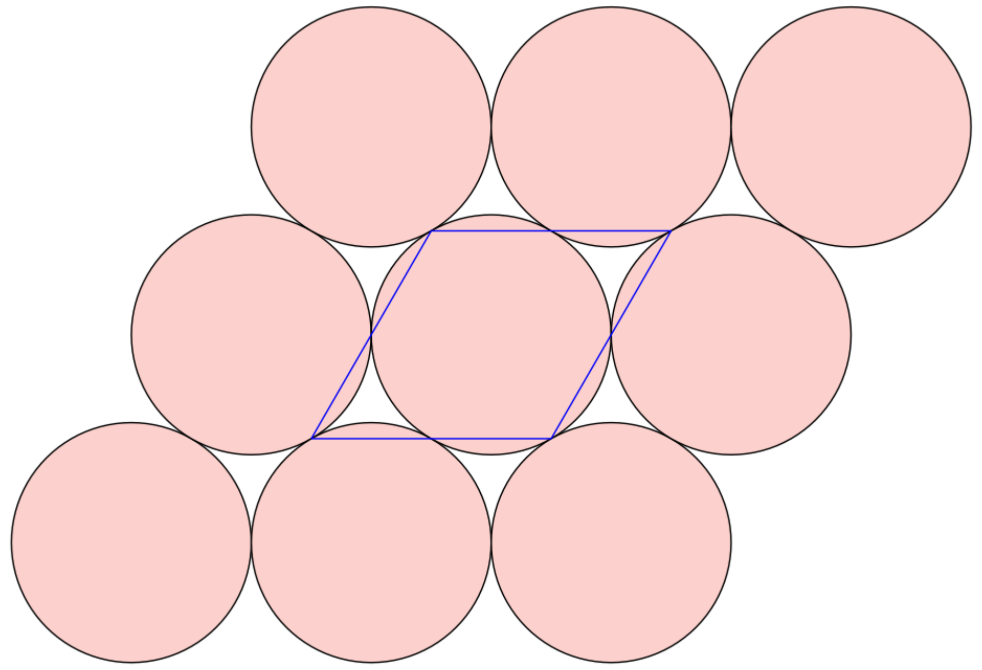
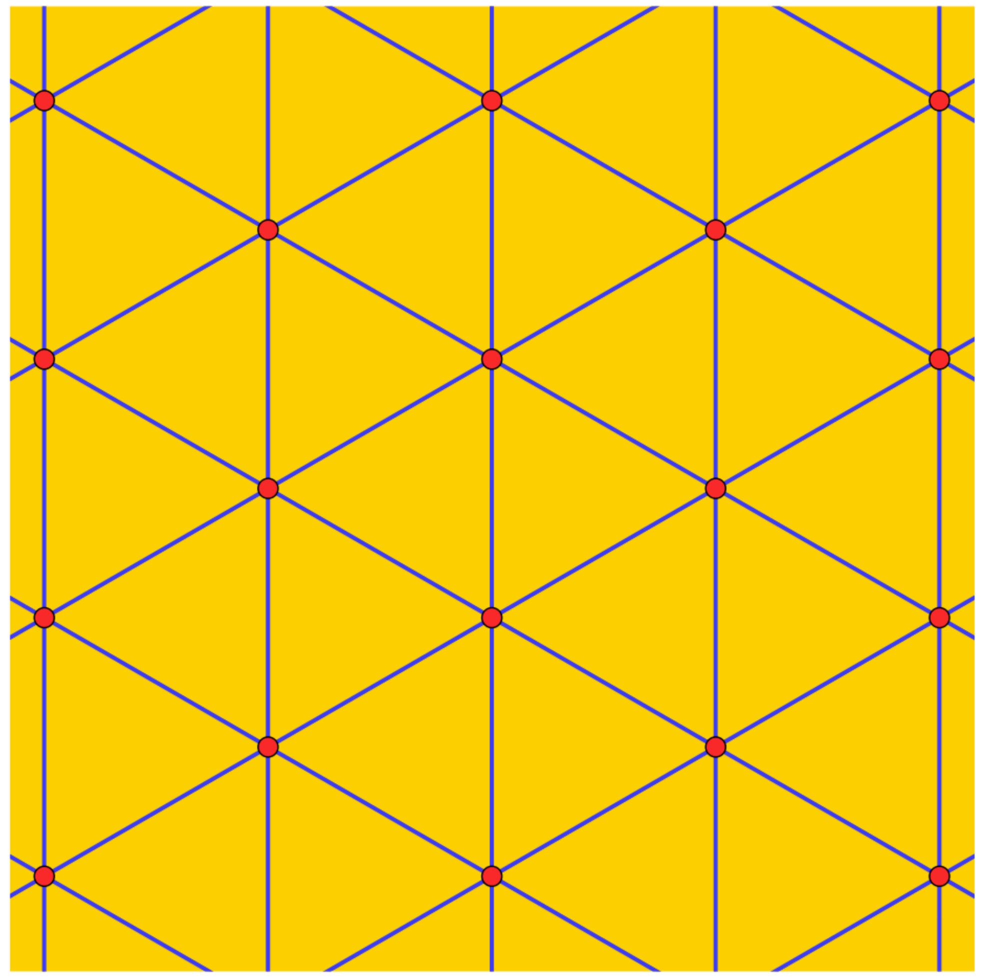
$\rho\left(\mathscr{K}_{p2/p2gg/pg/p3/p1\,\mathbf{max}}\right) = \frac{\sqrt{3}}{6}\pi = 0.9068996\ldots$



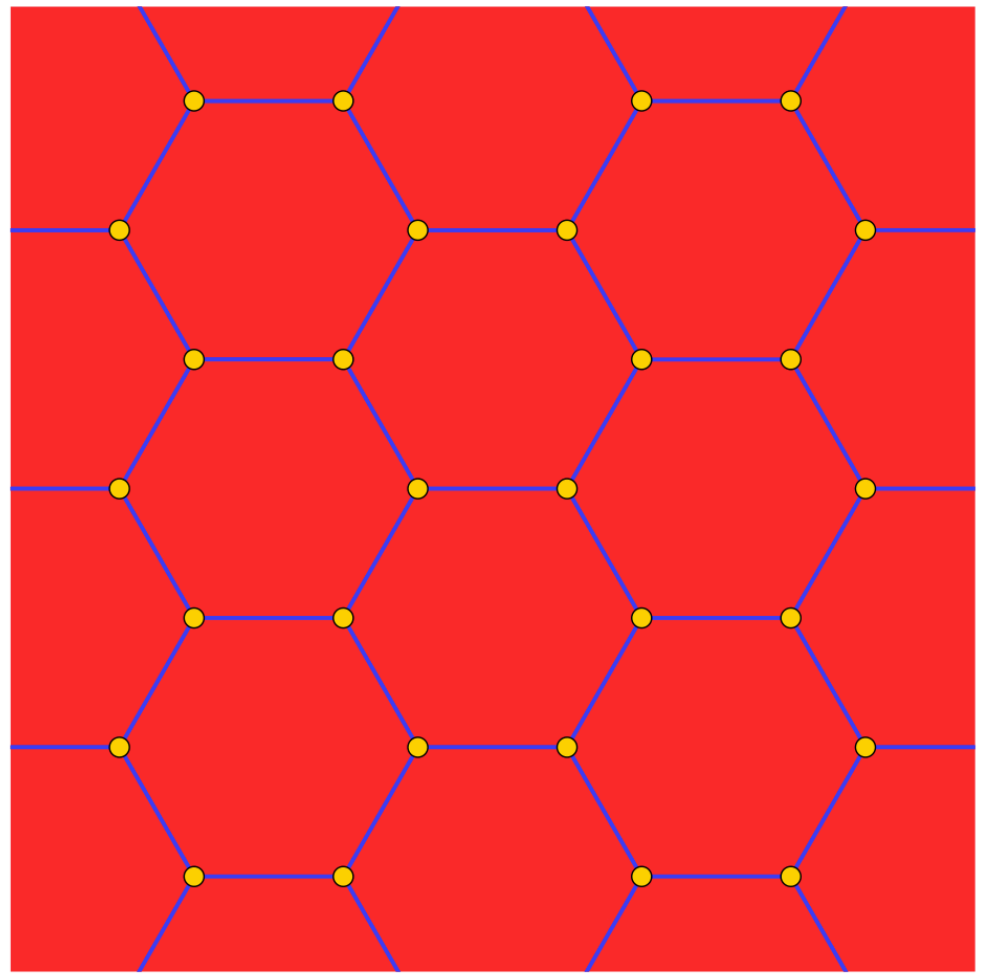
Densest Disc Packing

Regular tessellation



Triangular tiling

Dual tessellation



Hexagonal tiling

1. Triangular tiling. (2024, November 25). In *Wikipedia, The Free Encyclopedia*. https://en.wikipedia.org/wiki/Triangular_tiling
2. Hexagonal tiling. (2024, November 25). In *Wikipedia, The Free Encyclopedia*. https://en.wikipedia.org/wiki/Hexagonal_tiling

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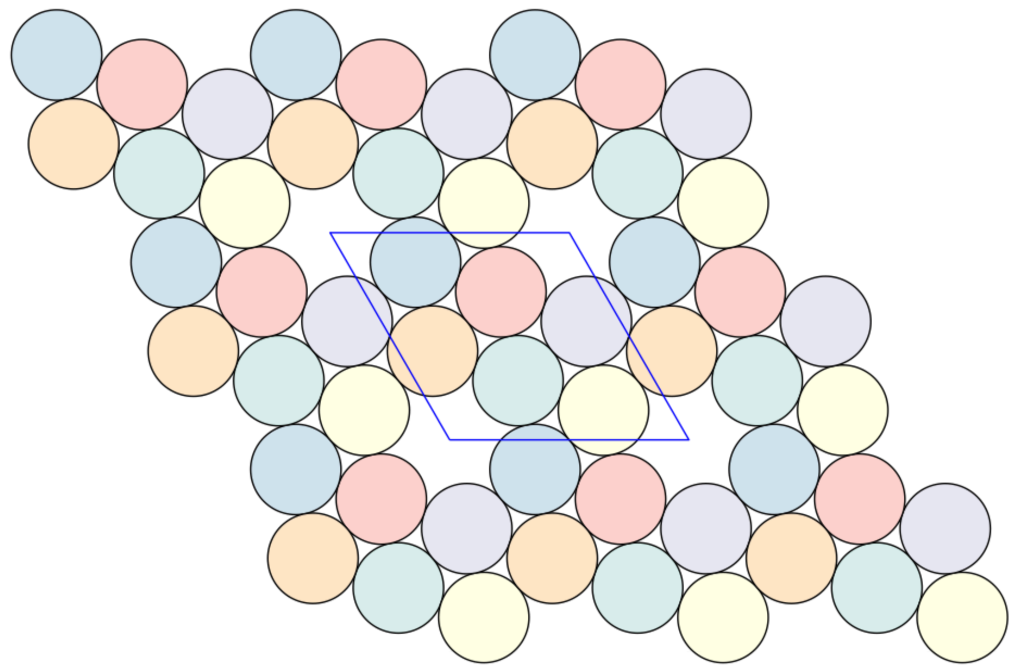
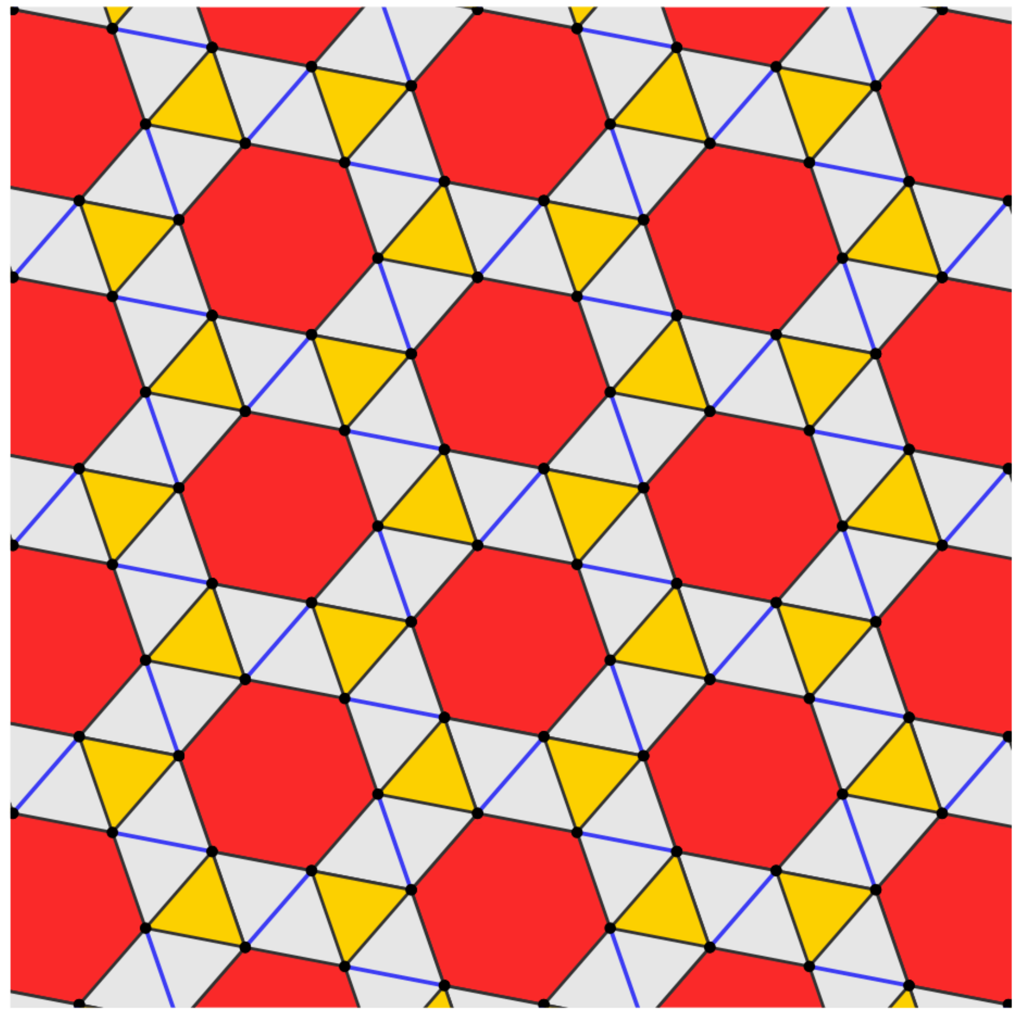
$$\rho\left(\mathscr{K}_{p6_{\textbf{max}}}\right) = \frac{\sqrt{3}}{7}\pi = 0.7773425\ldots$$

Regular tessellation

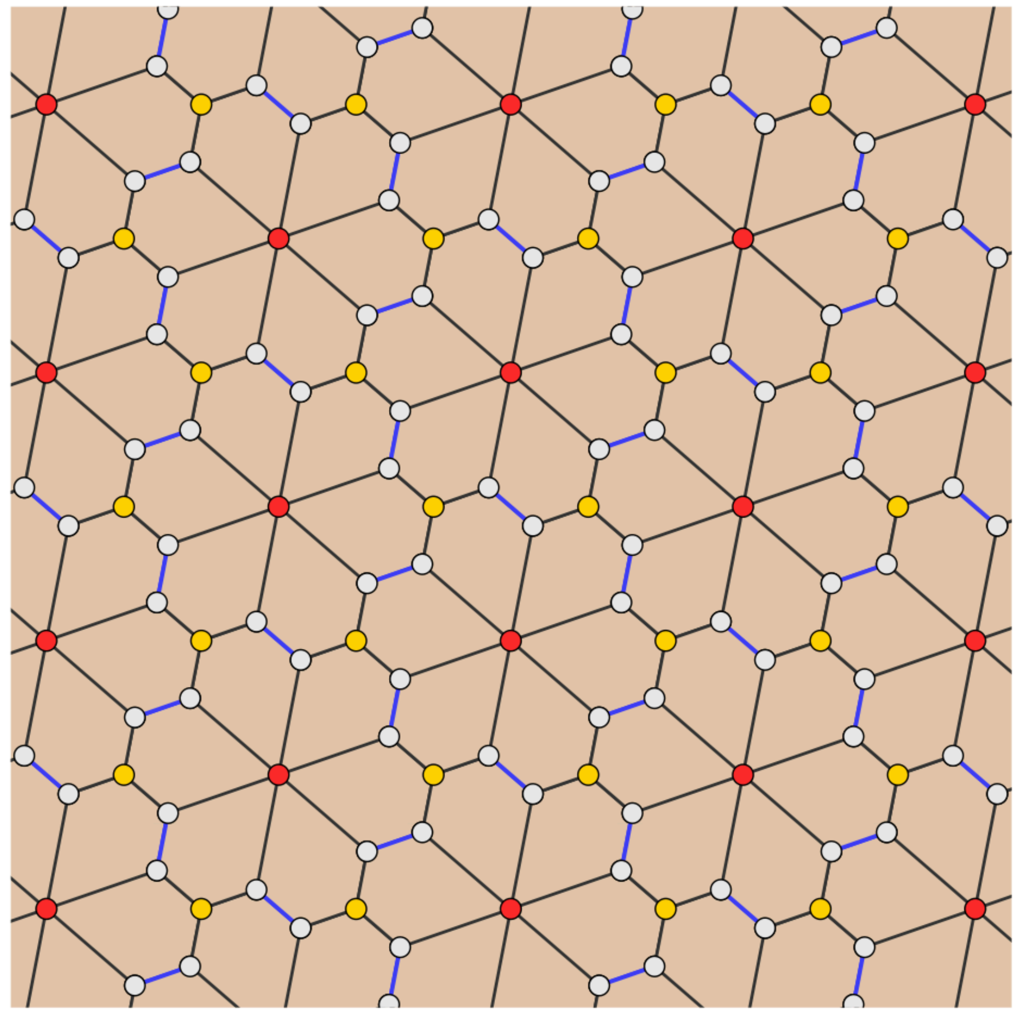
Dual tessellation



Densest $p6$ disc packing



Snub trihexagonal tiling



Floret pentagonal tiling

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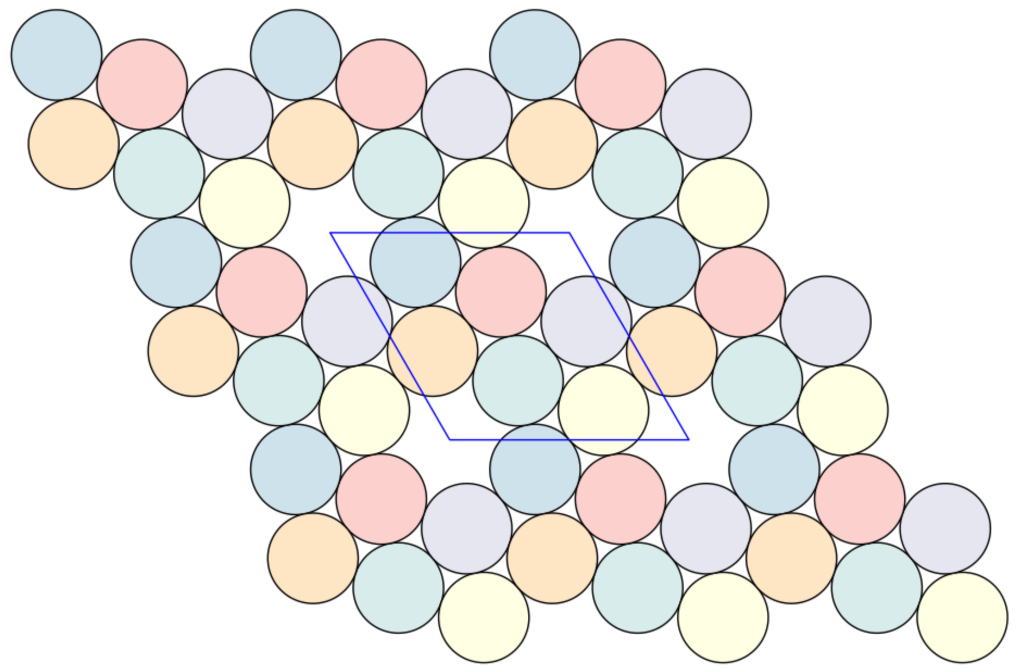
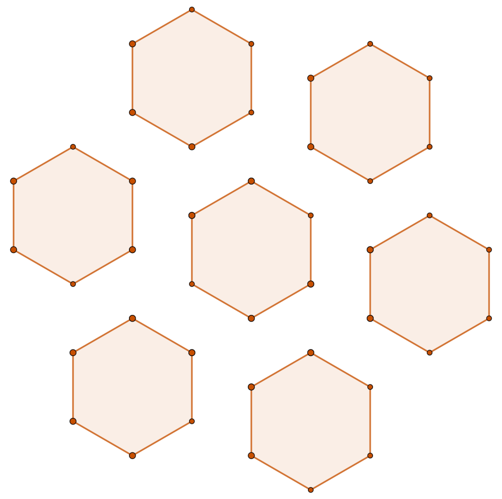
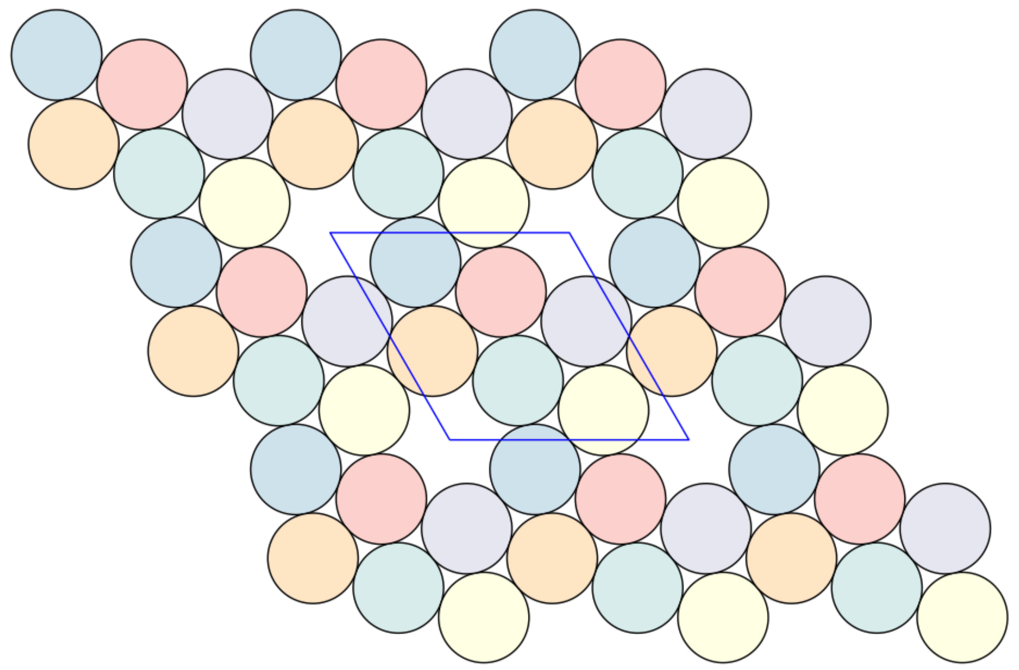


Densest $p6$ disc packing



Case of The Pairwise Potential $\phi_{(i,j)} = u_{(i,j)}$ ($\phi^{\textbf{electrostatic}}_{(i,j)} = 0$).

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



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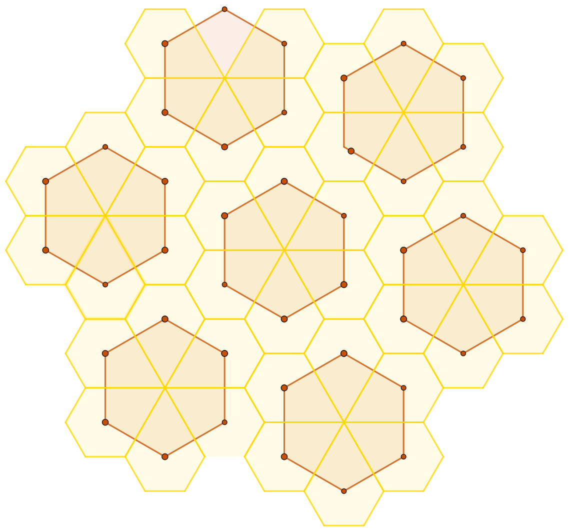

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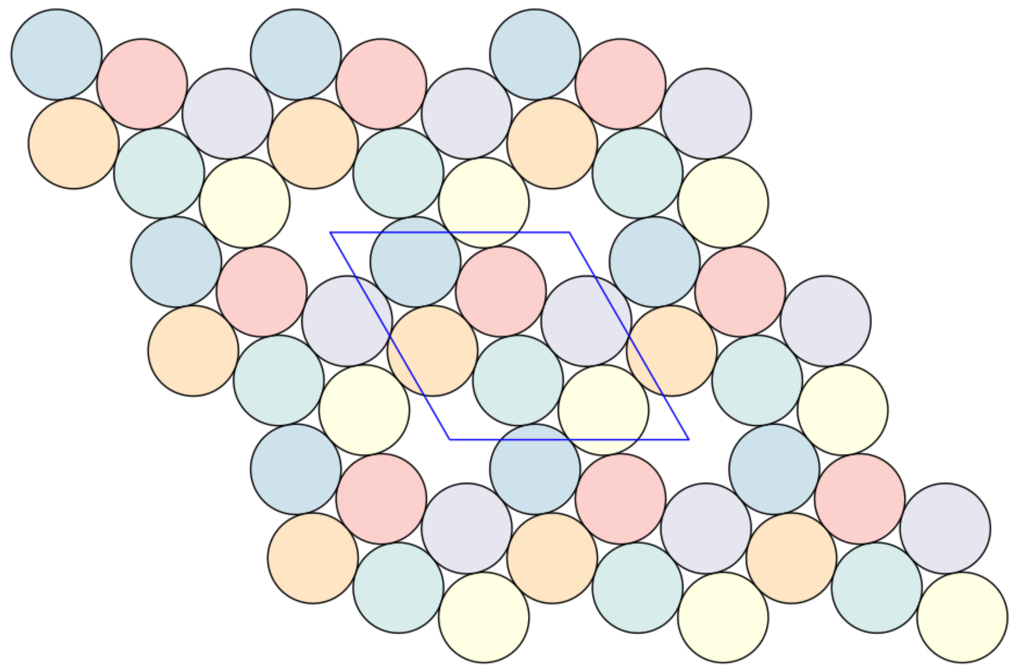

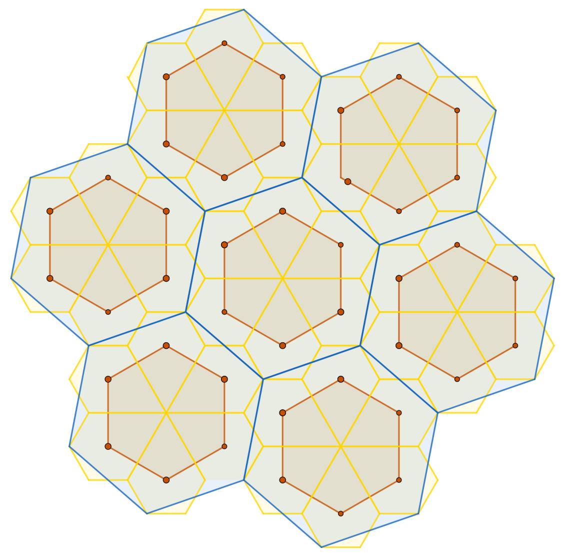

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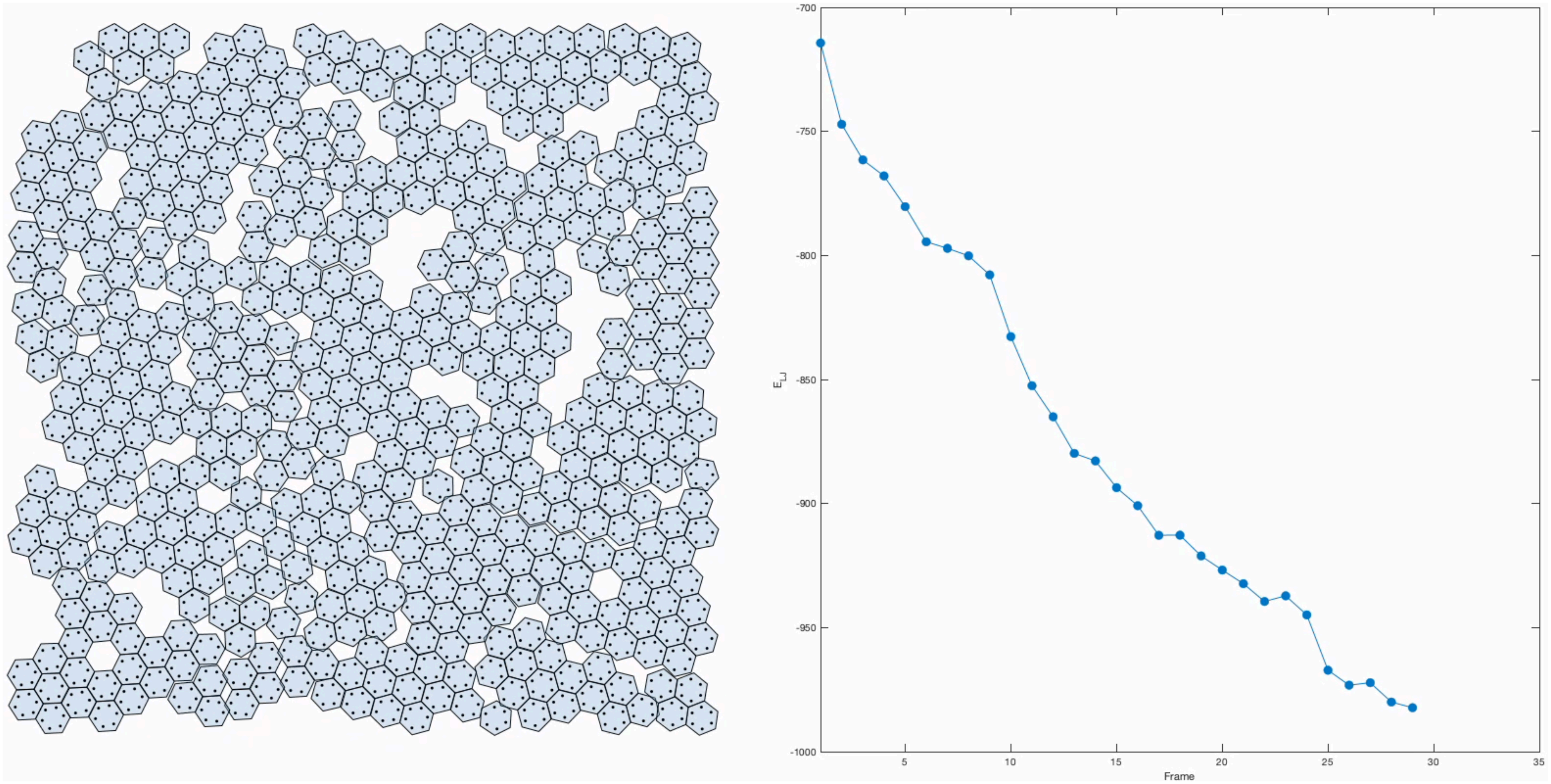

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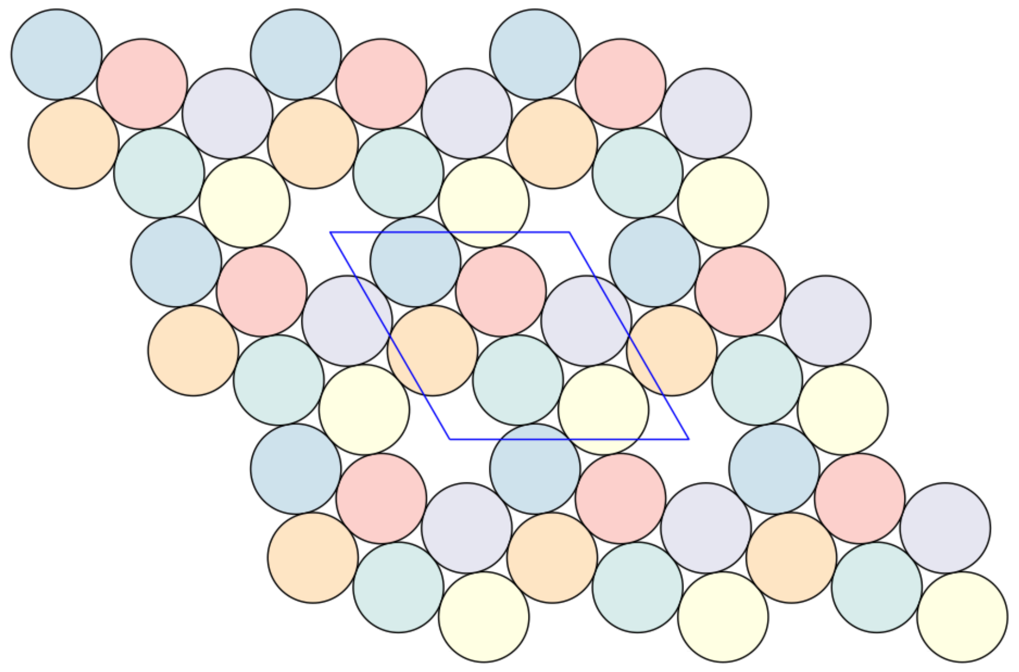

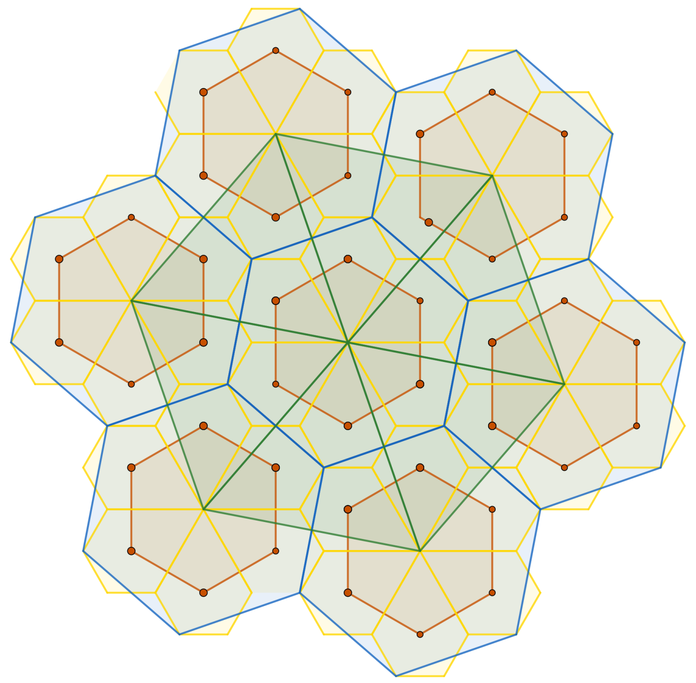

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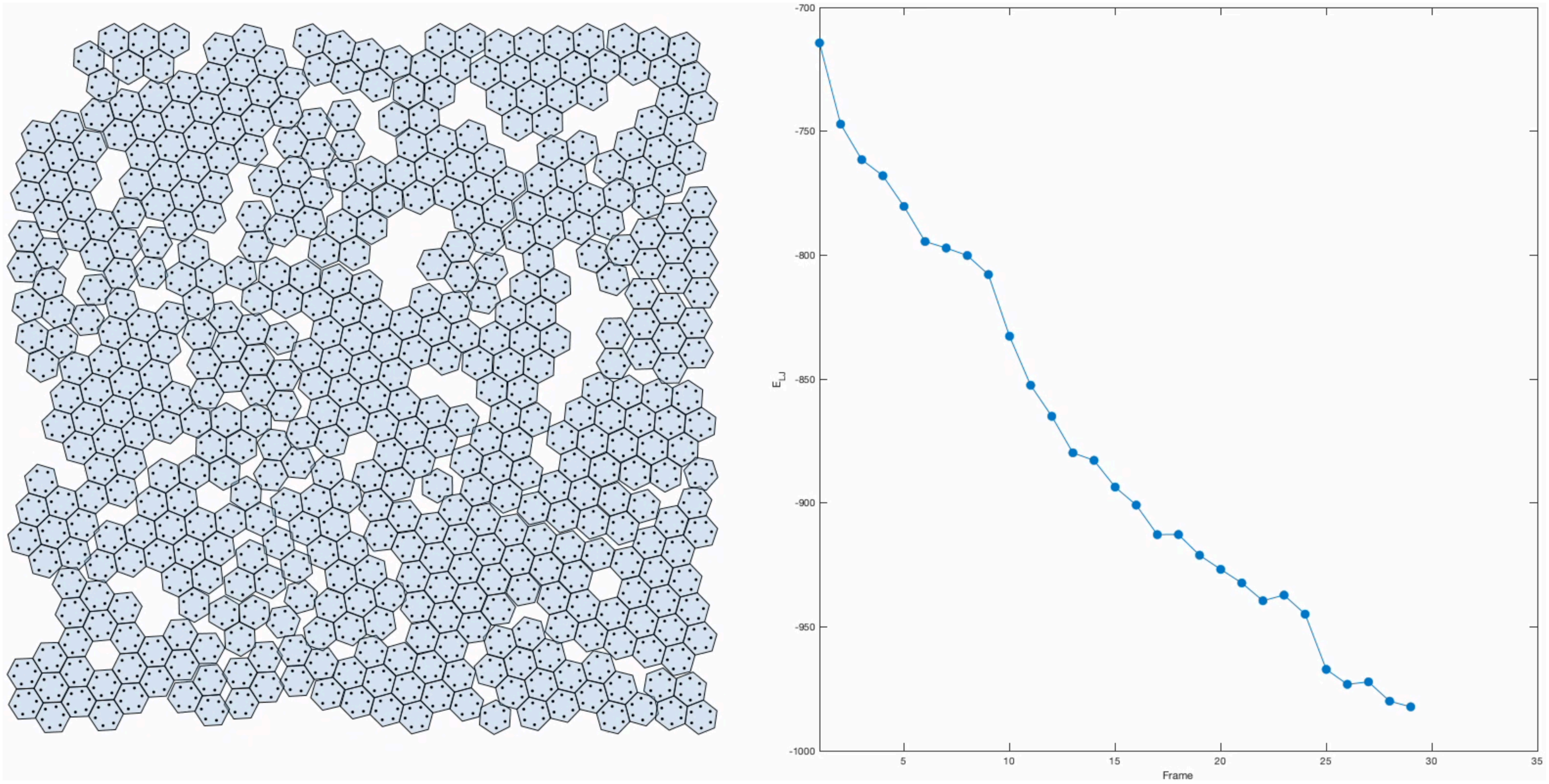

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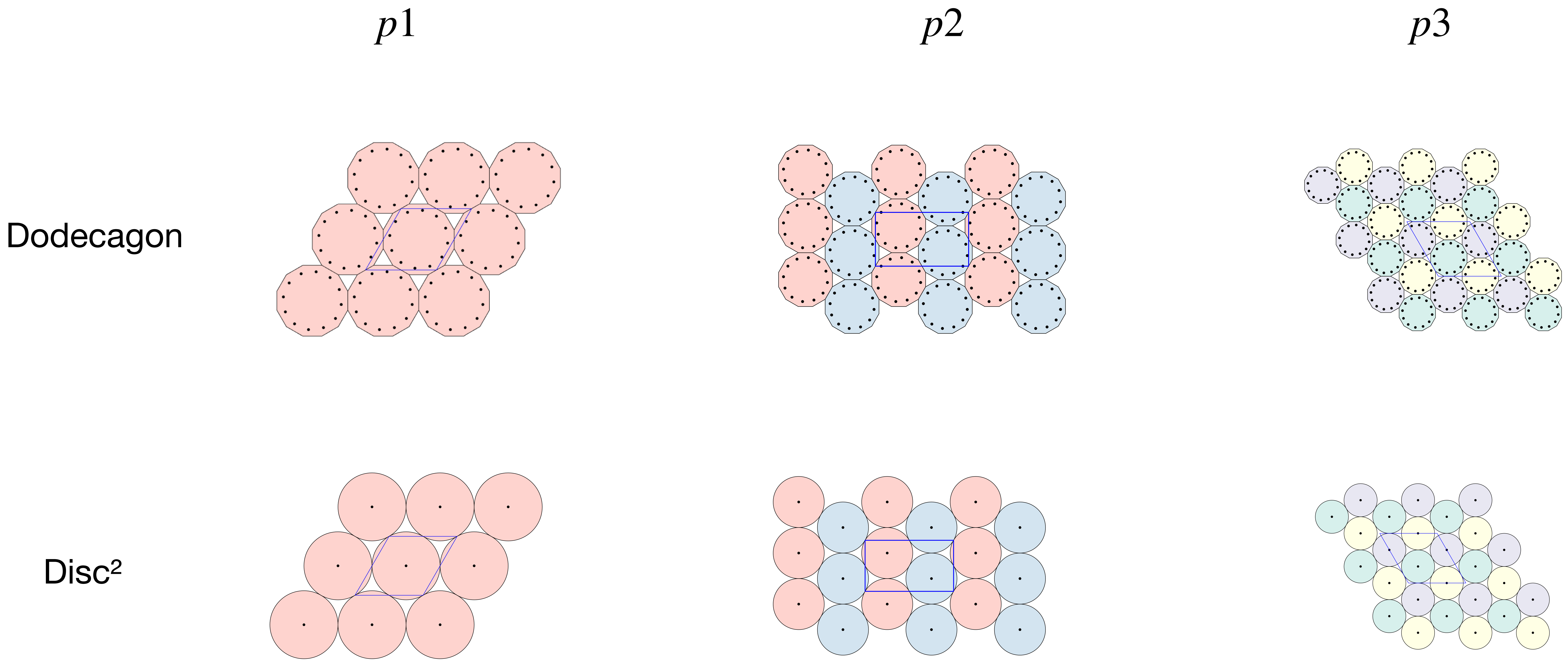
Conjecture. For any regular molecule with six-fold rotational symmetry and Lennard-Jones-like inter atomic potential, the ground state configuration is given by the densest packing of the corresponding regular polygon.



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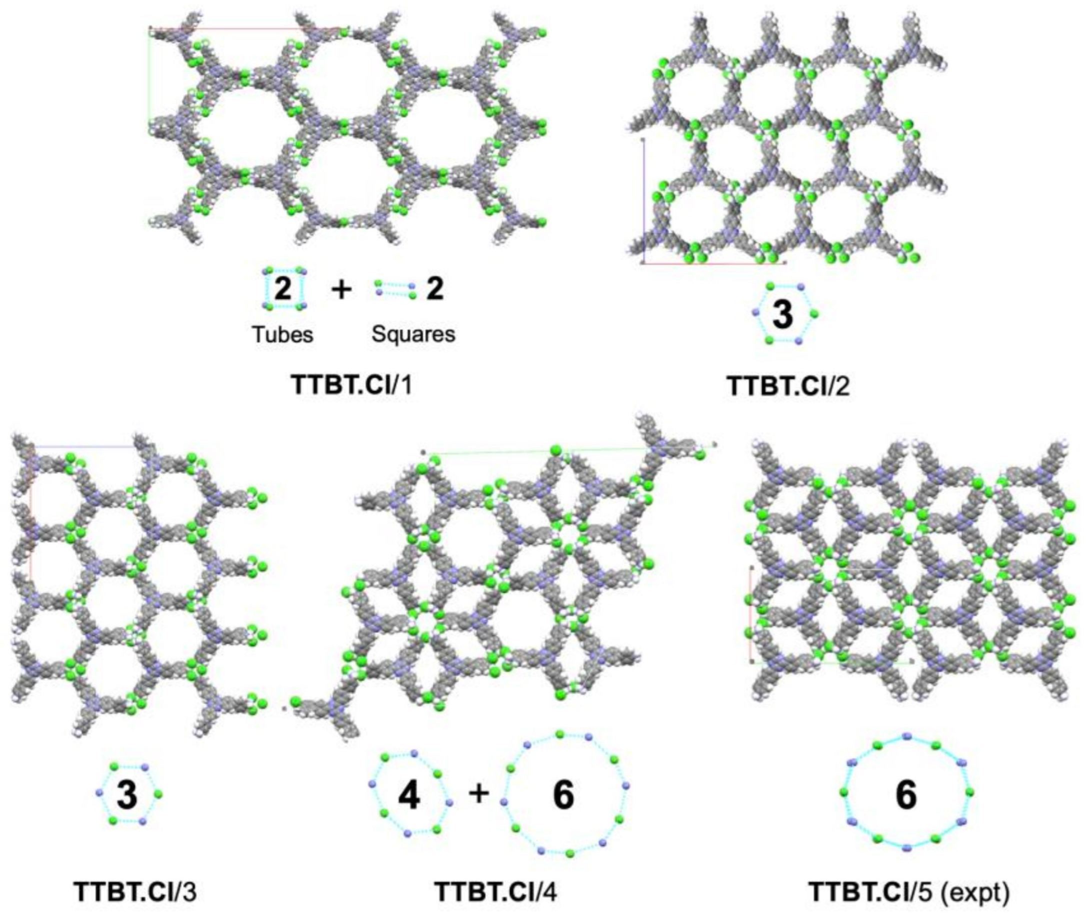
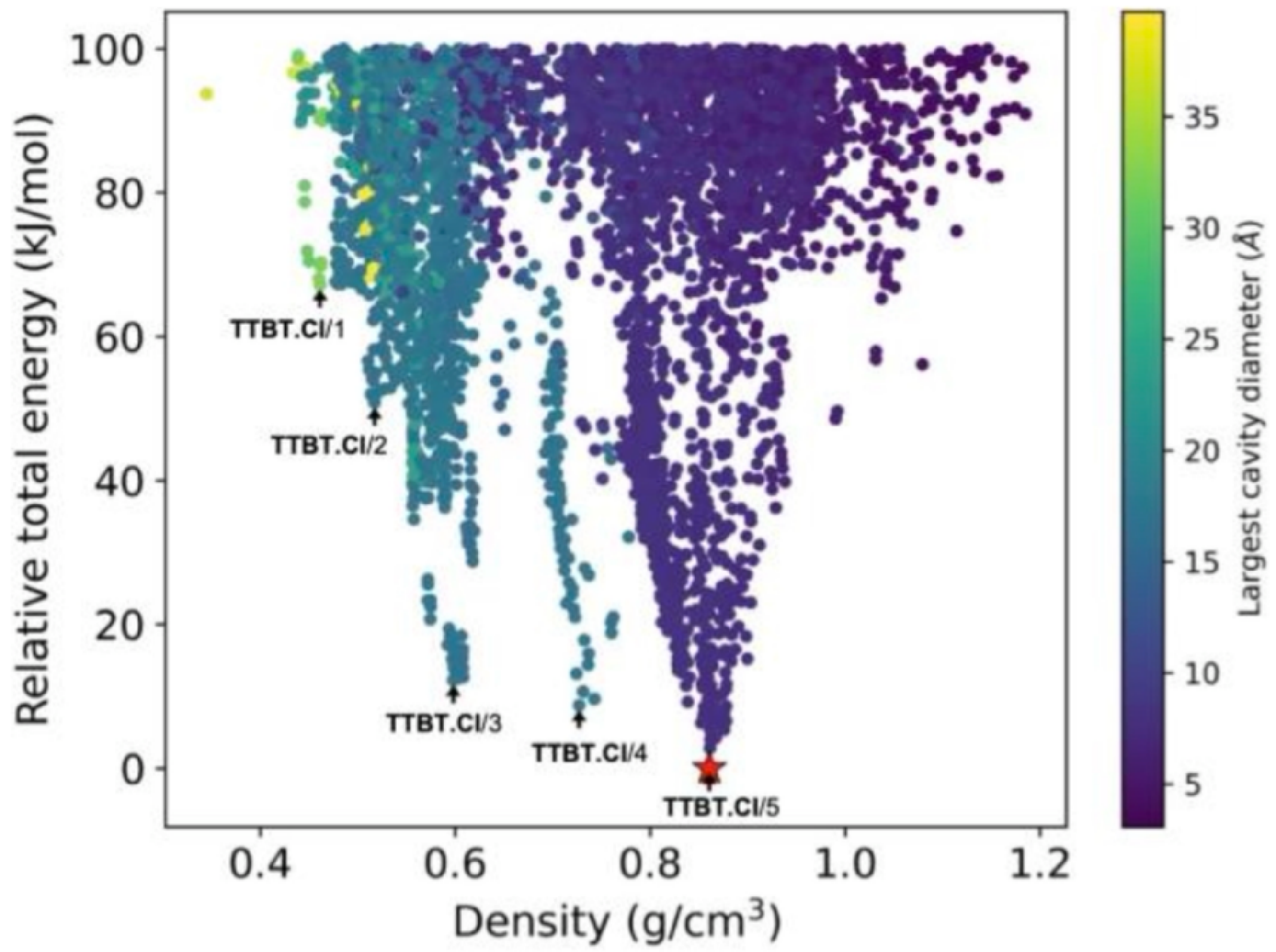
Non-Metal Organic Frameworks[1]





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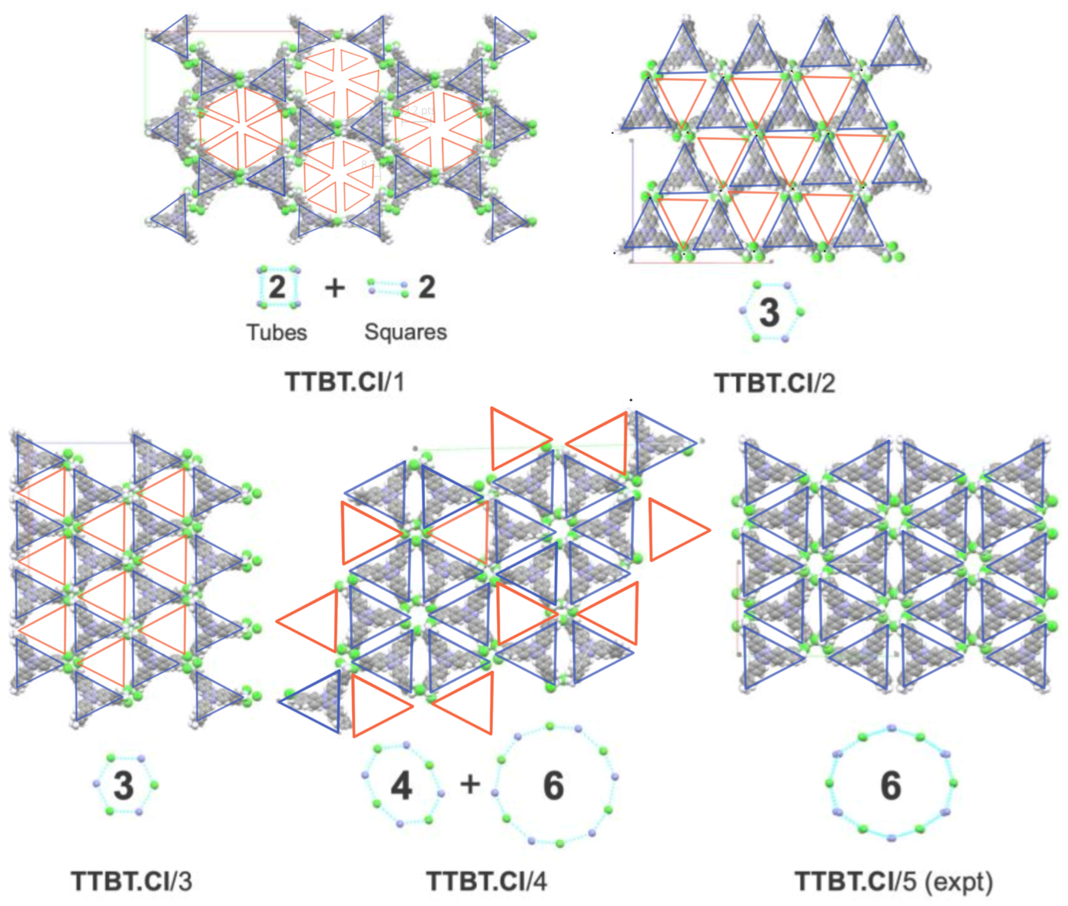

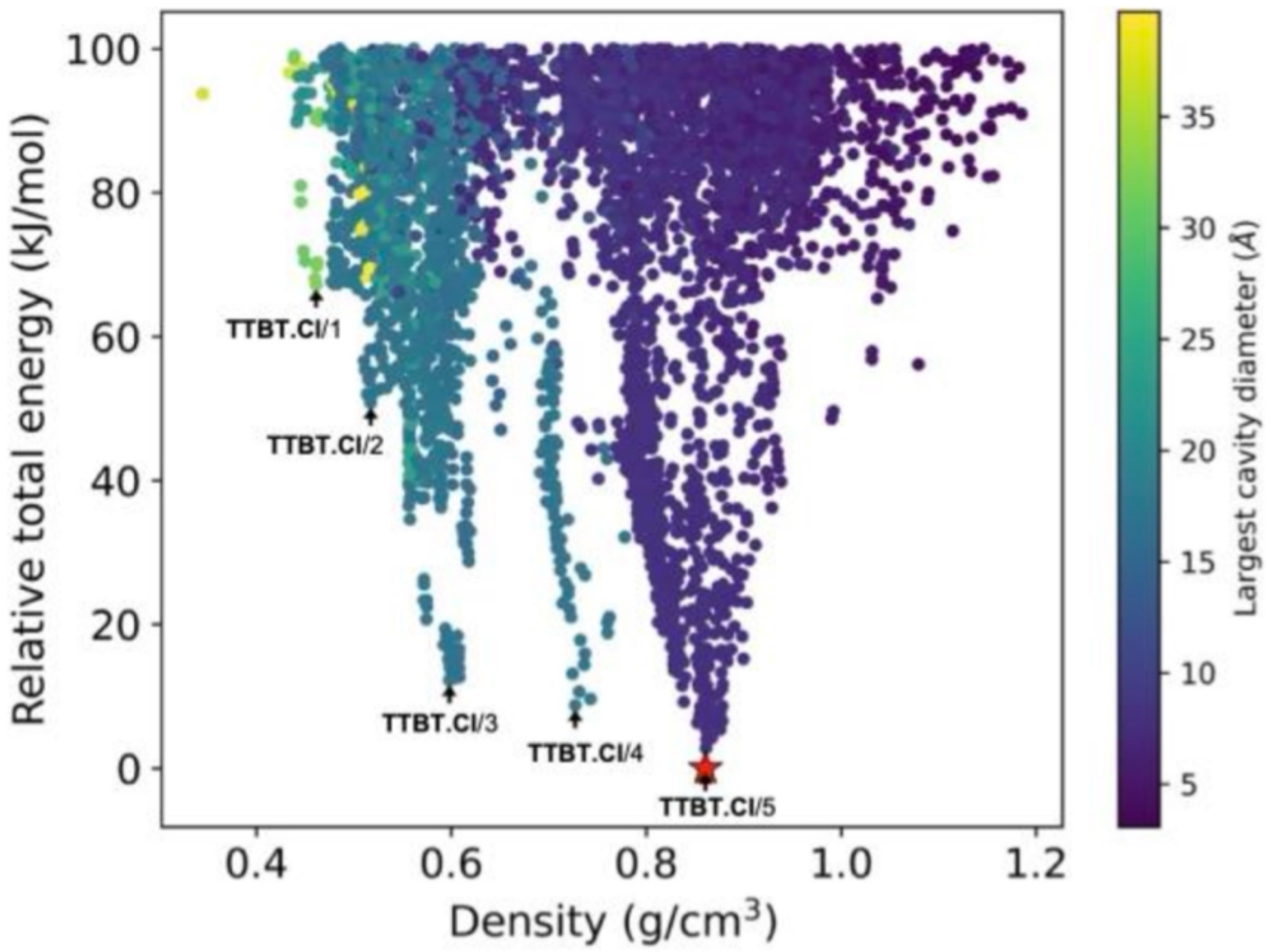

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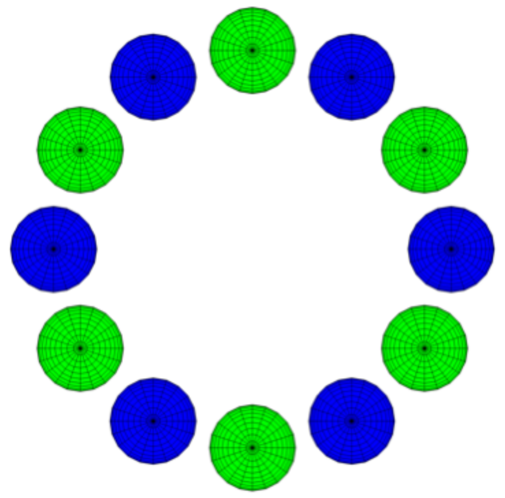
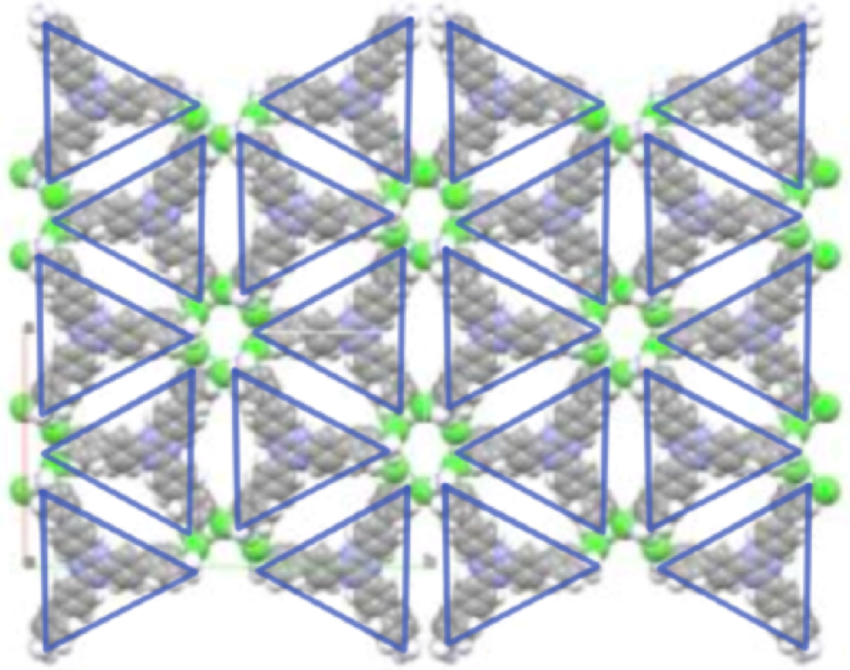
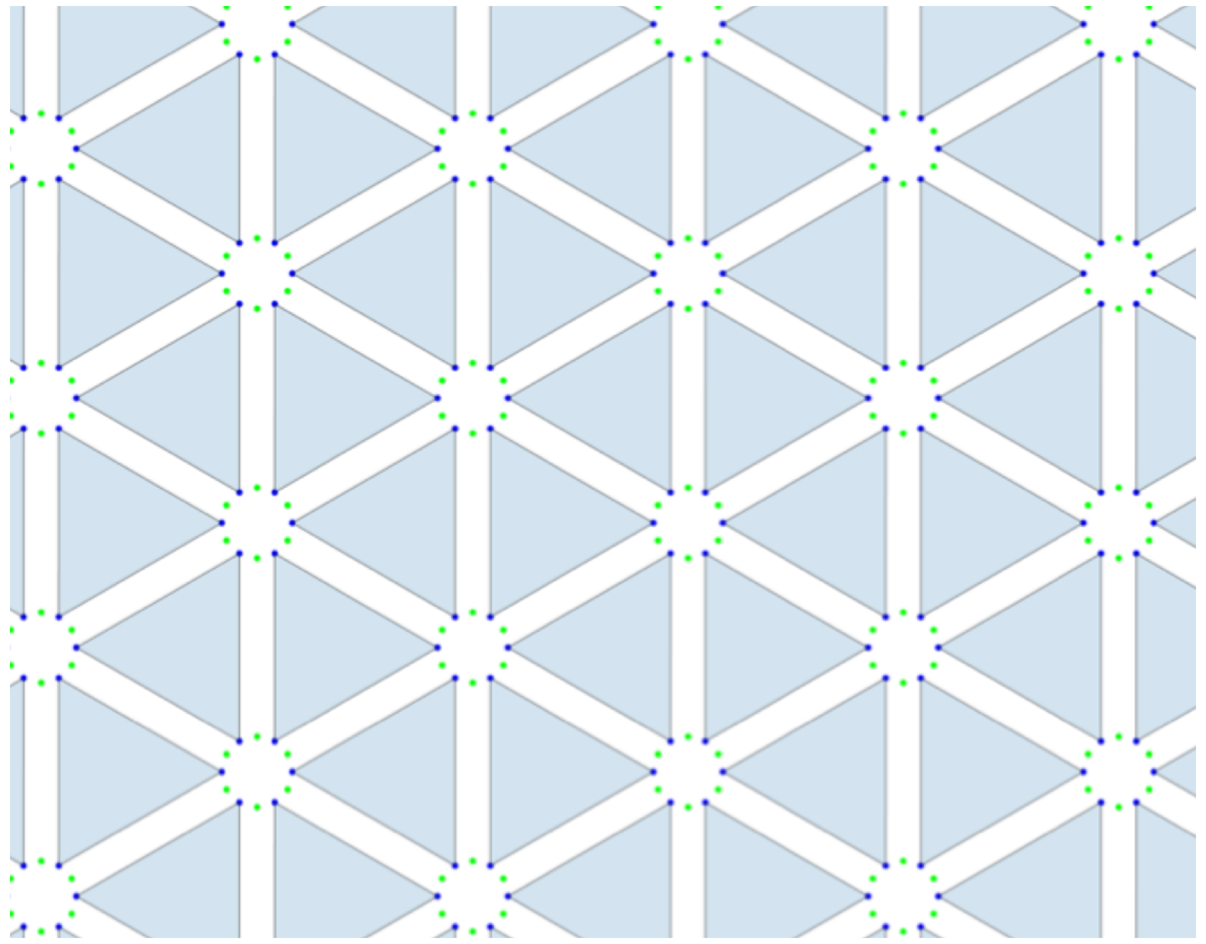
Coulomb potential. $$\phi_{(i,j)} = \begin{cases} -\frac{1}{r_{(i,j)}}, i \in \mathcal{I}, j \in \mathcal{J} \\ \frac{1}{r_{(i,j)}}, i,j \in \mathcal{I}, i \neq j \\ \frac{1}{r_{(i,j)}}, i,j \in \mathcal{J}, i \neq j \end{cases}$$

$$E_C = \sum_{i,j \in I \cup J} \phi_{(i,j)} = 0$$





TTBT.Cl/5 (expt)



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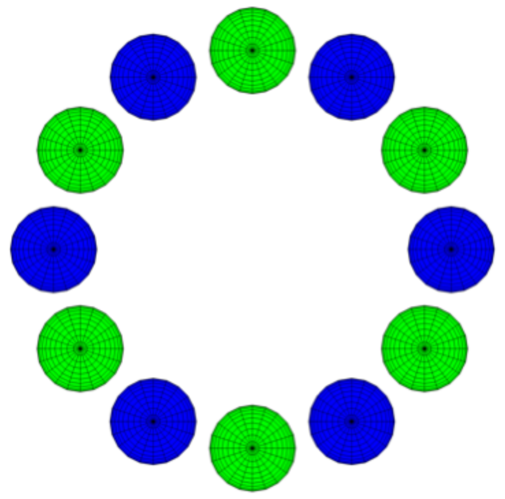

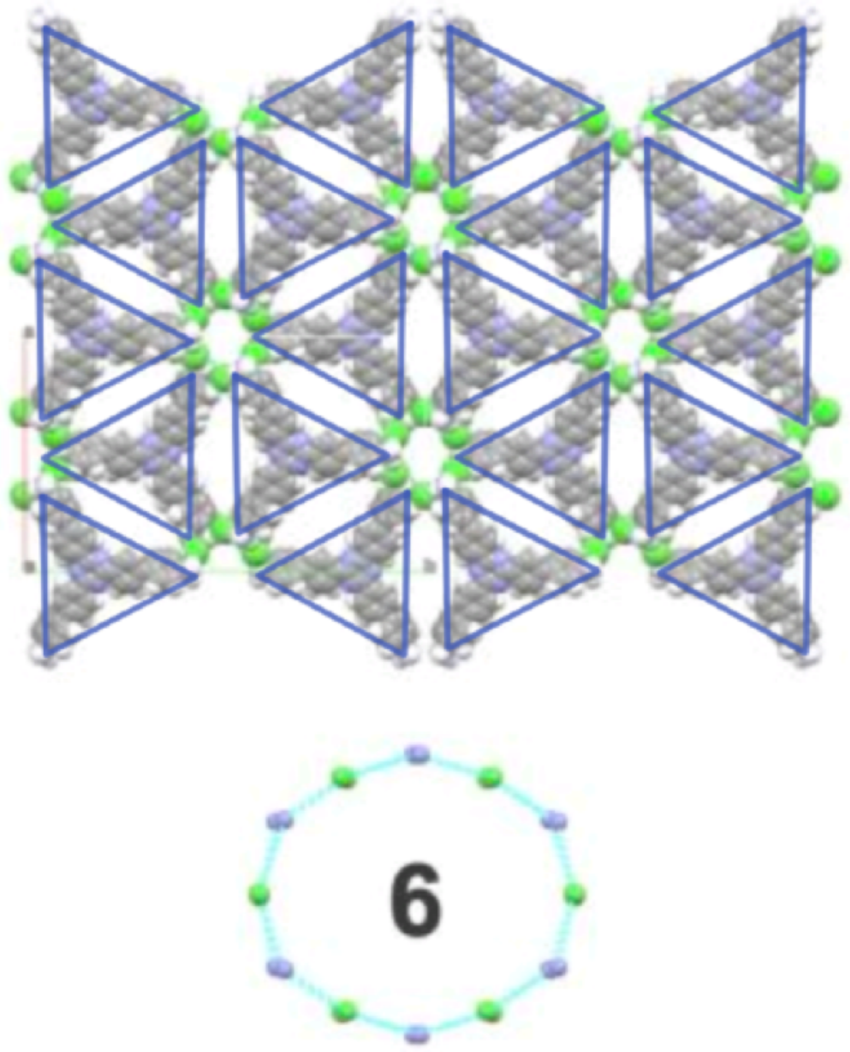

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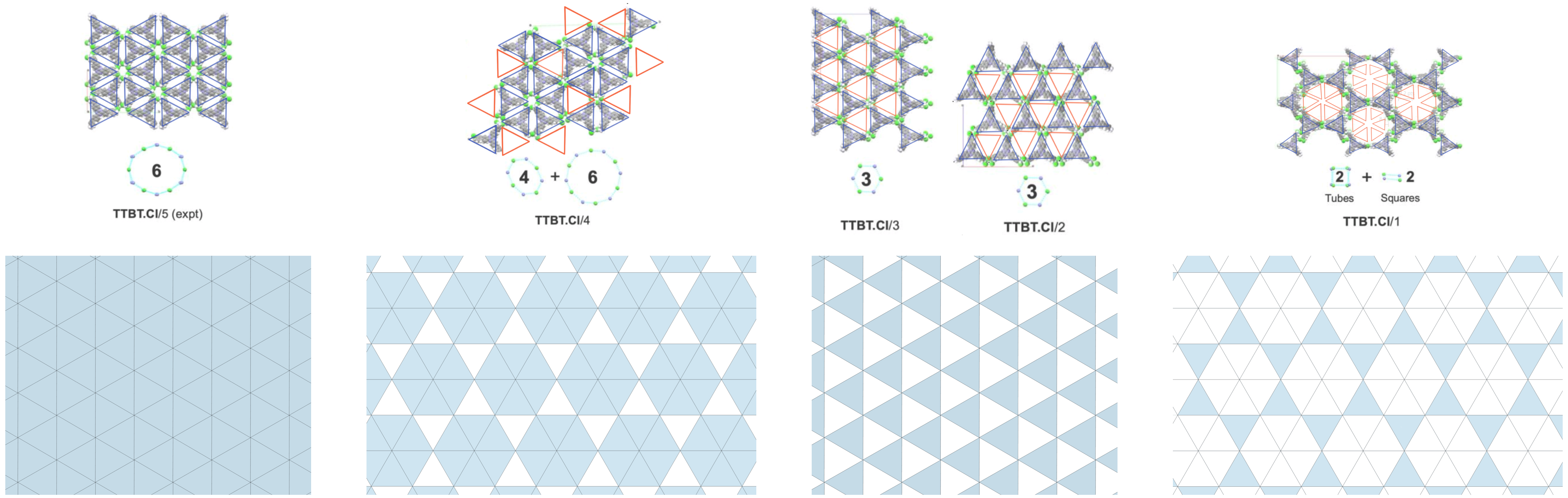

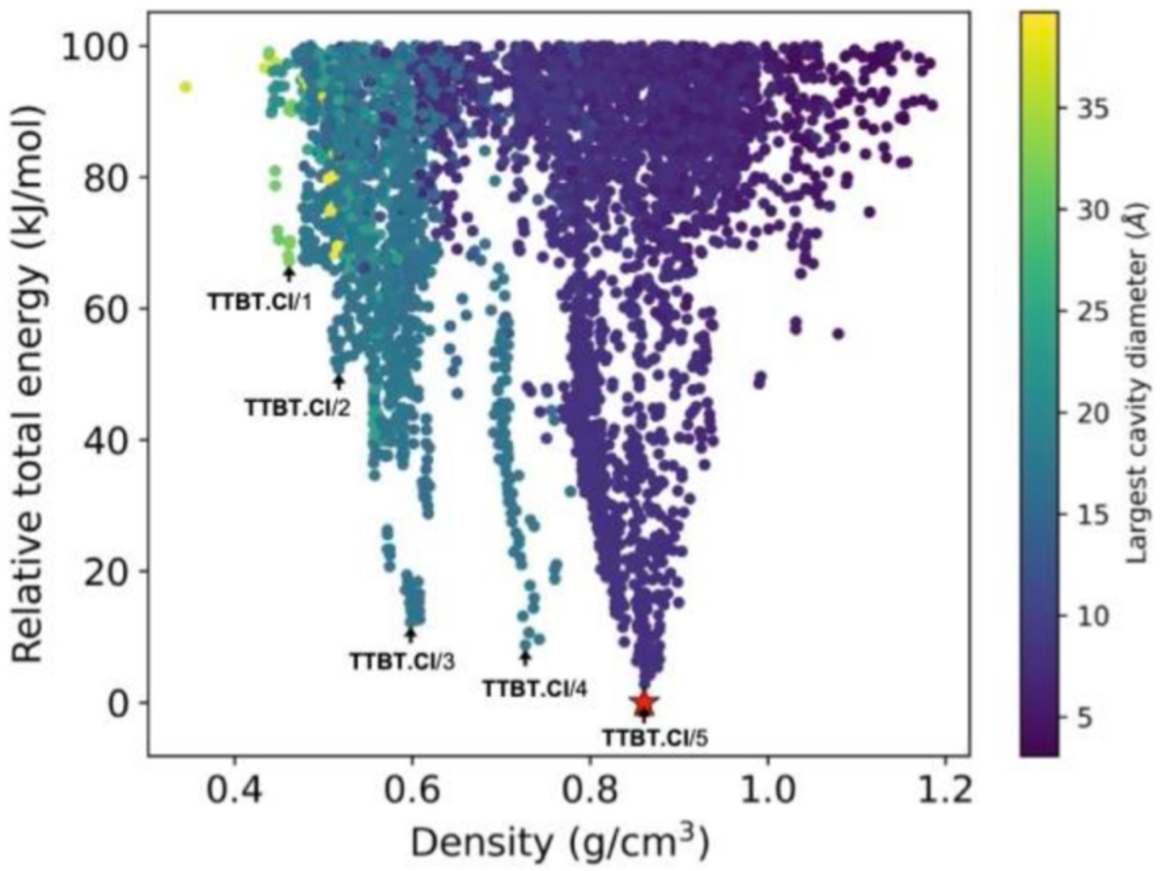

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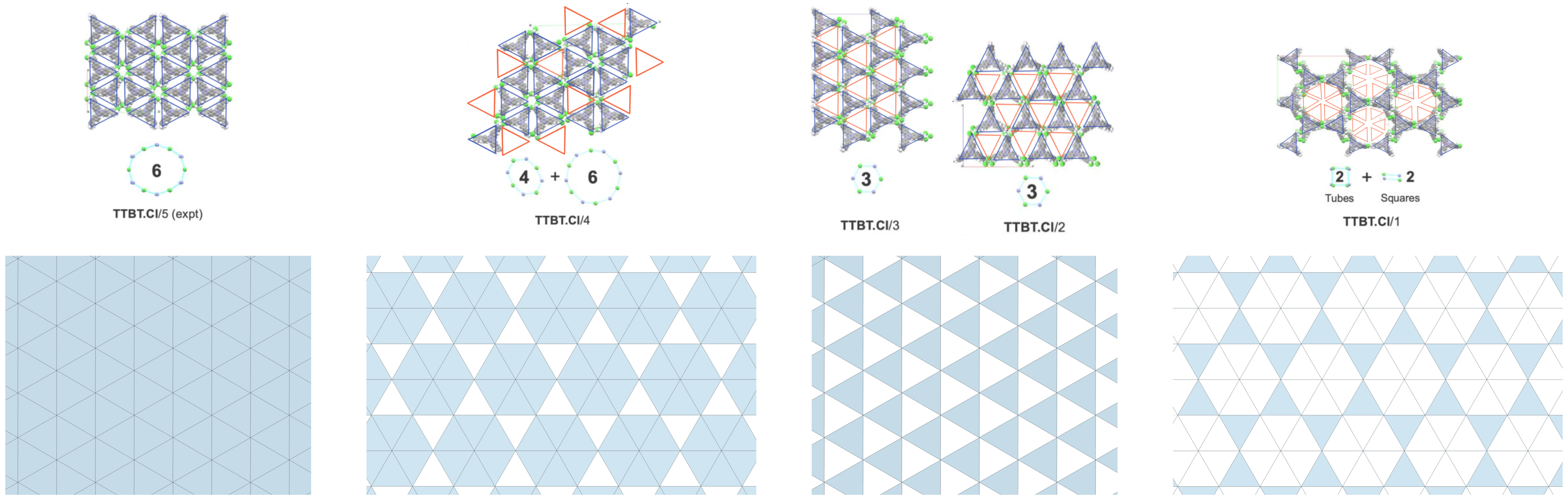

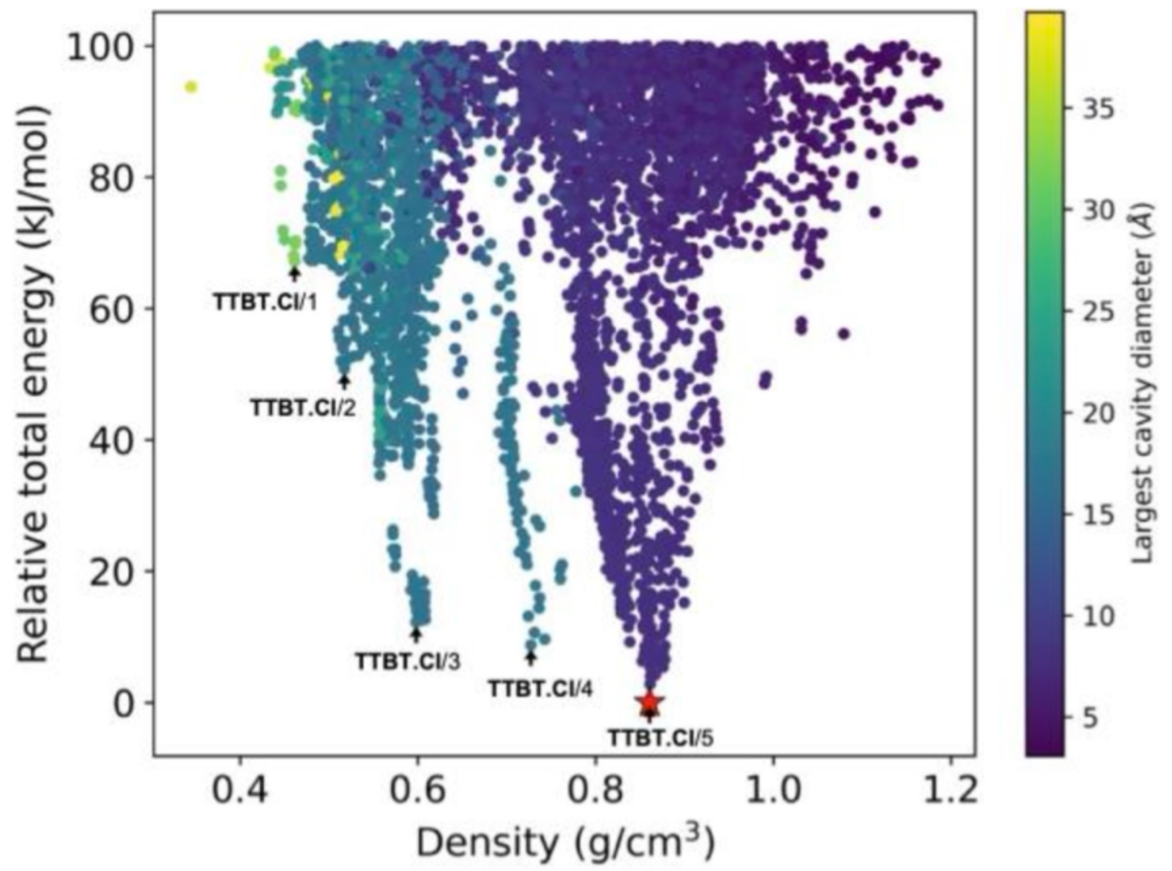

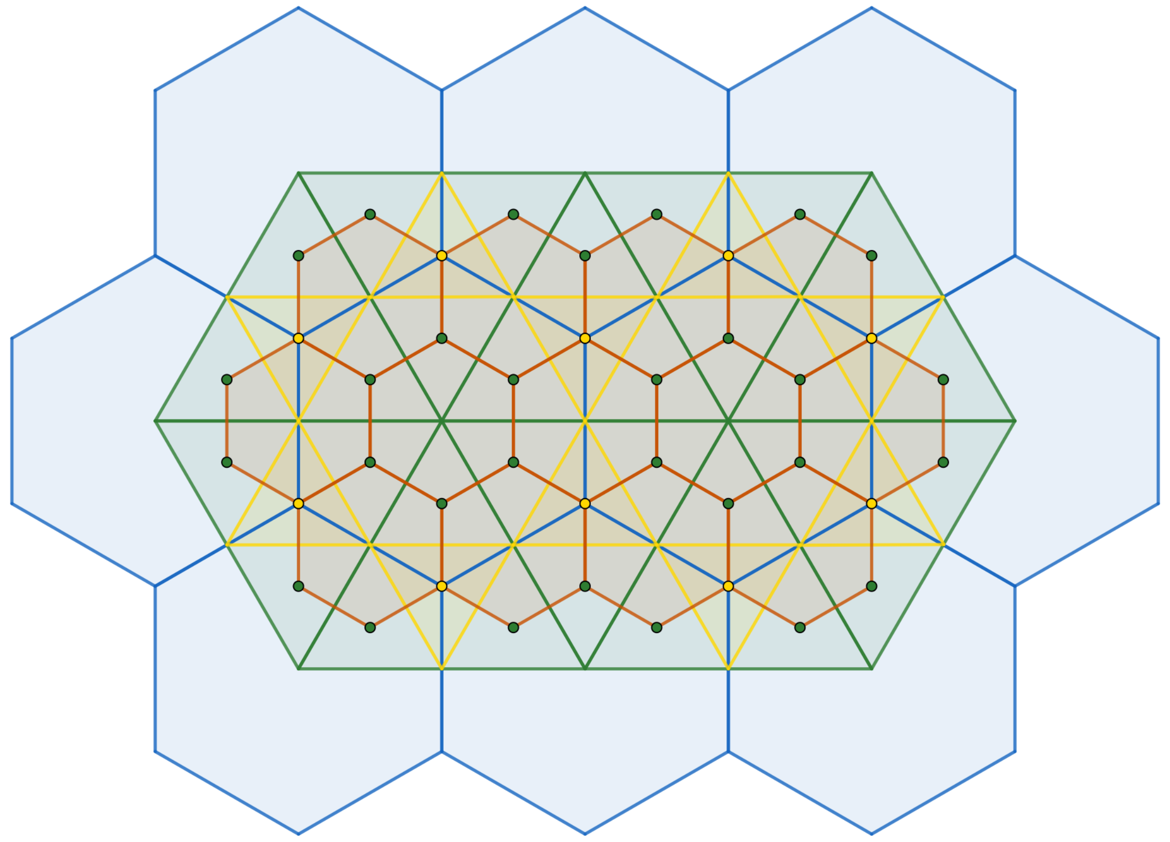

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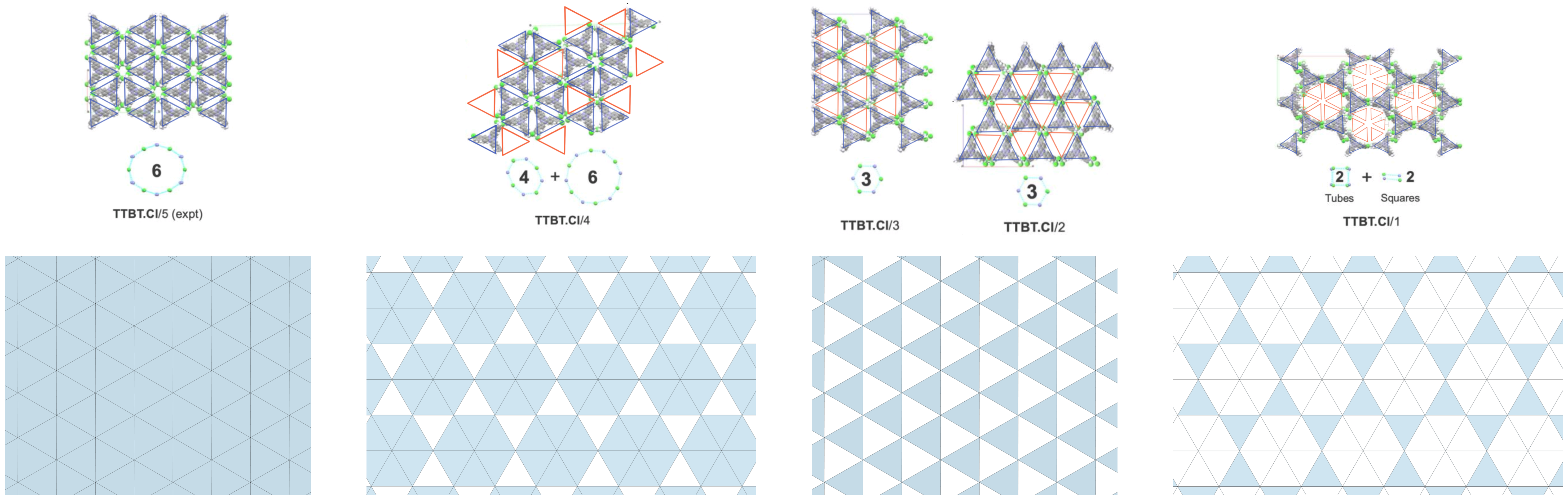
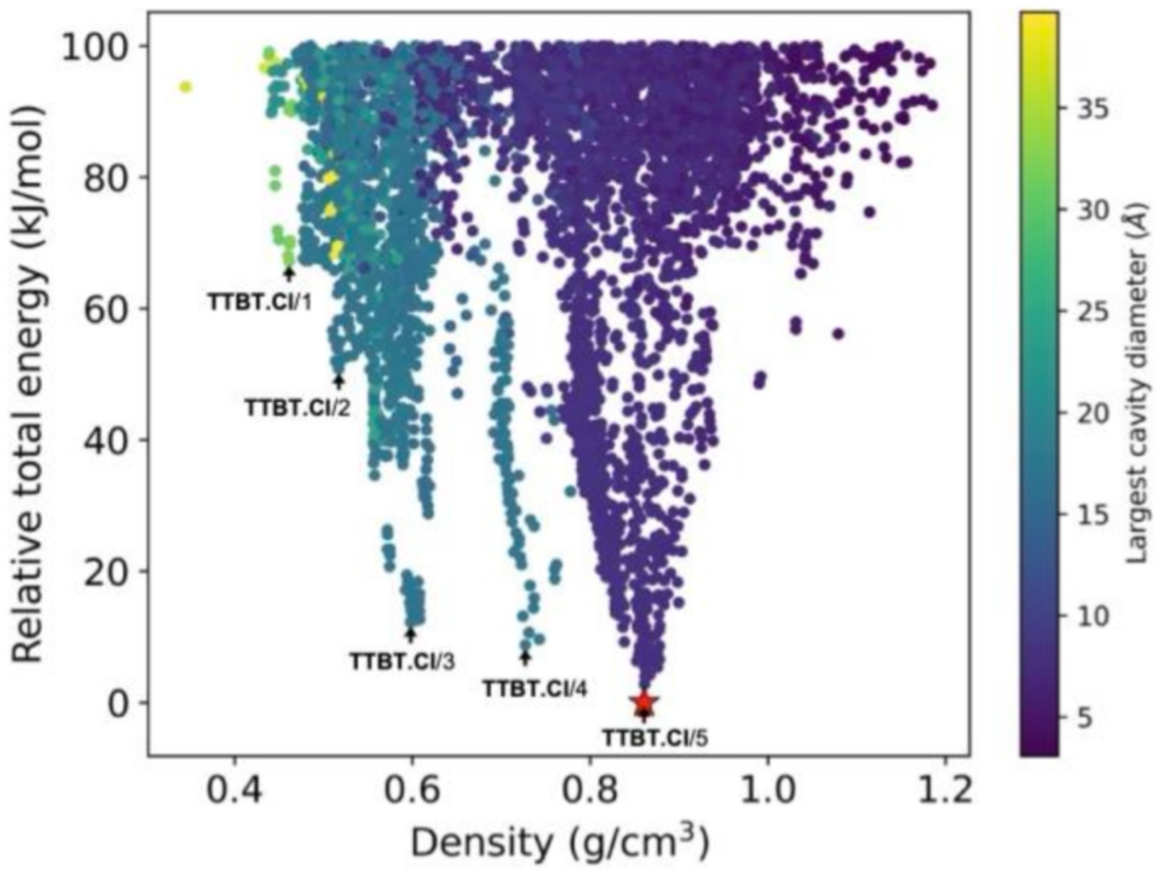
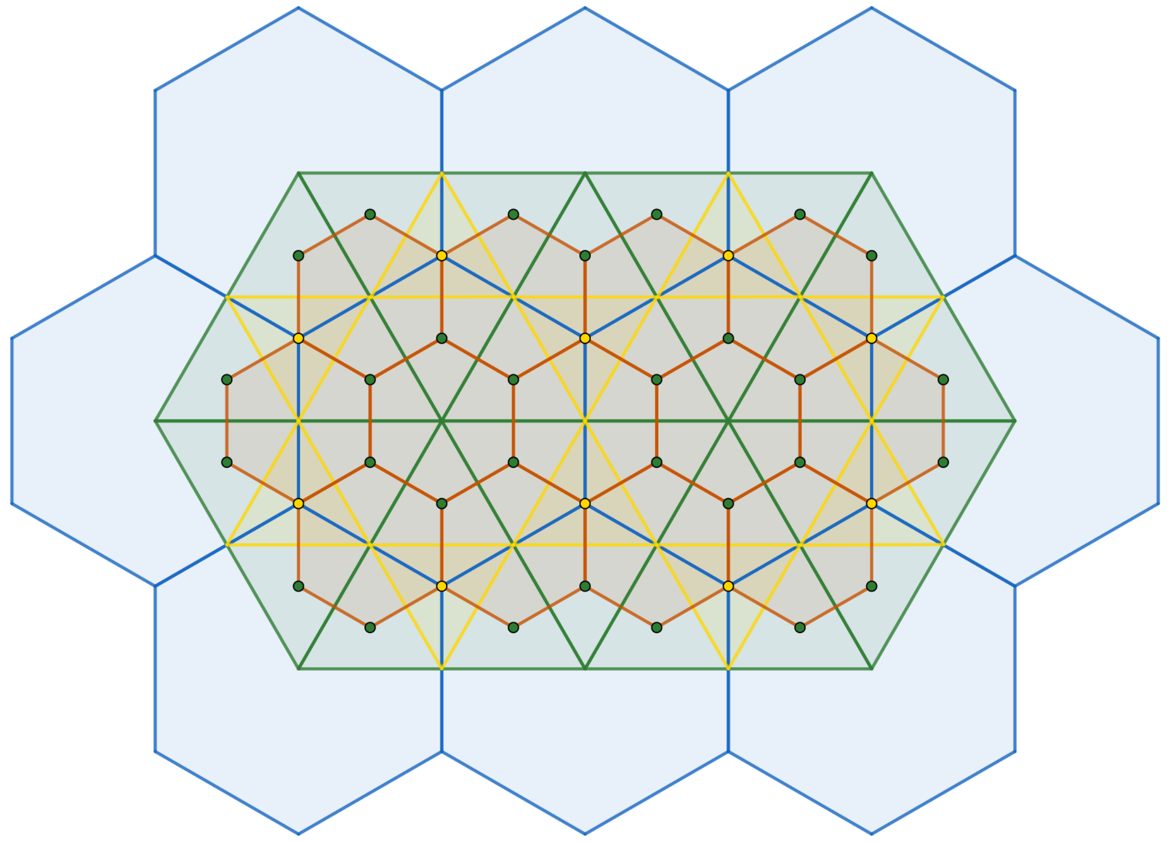


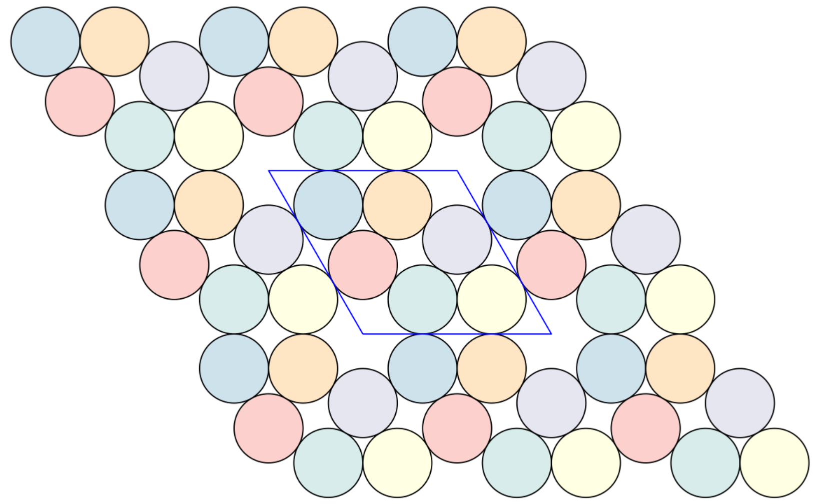


$$\rho\left(\mathscr{K}_{p31m_{\textbf{max}}}\right) = \frac{2\sqrt{3}-3}{2}\pi = 0.7290091\ldots$$

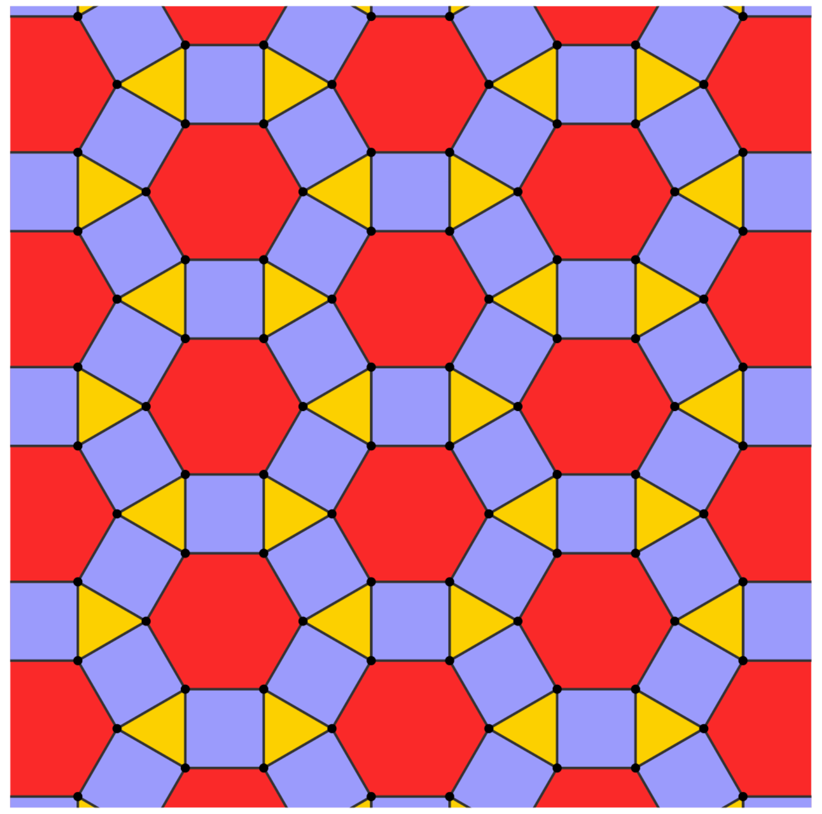
Regular tessellation

Dual tessellation

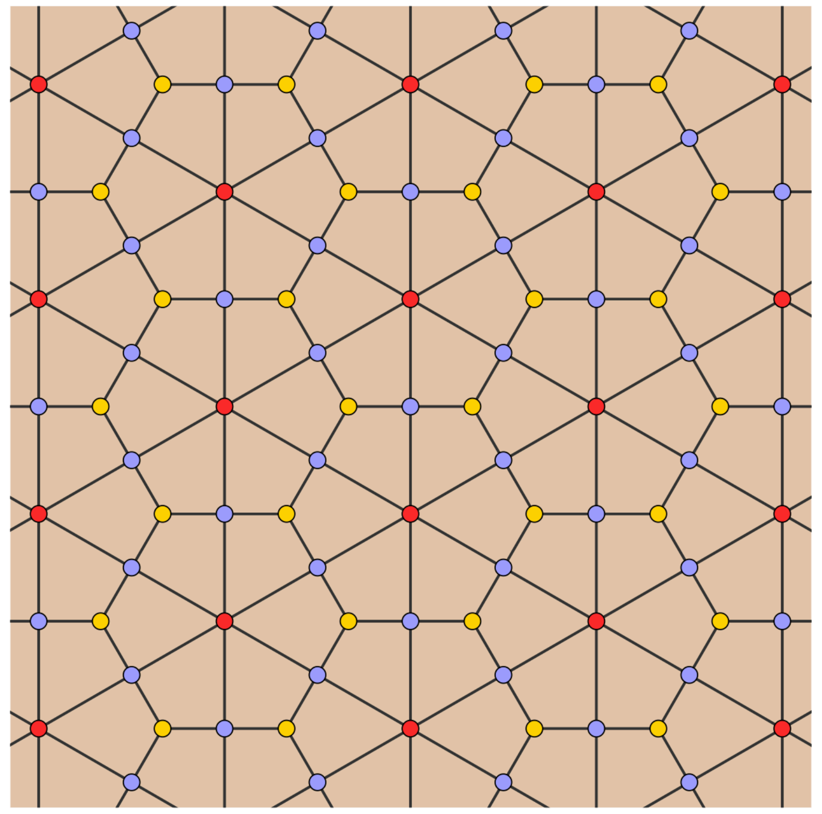




Densest $p31m$ disc packing



Rhombitrihexagonal tiling



Deltoidal trihexagonal tiling

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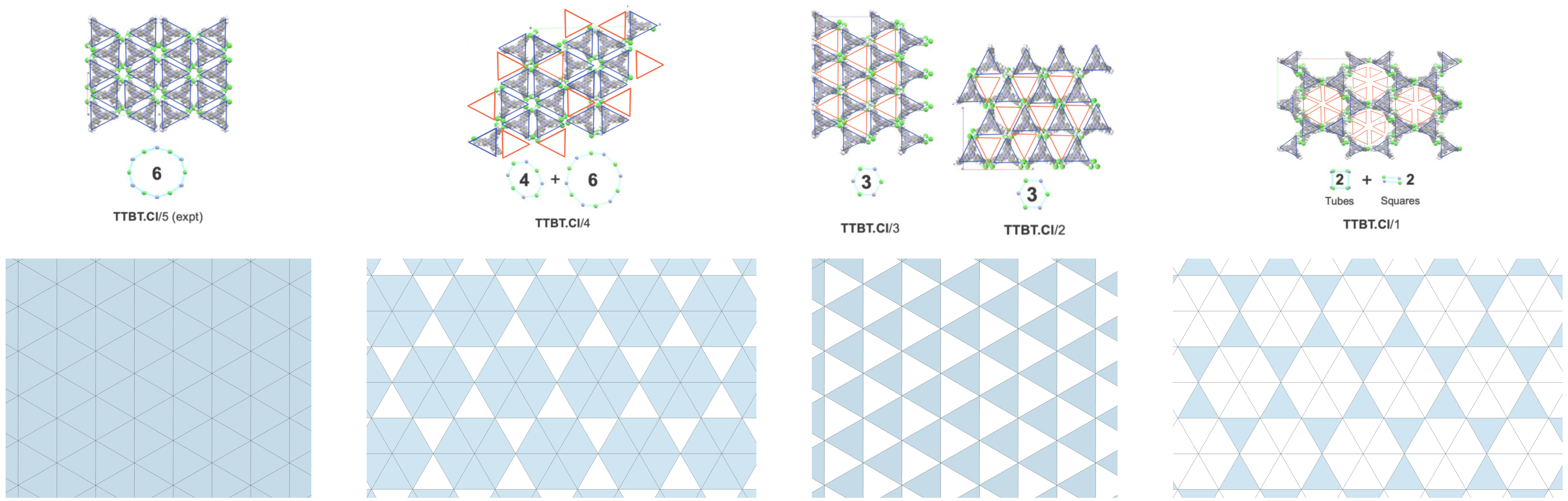
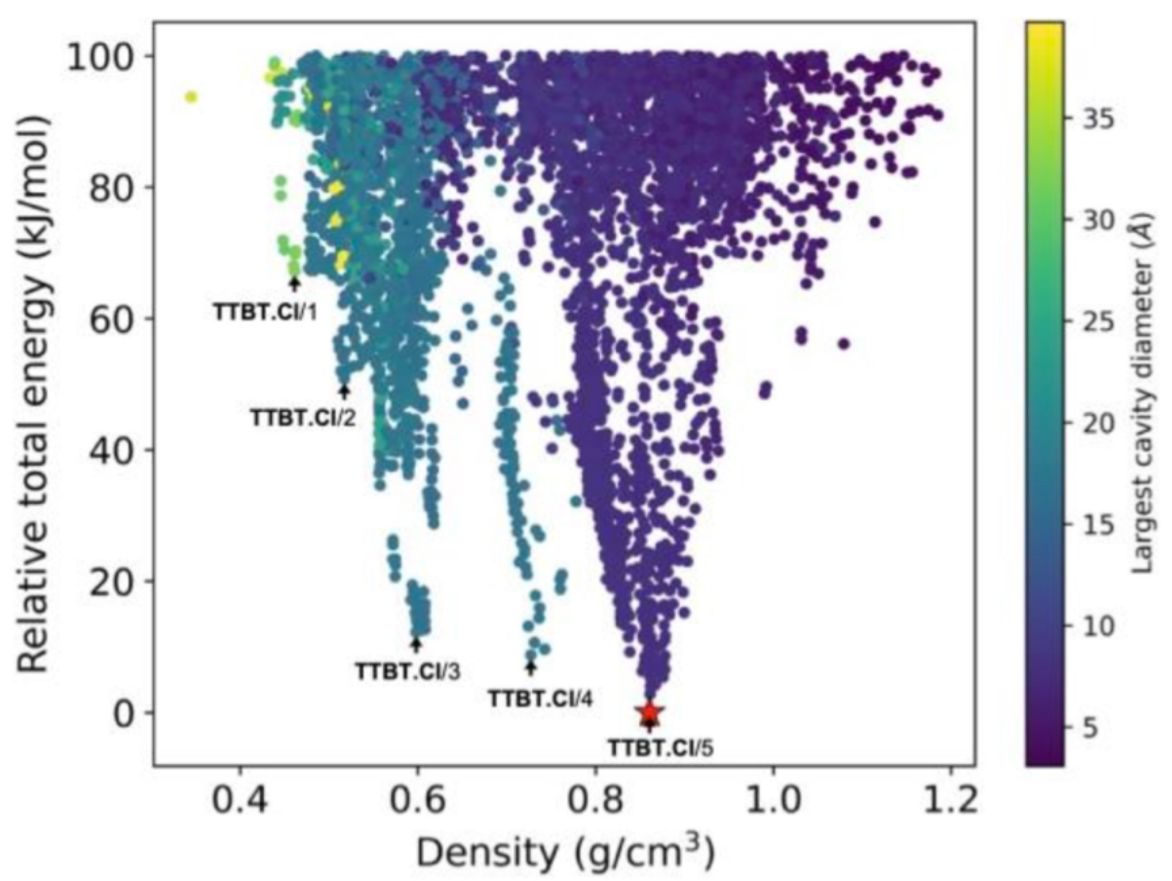
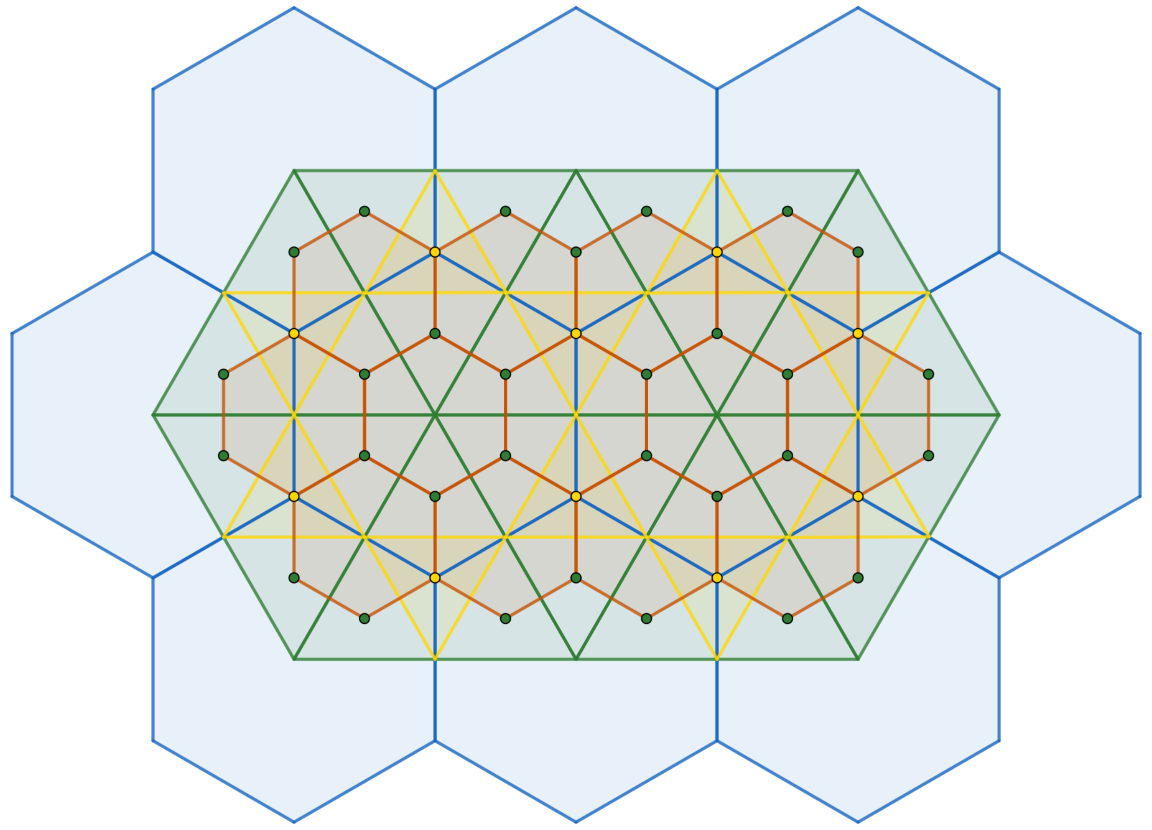
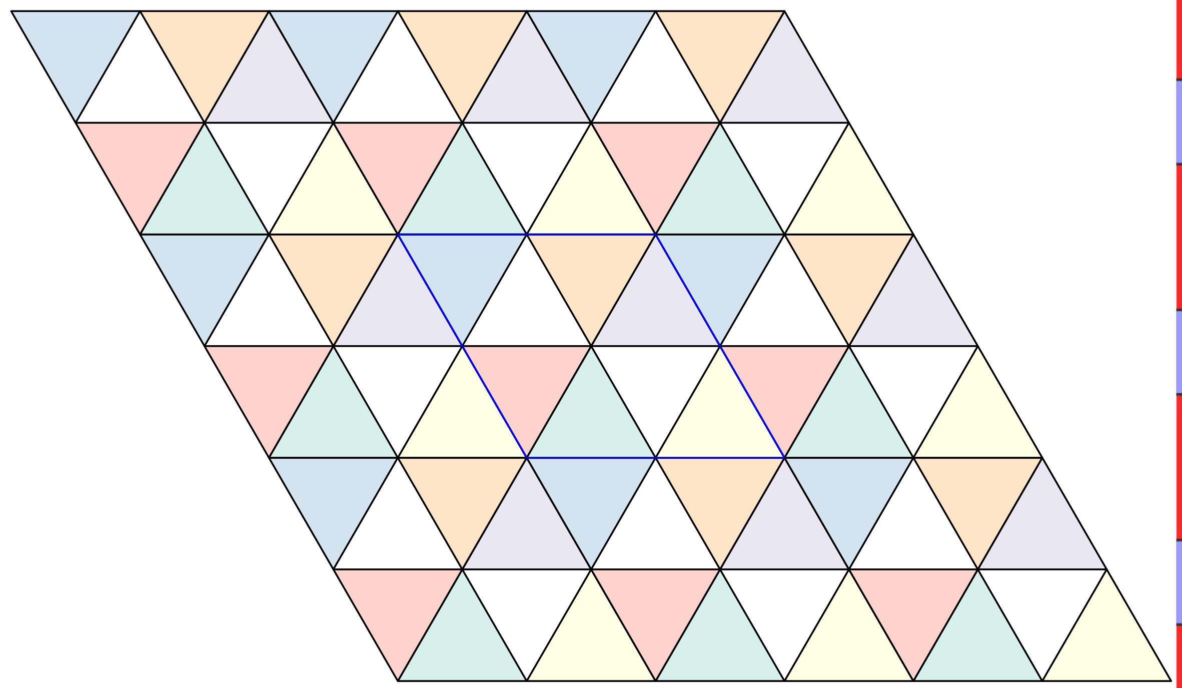




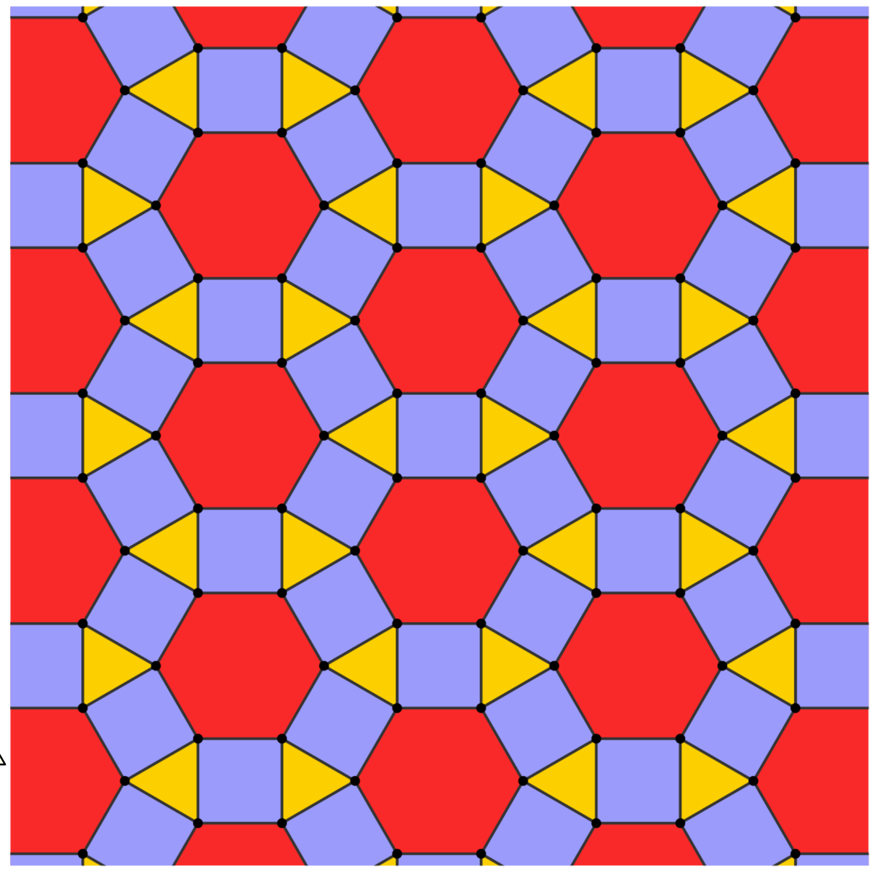


$$\rho\left(\mathscr{K}_{p31m\textbf{max}}\right) = \frac{3}{4}$$



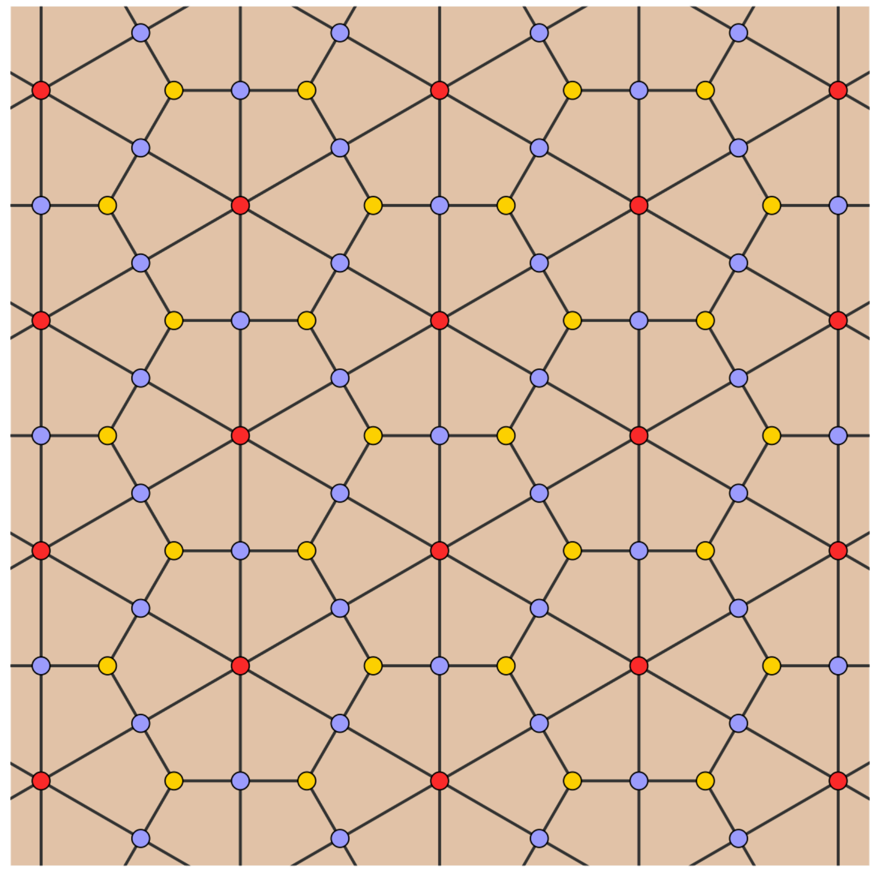
Densest $p31m$ regular triangle packing

Regular tessellation



Rhombitrihexagonal tiling

Dual tessellation



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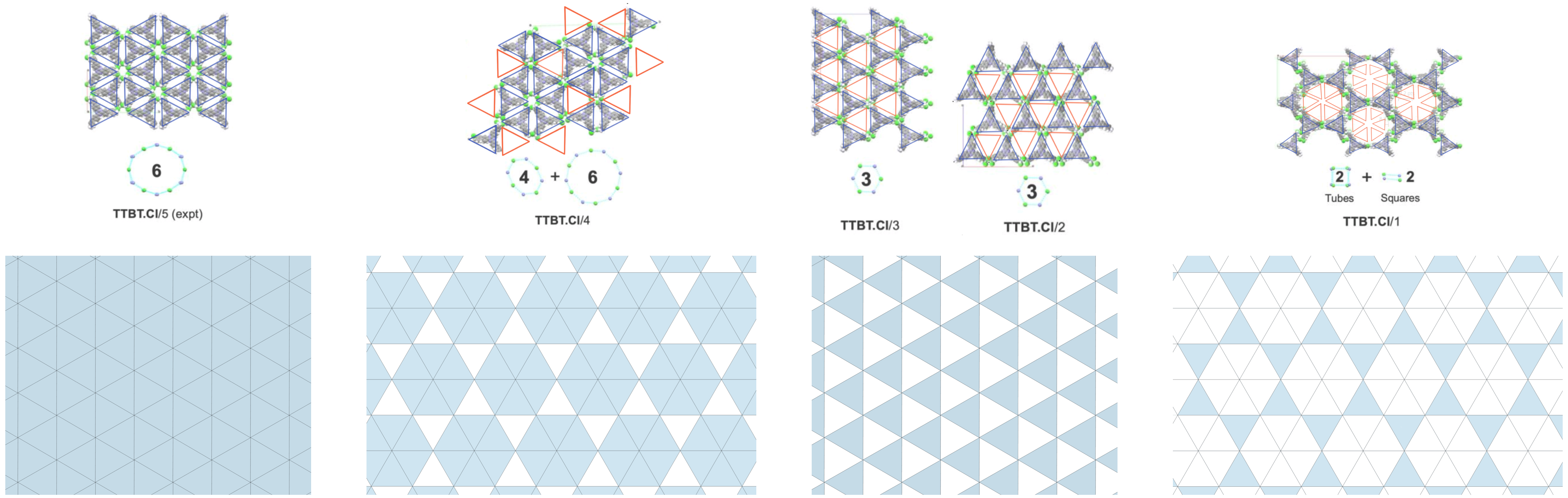

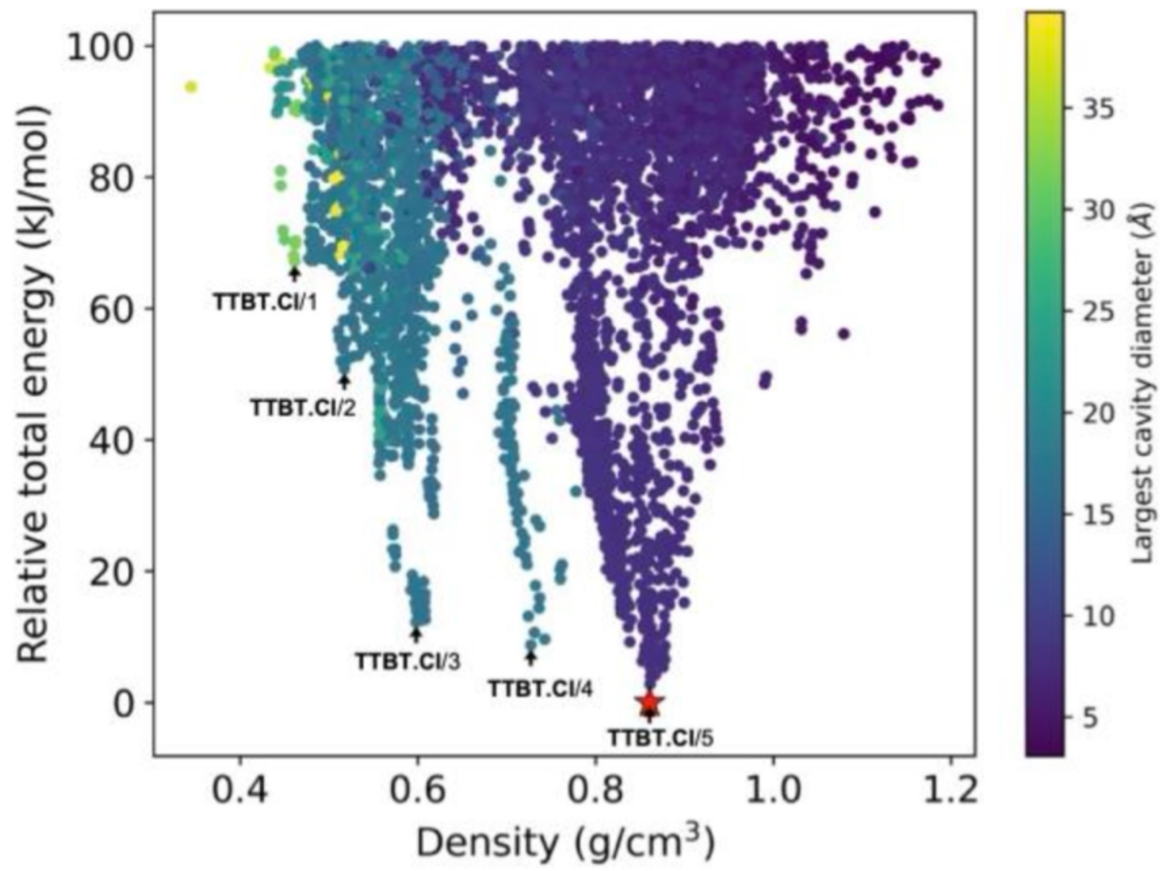

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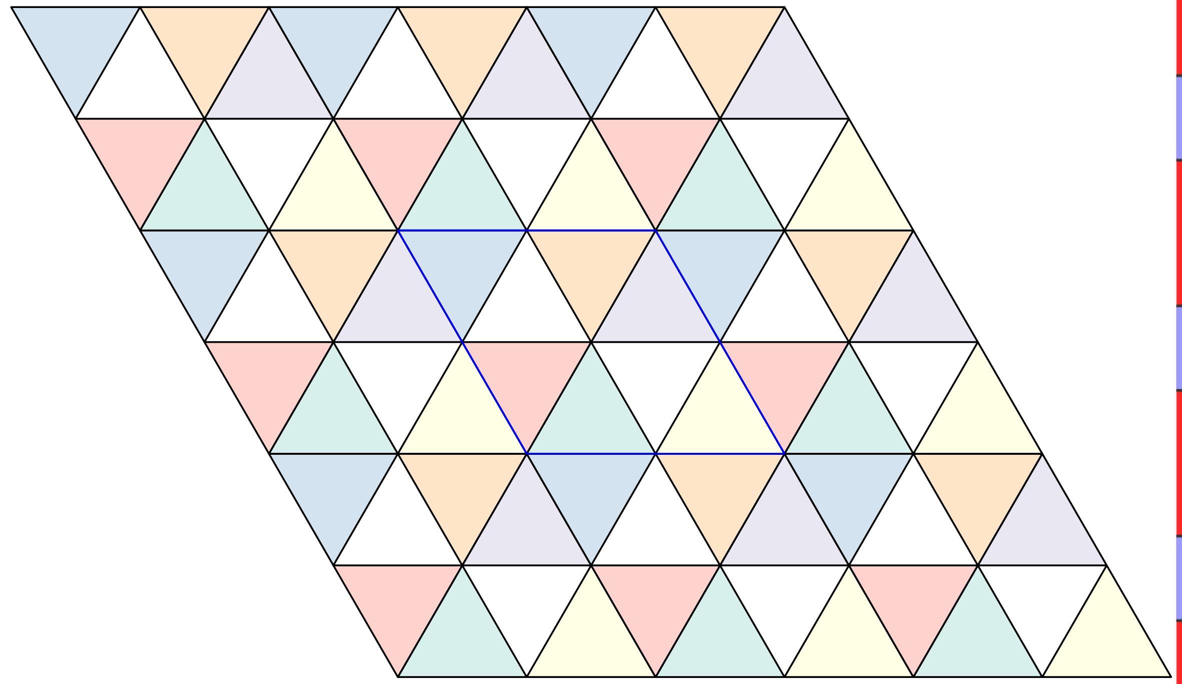
Regular tessellation

Dual tessellation



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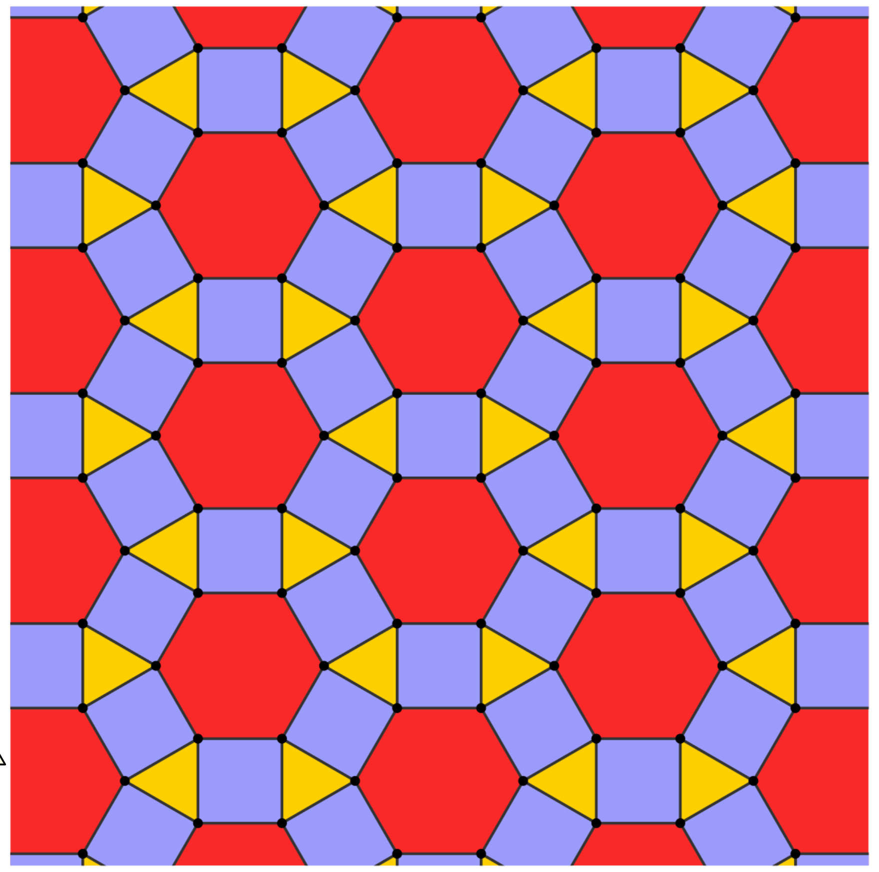

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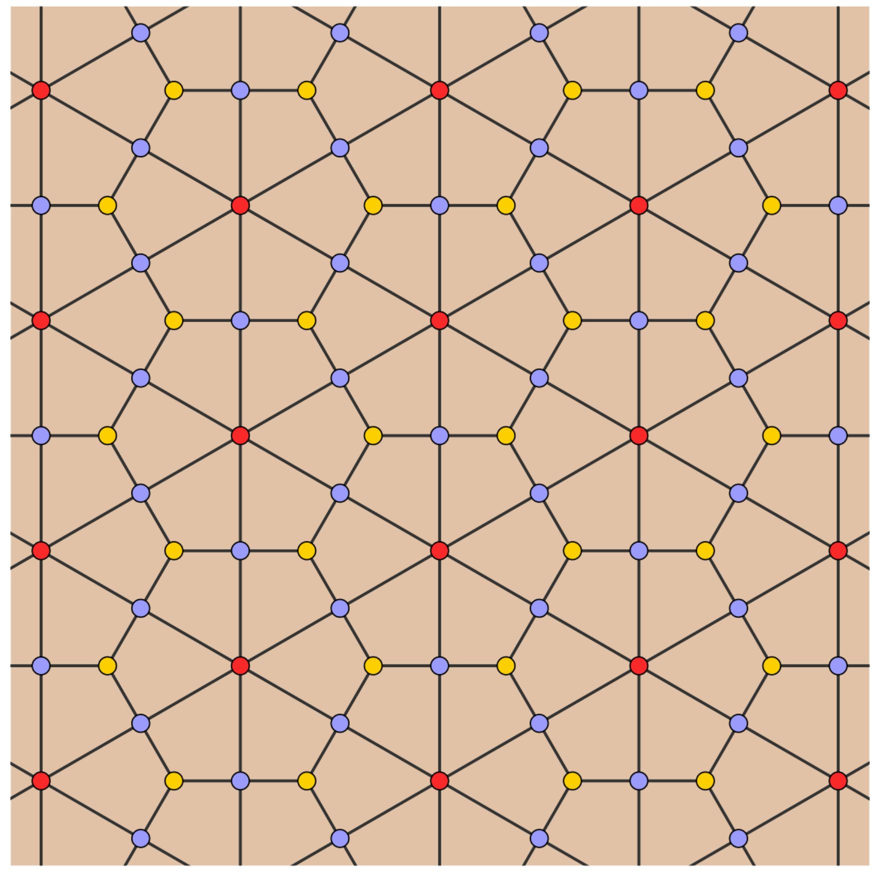

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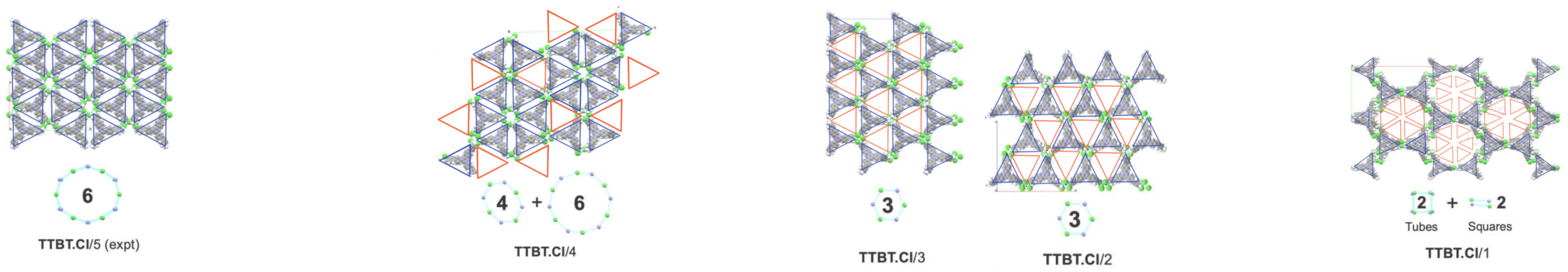

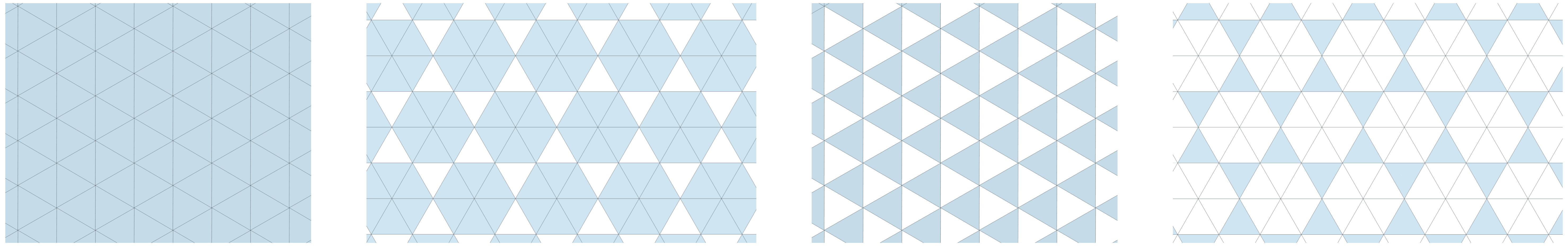

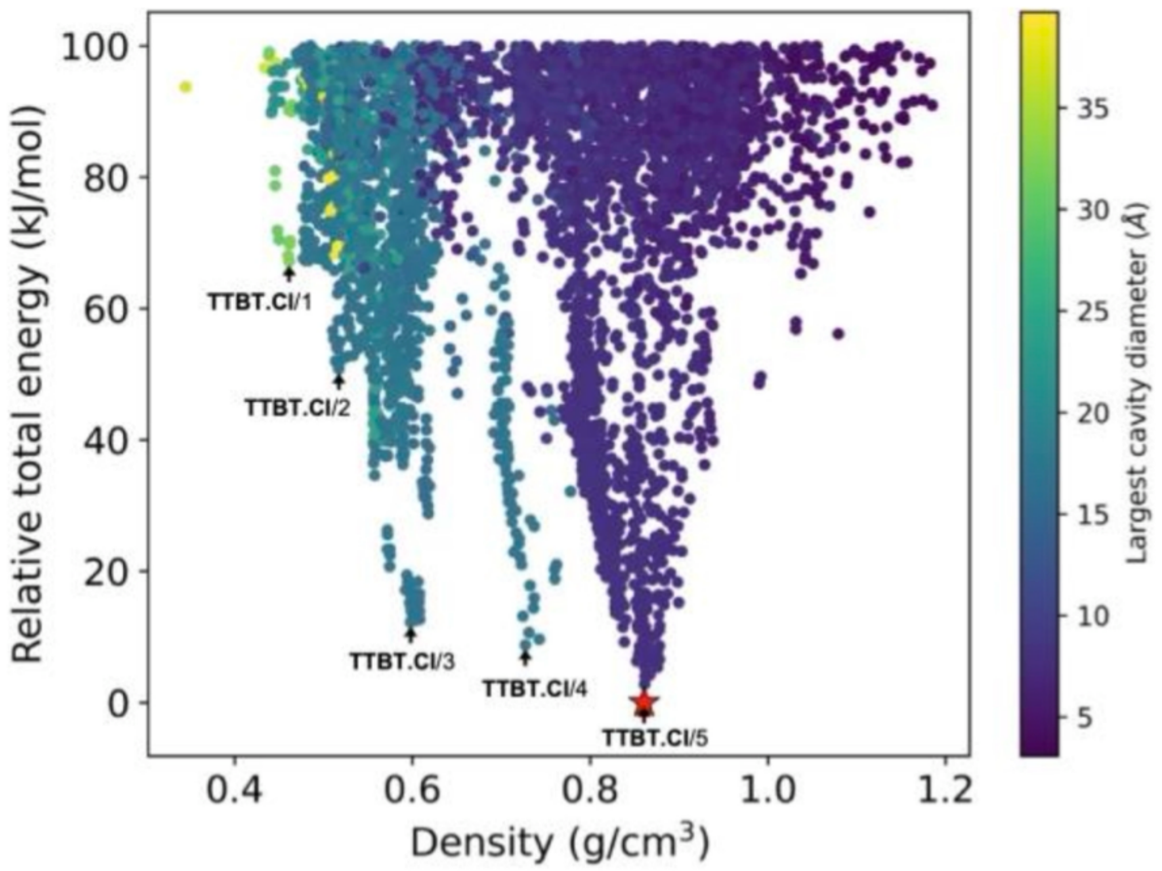

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Vertex configuration. 3.4.6.4

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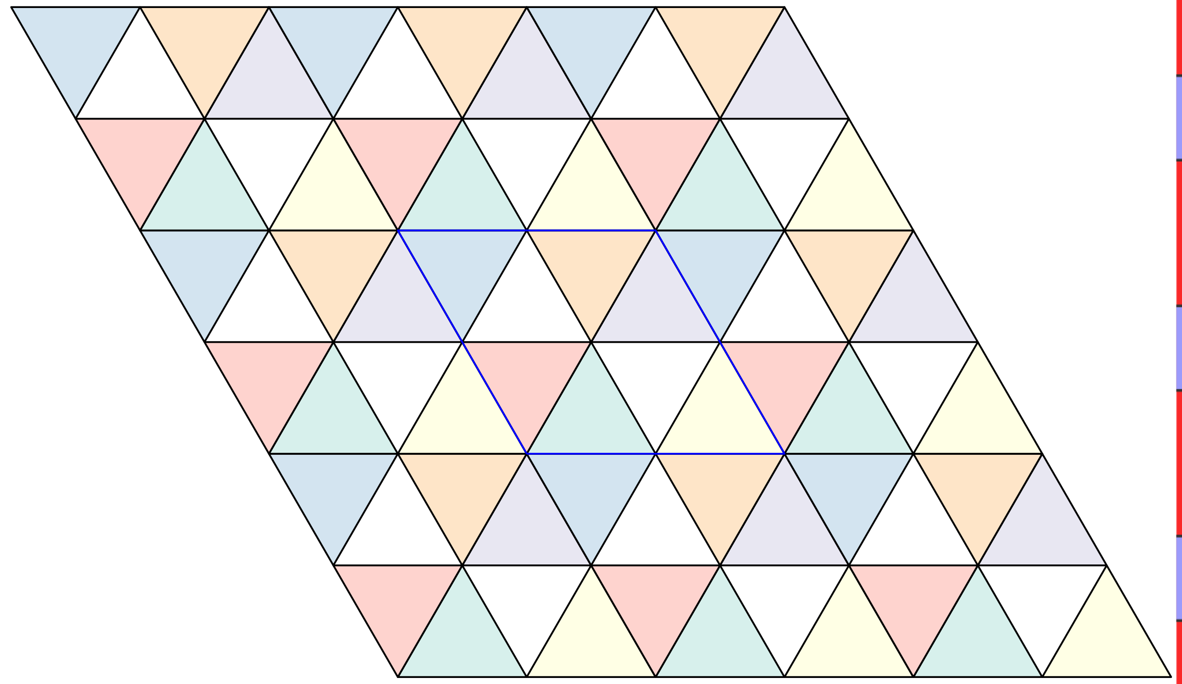
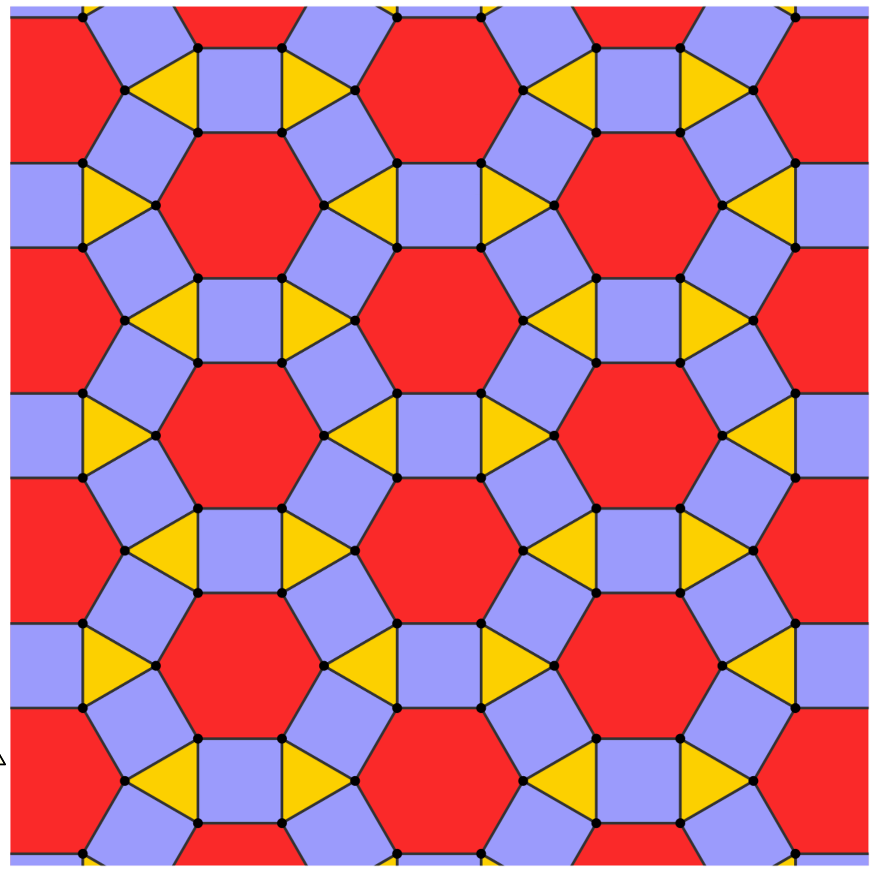
Regular tessellation

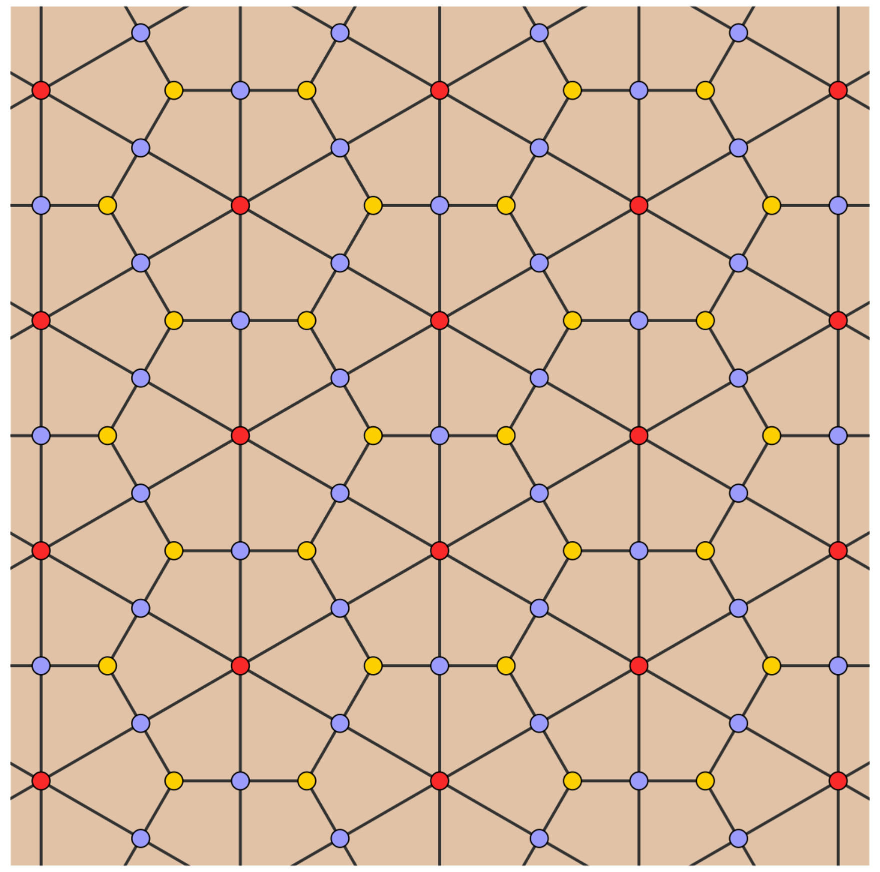
Dual tessellation



Densest $p31m$ regular triangle packing



Rhombitrihexagonal tiling



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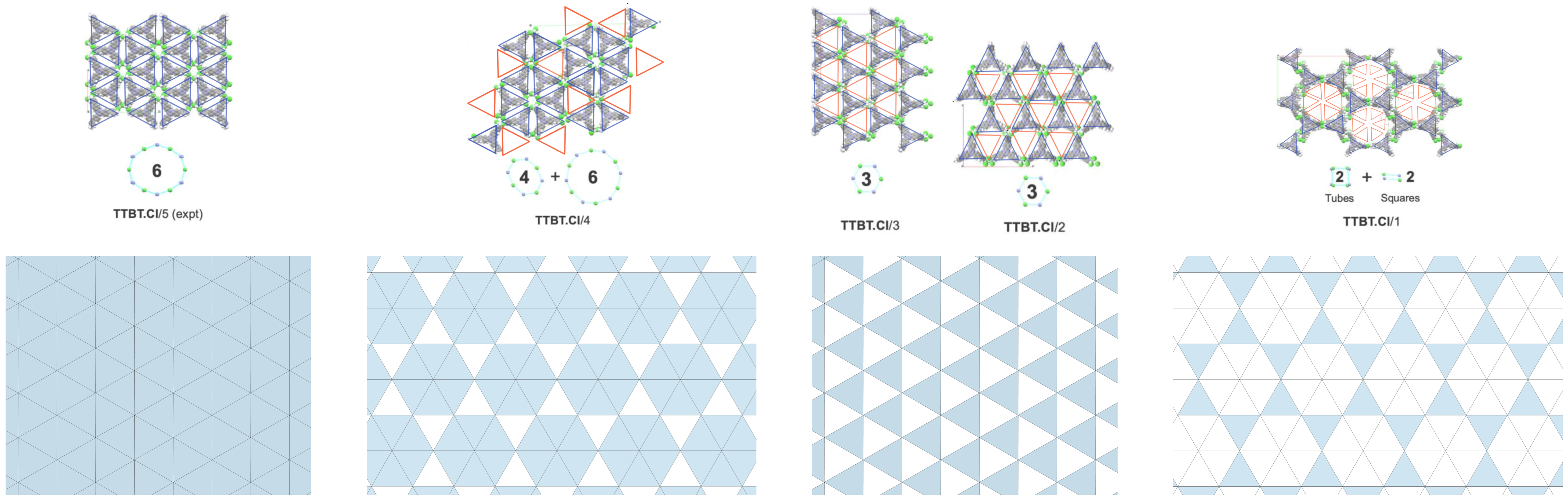

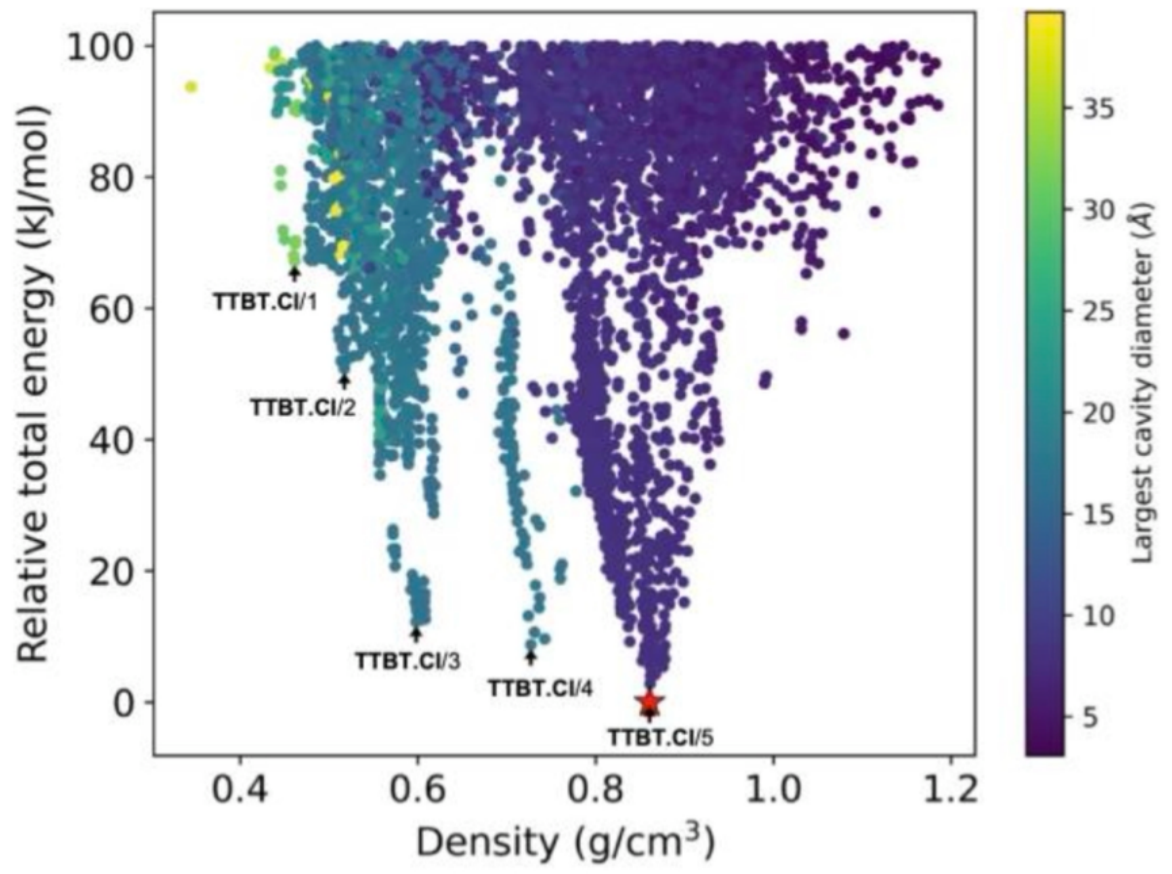

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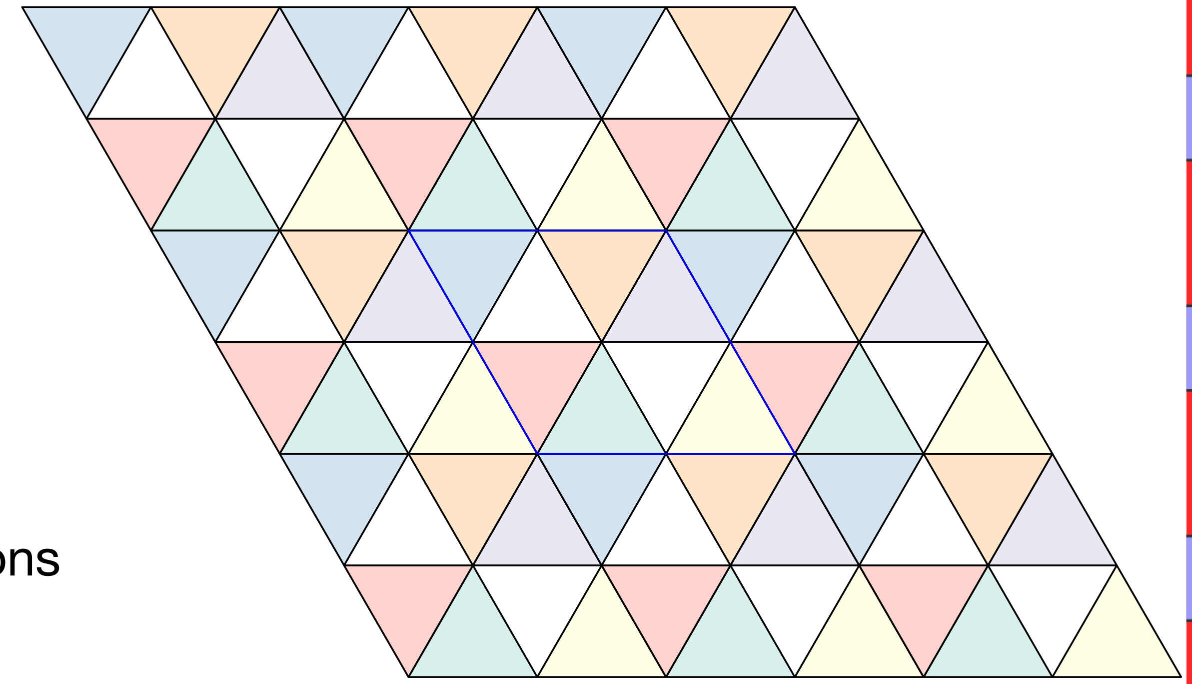
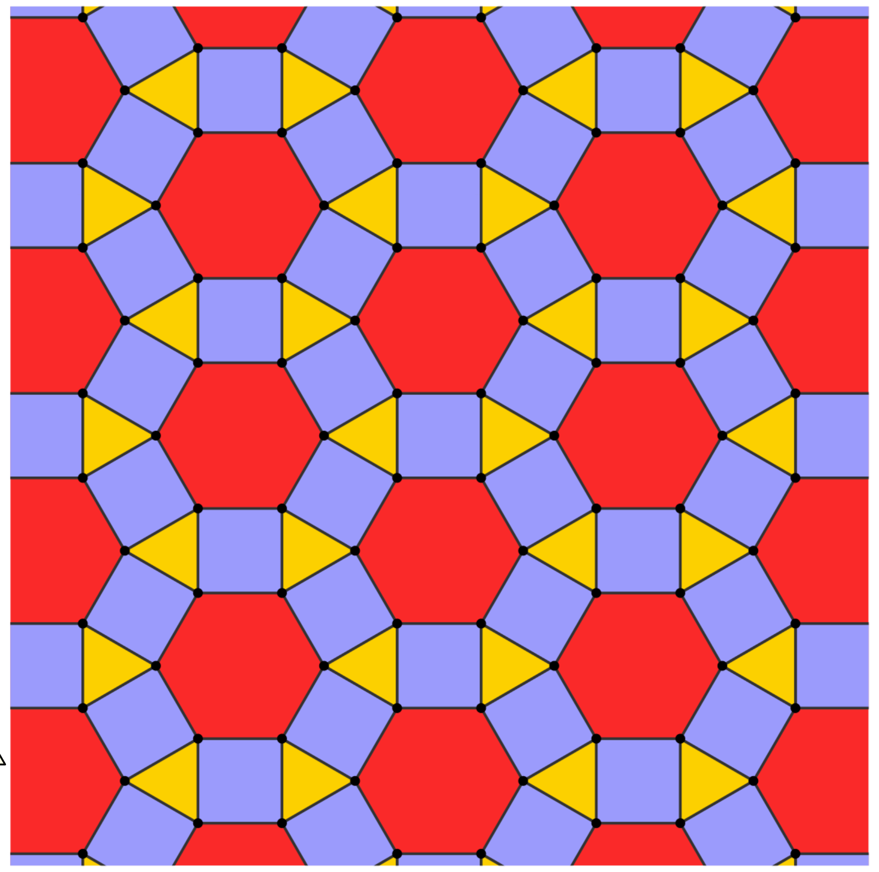
Crystallographic restriction theorem[3]. If a discrete group of rotations in the plane has more than one centre of rotation, then the only rotations that can occur are 2-fold, 3-fold, 4-fold, and 6-fold.

$$\rho\left(\mathscr{K}_{p31m\textbf{max}}\right) = \frac{3}{4}$$



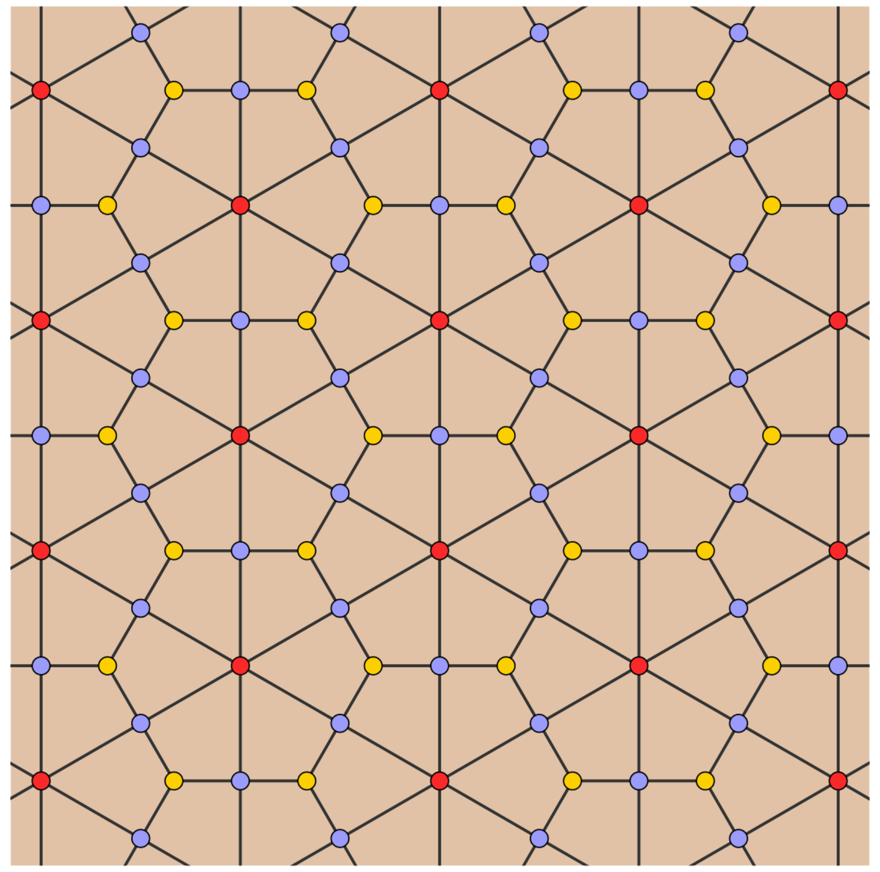
Densest $p31m$ regular triangle packing

Regular tessellation



Rhombitrihexagonal tiling

Dual tessellation



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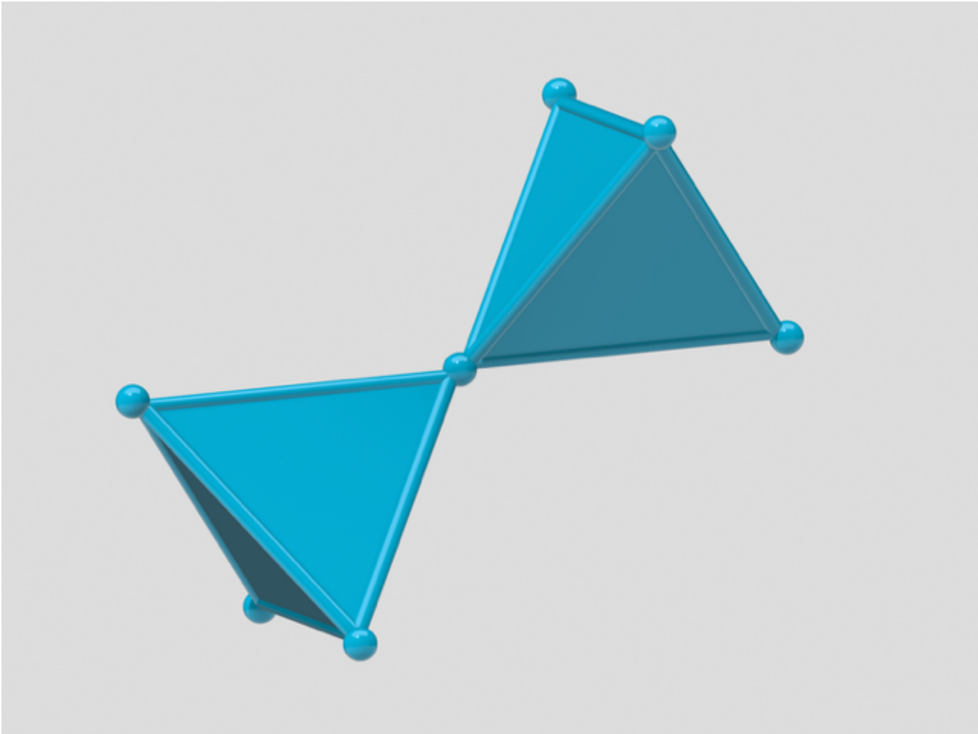

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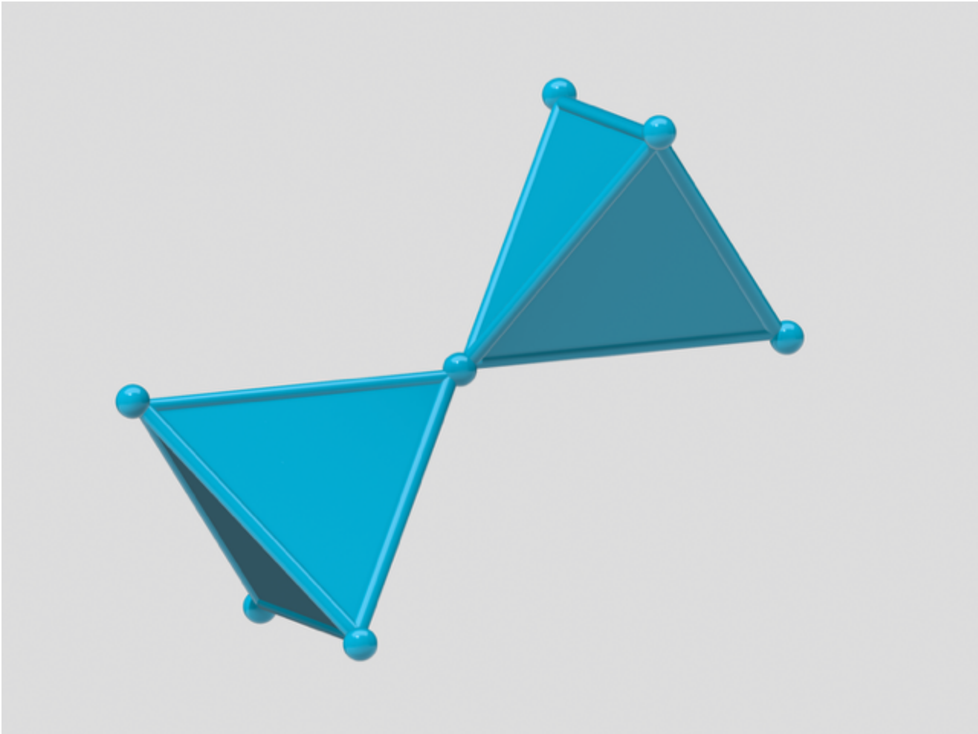

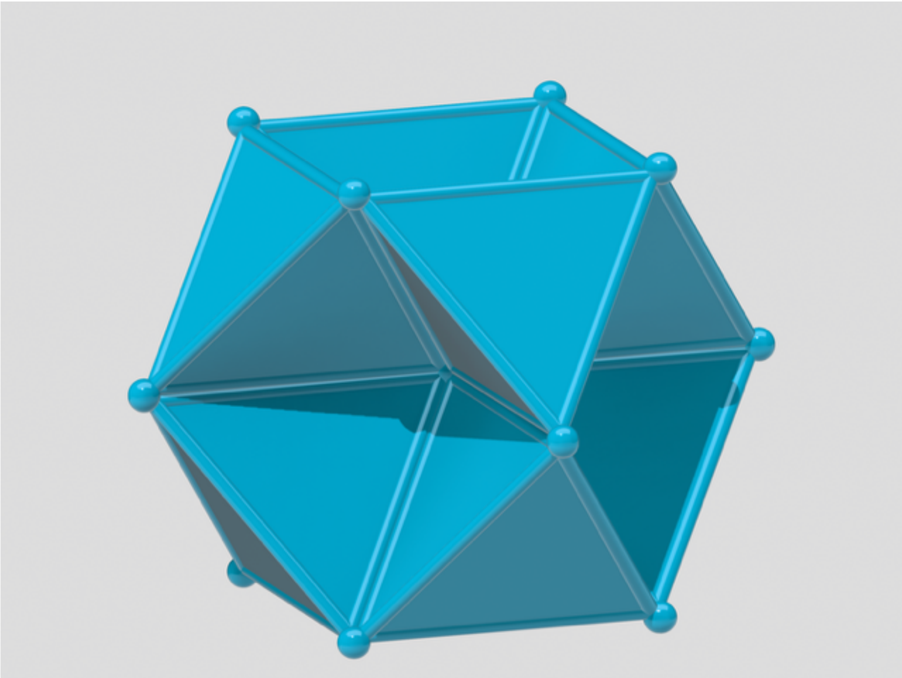

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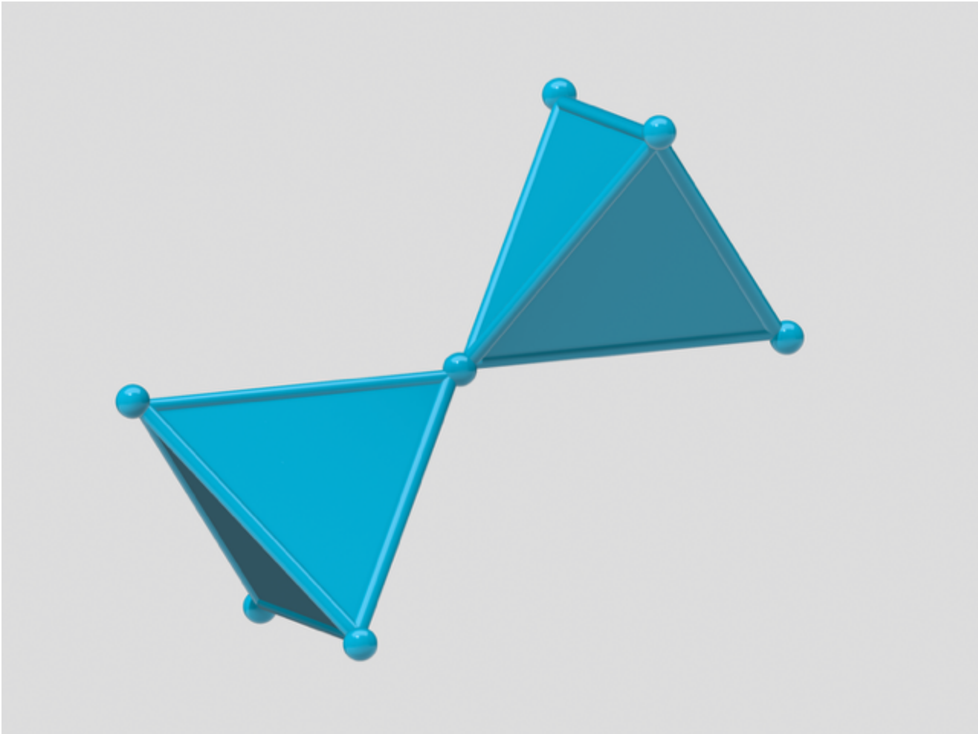

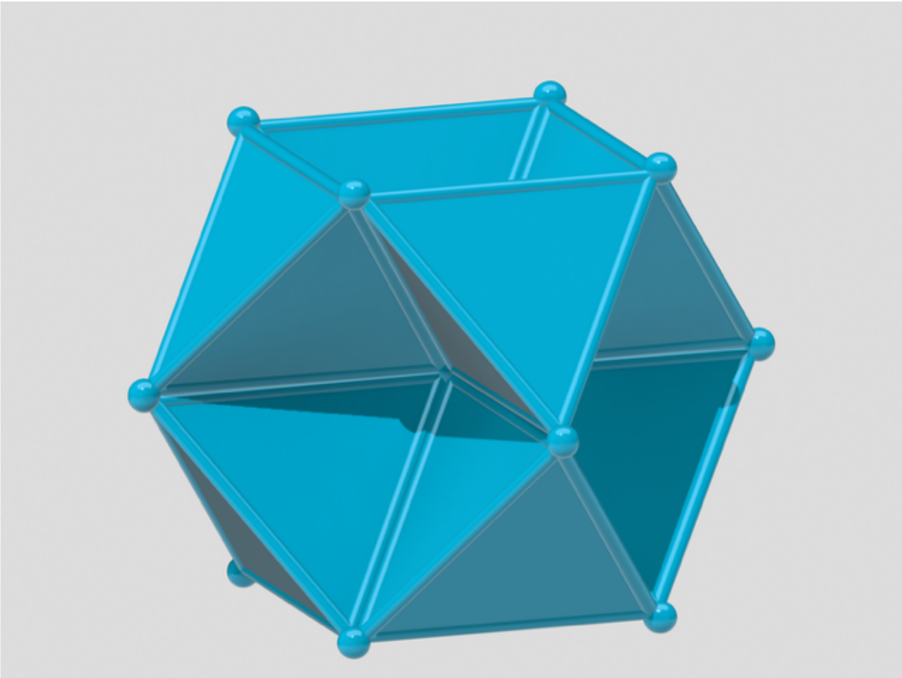

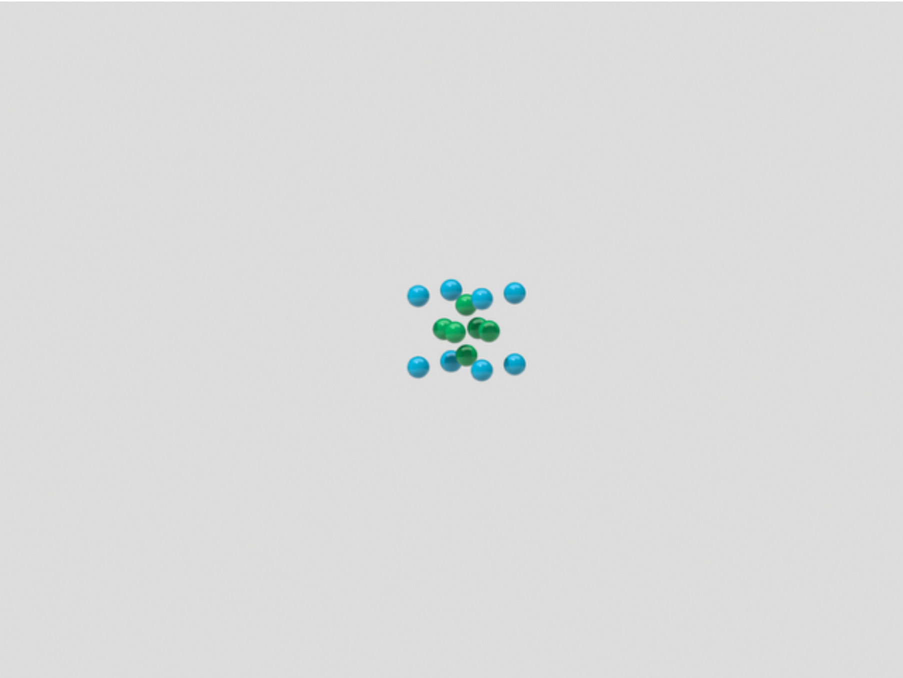

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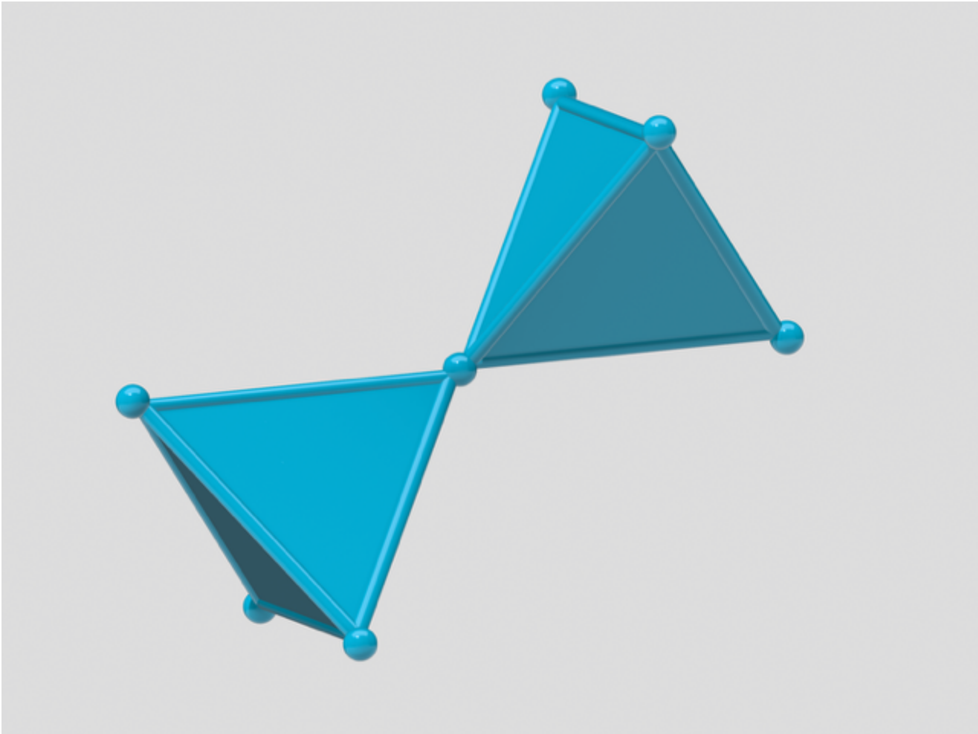
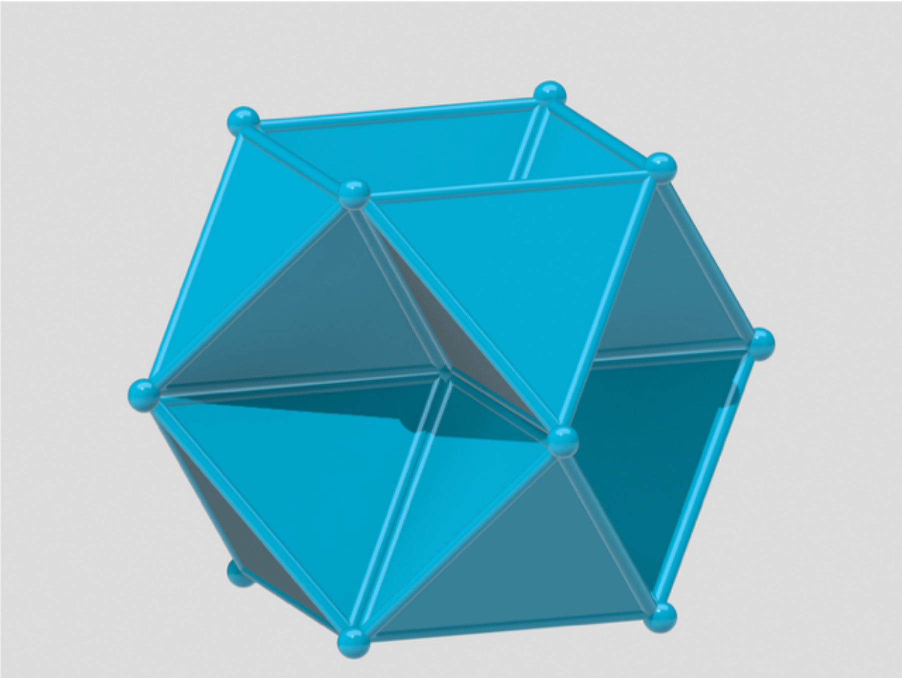
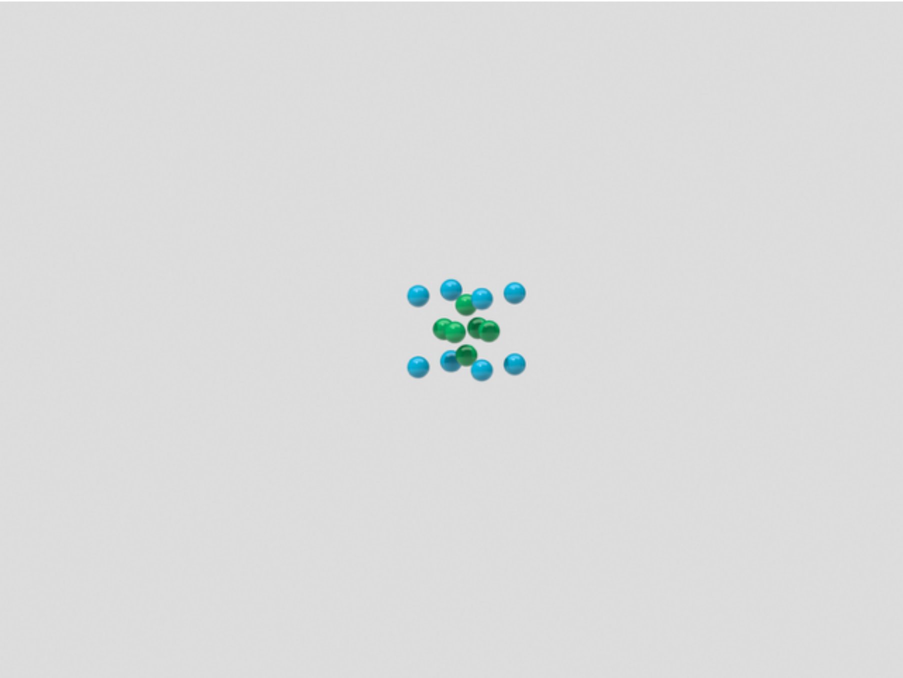
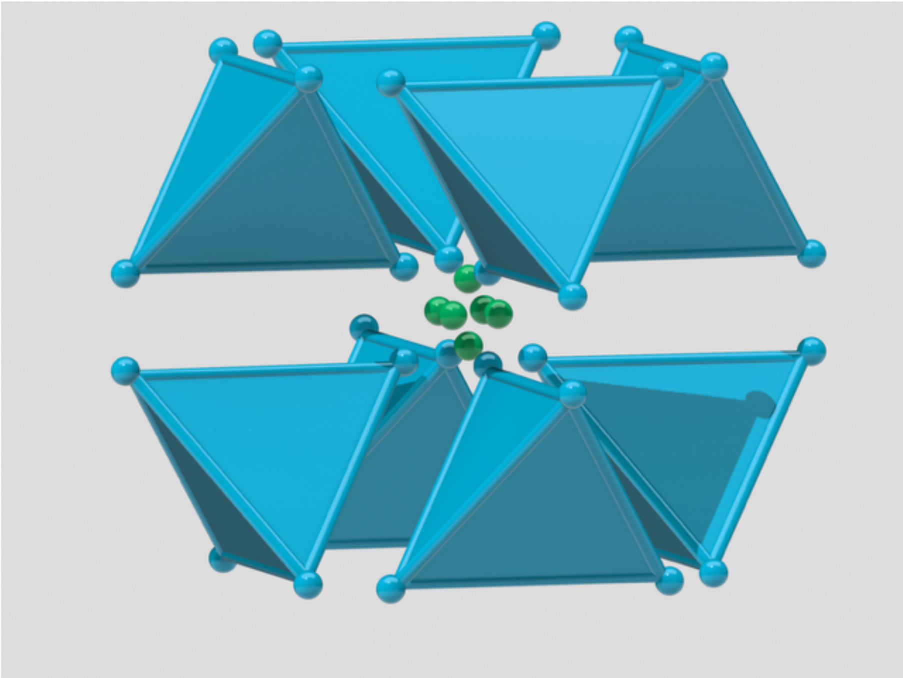

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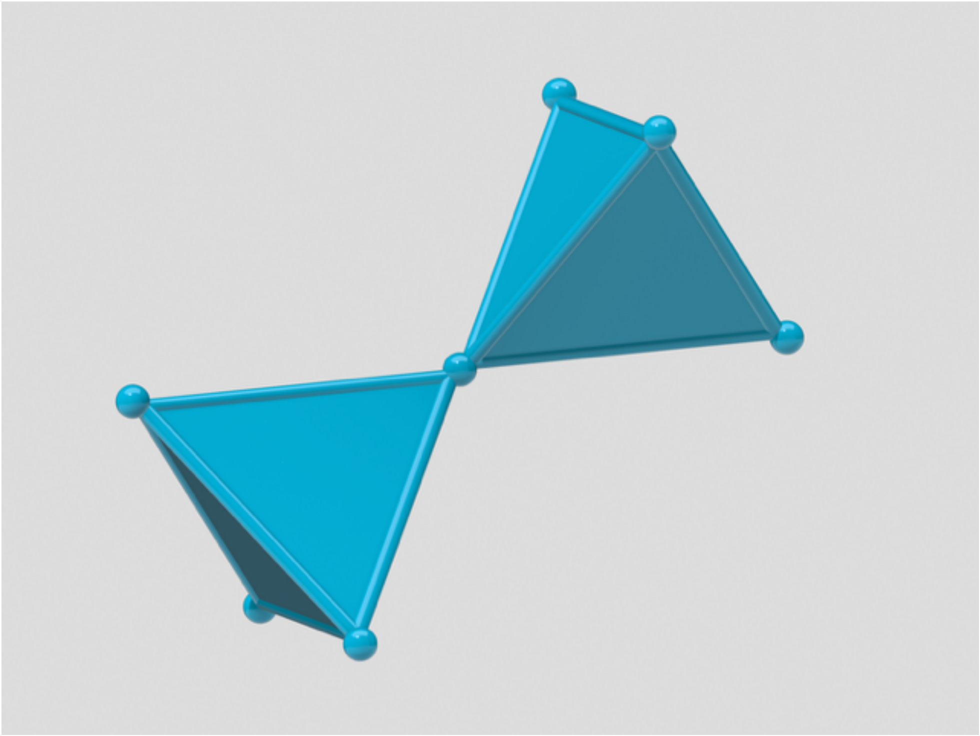

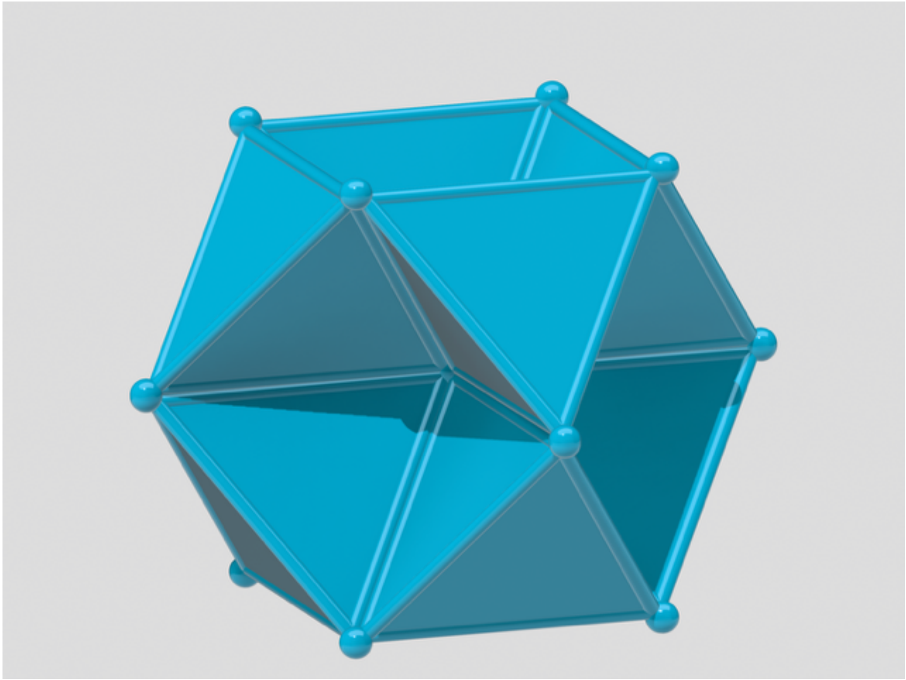

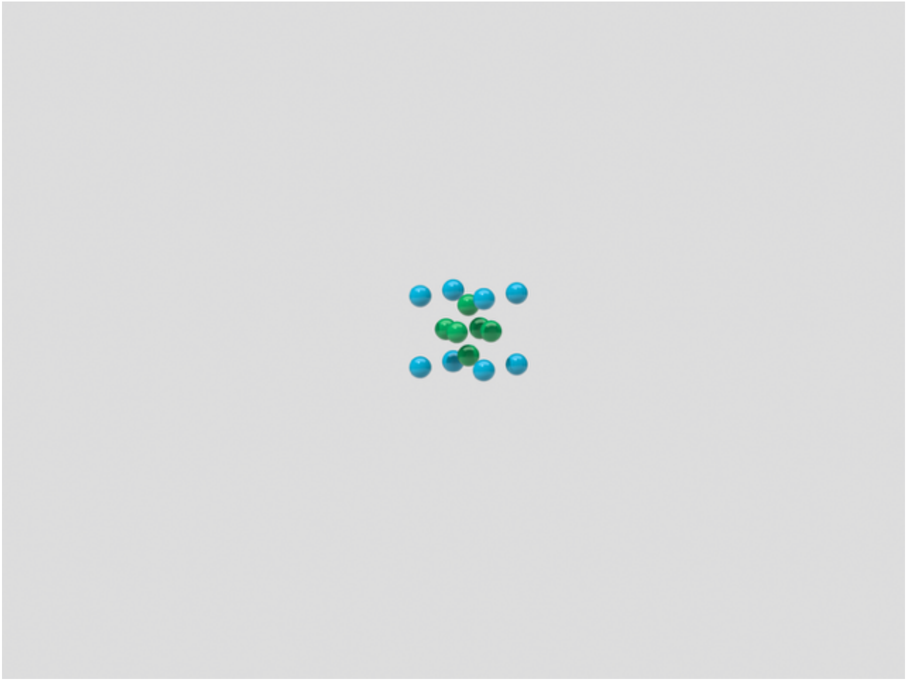

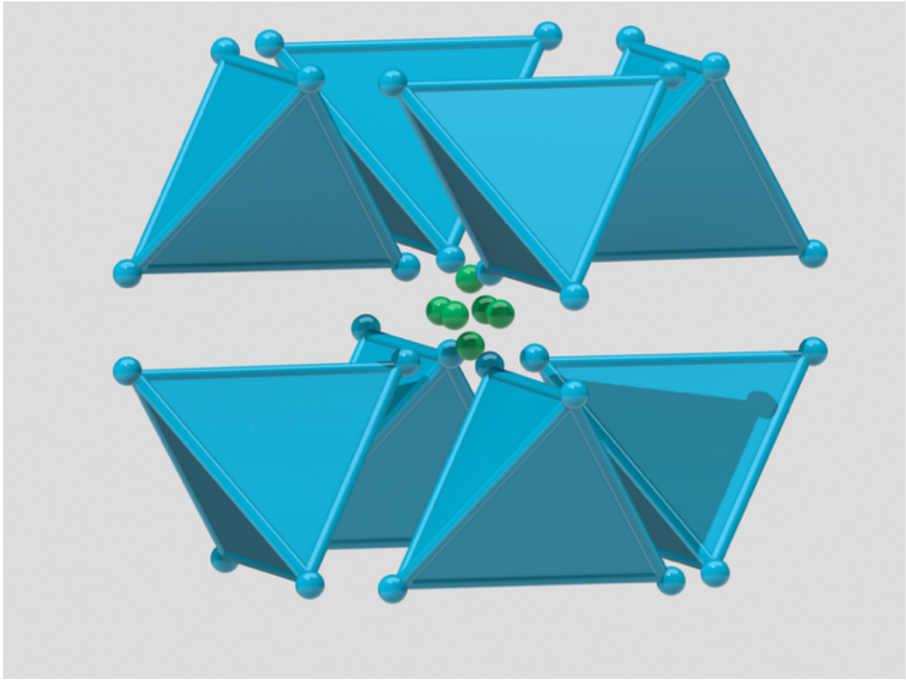

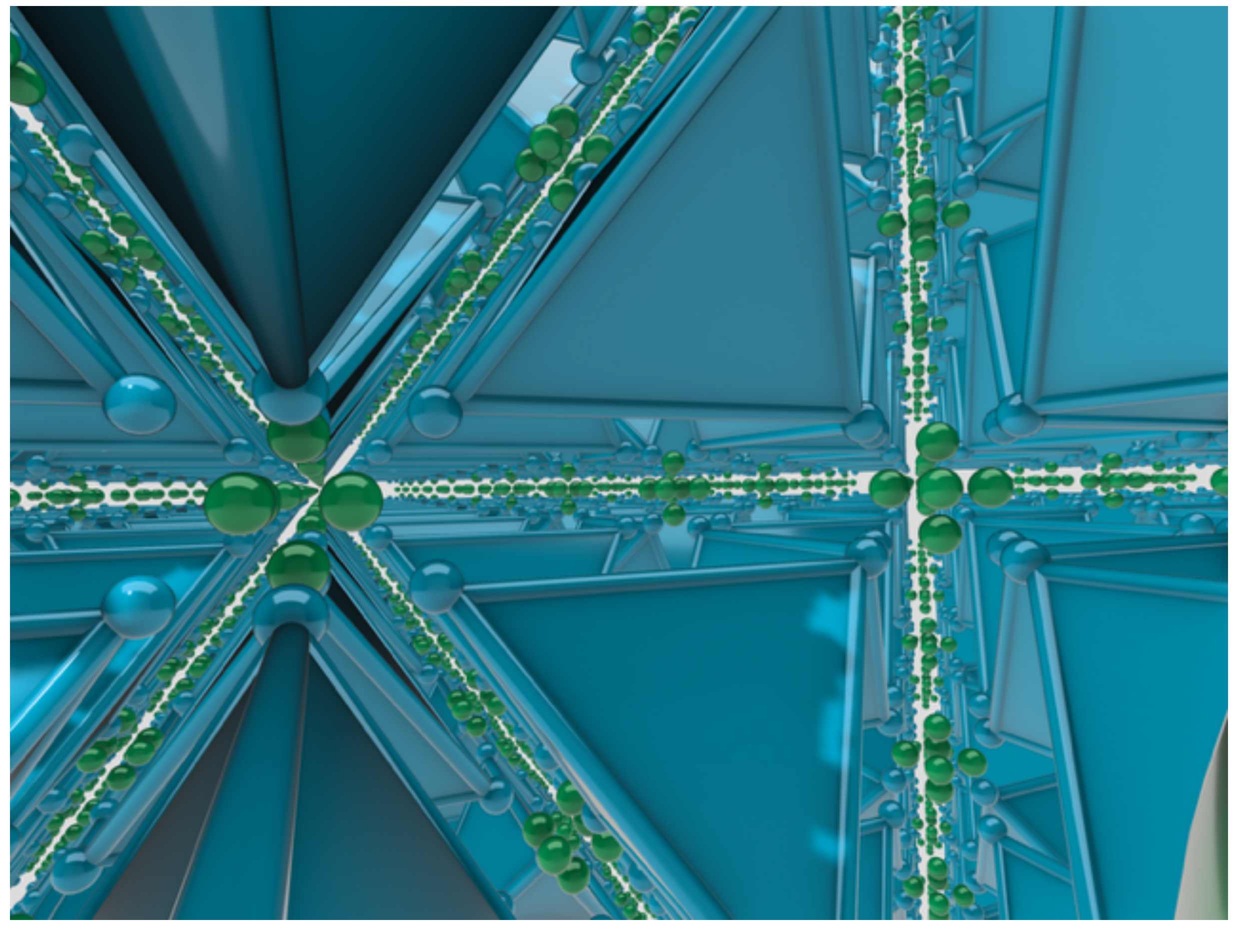

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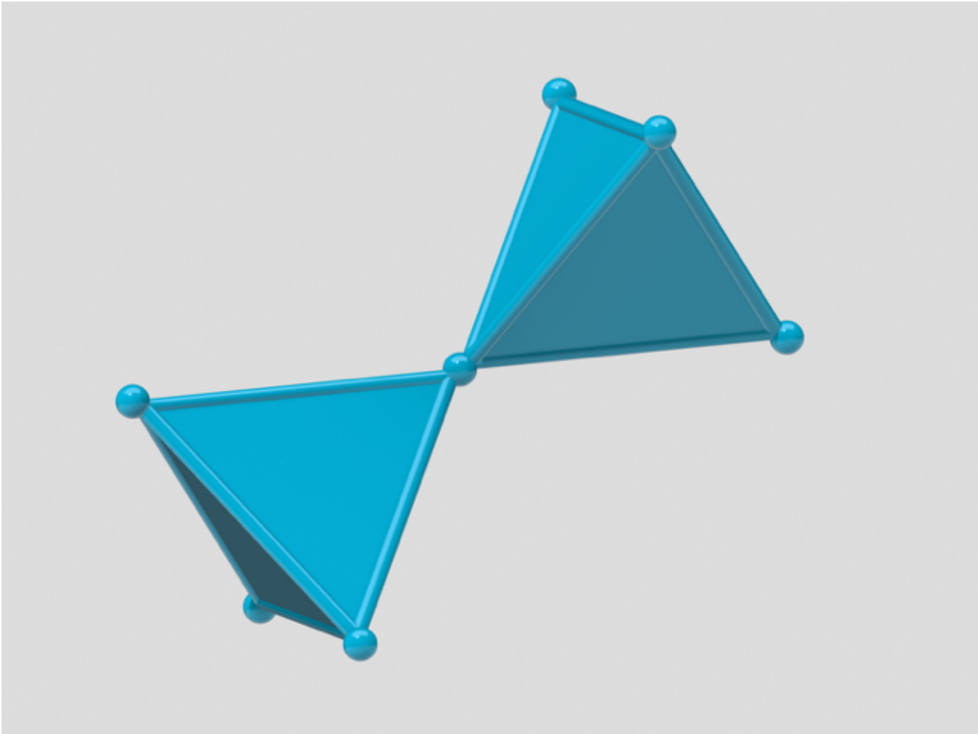
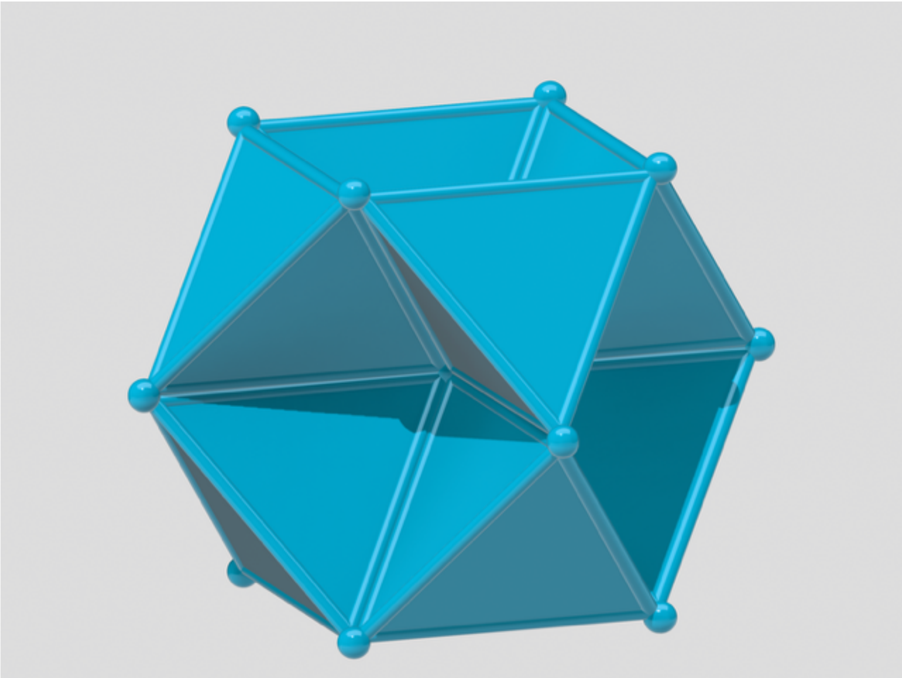
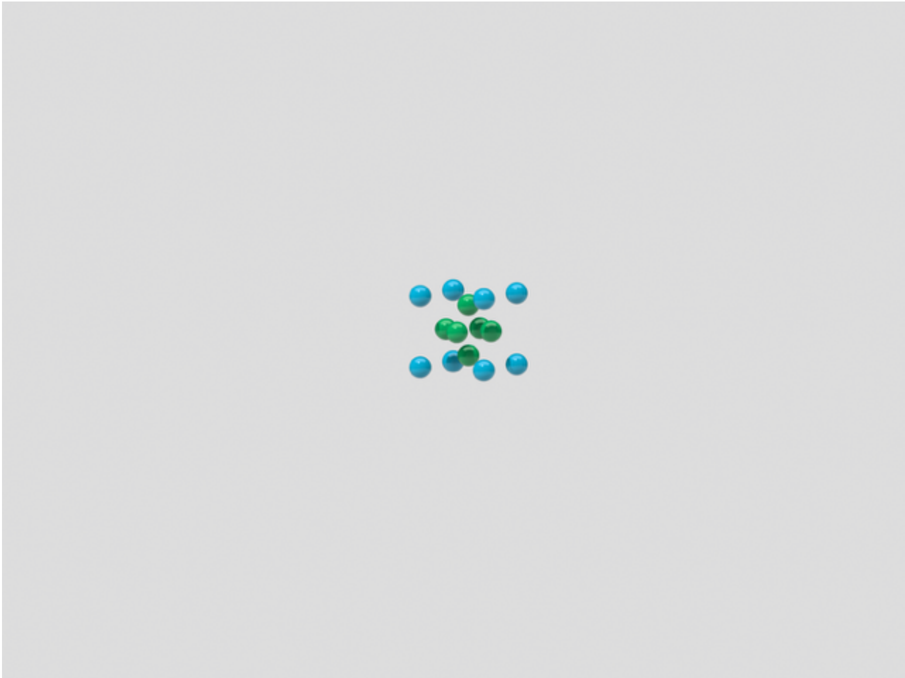
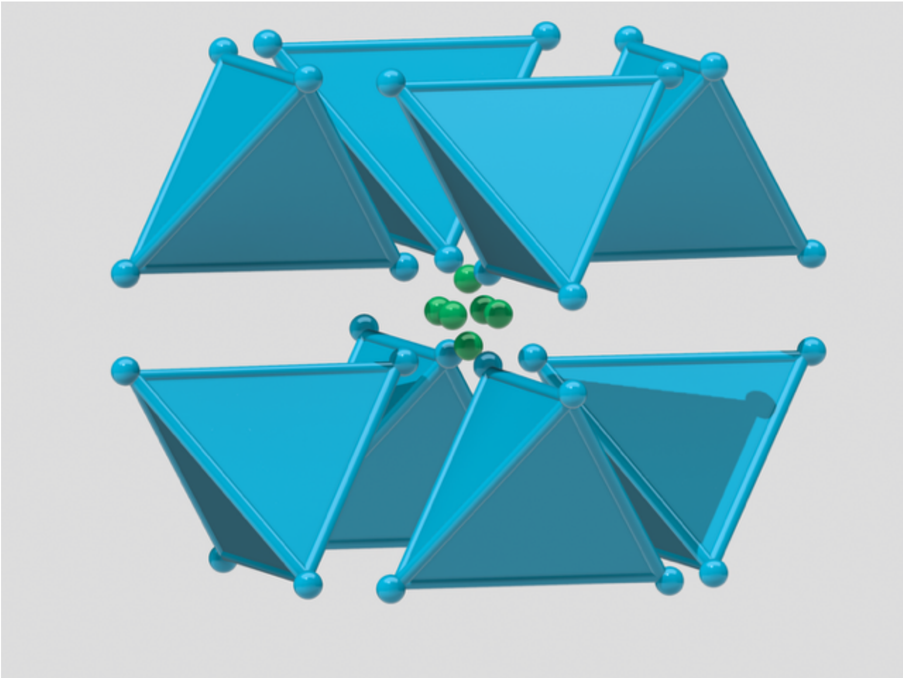
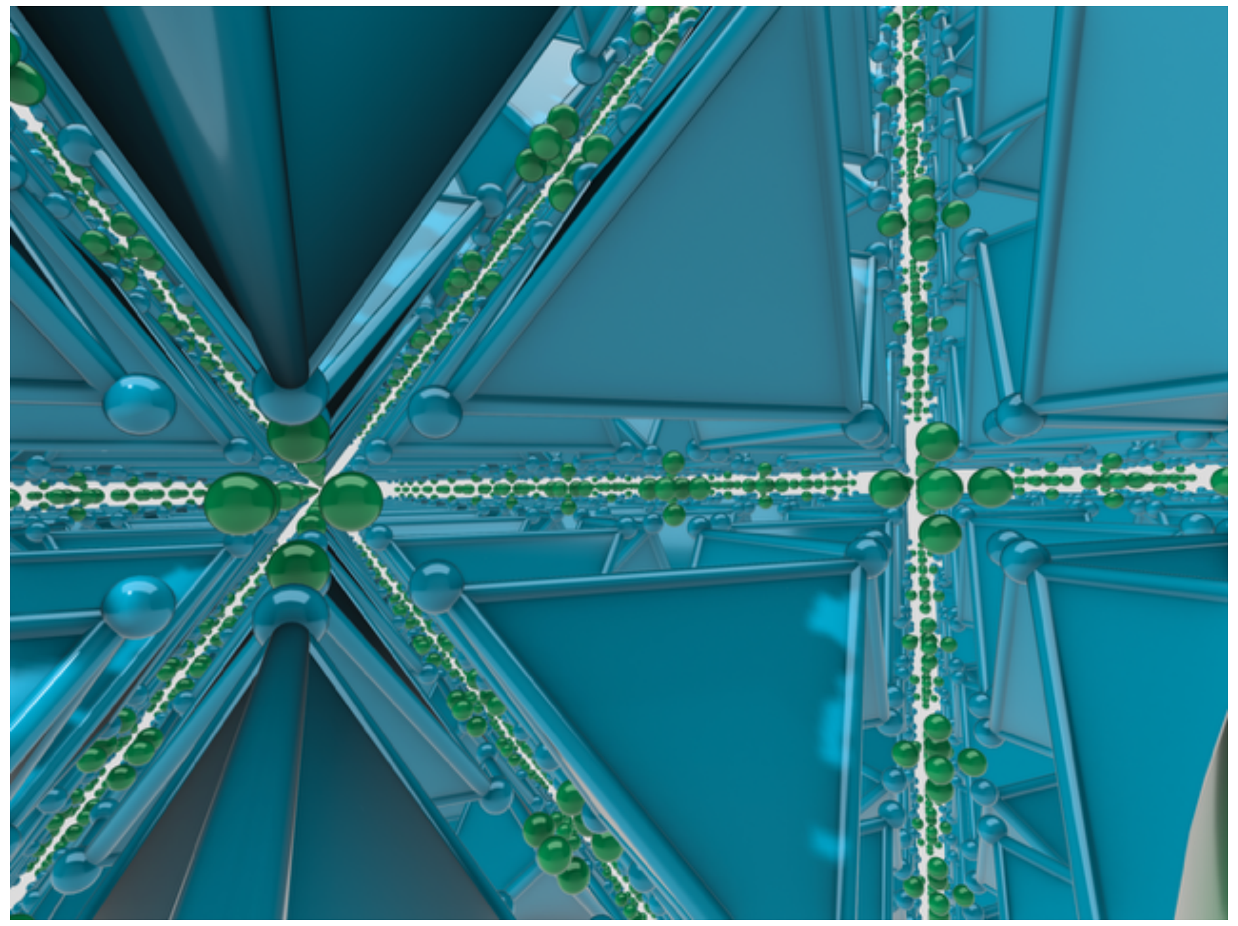
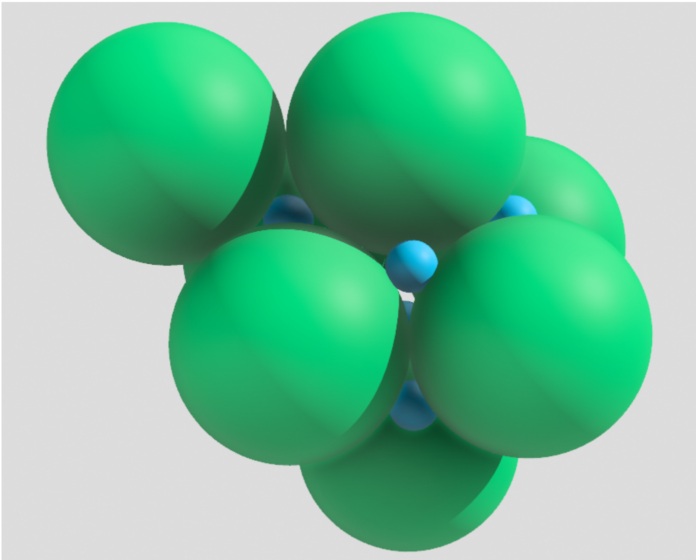

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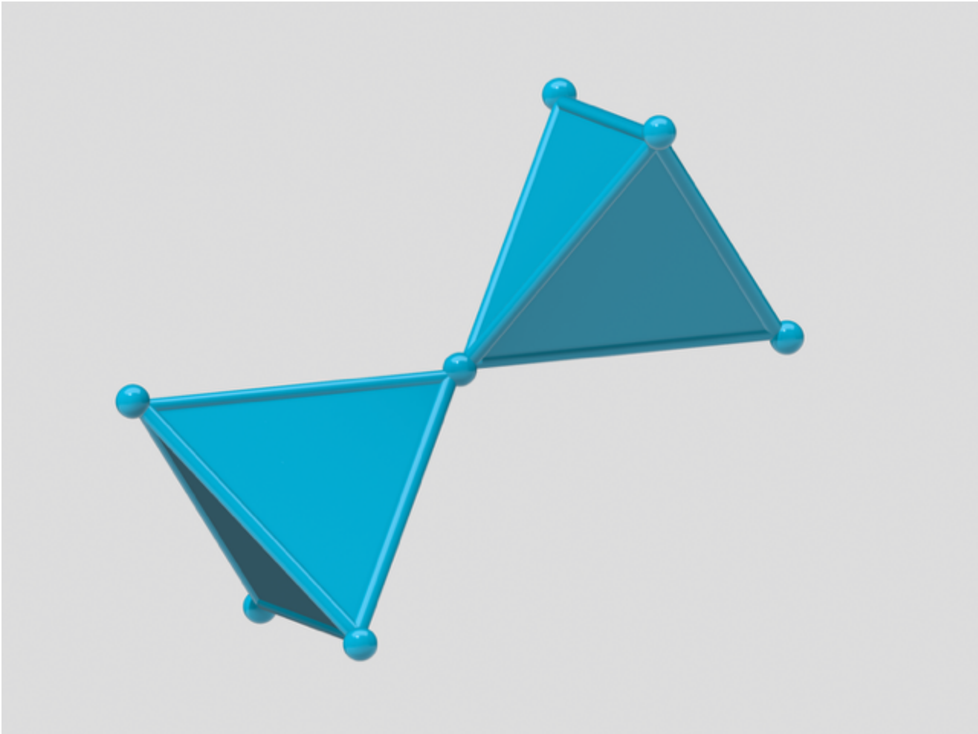
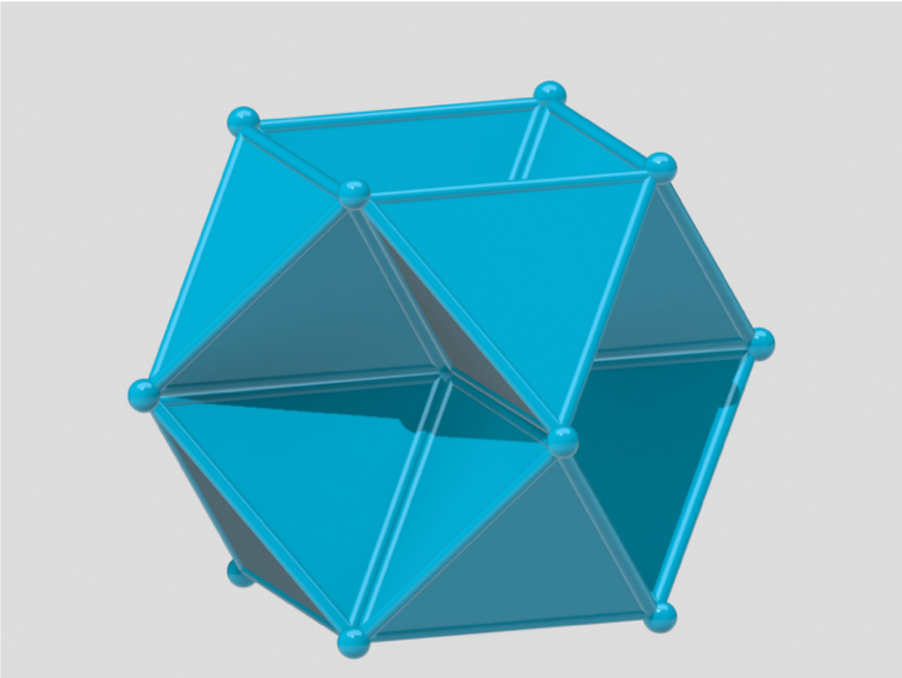
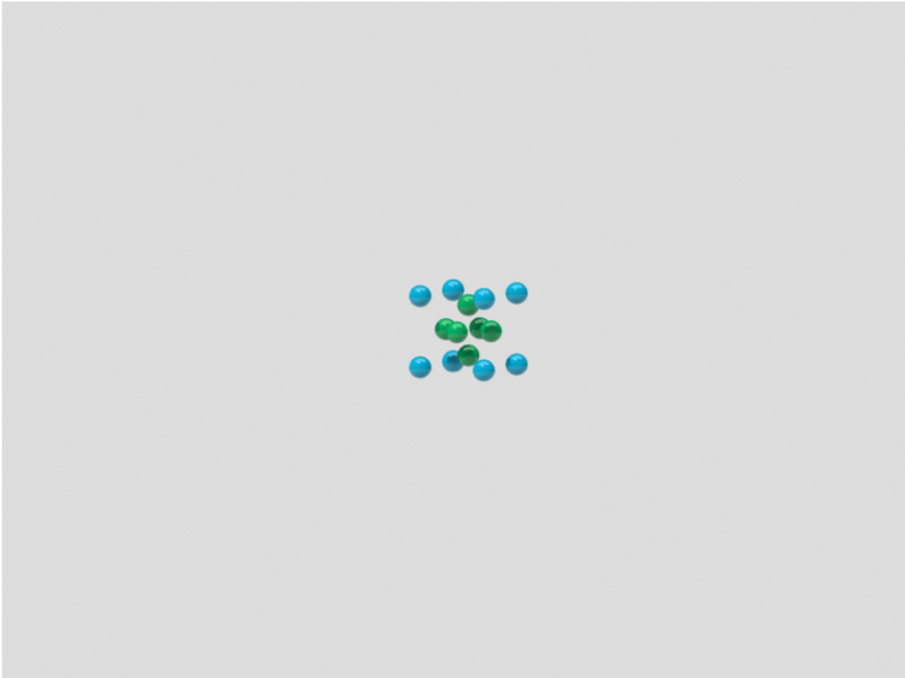
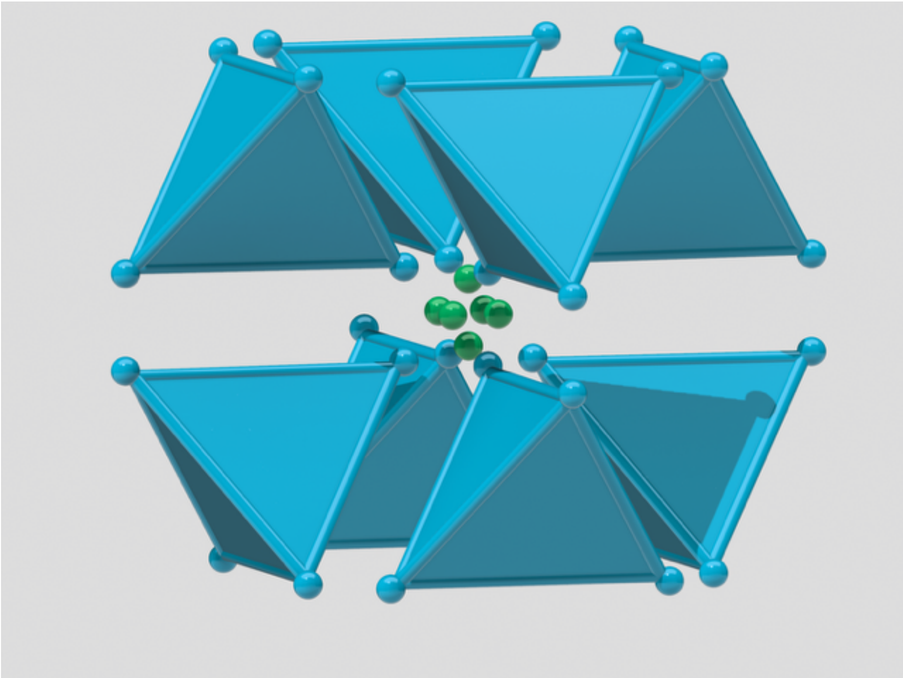
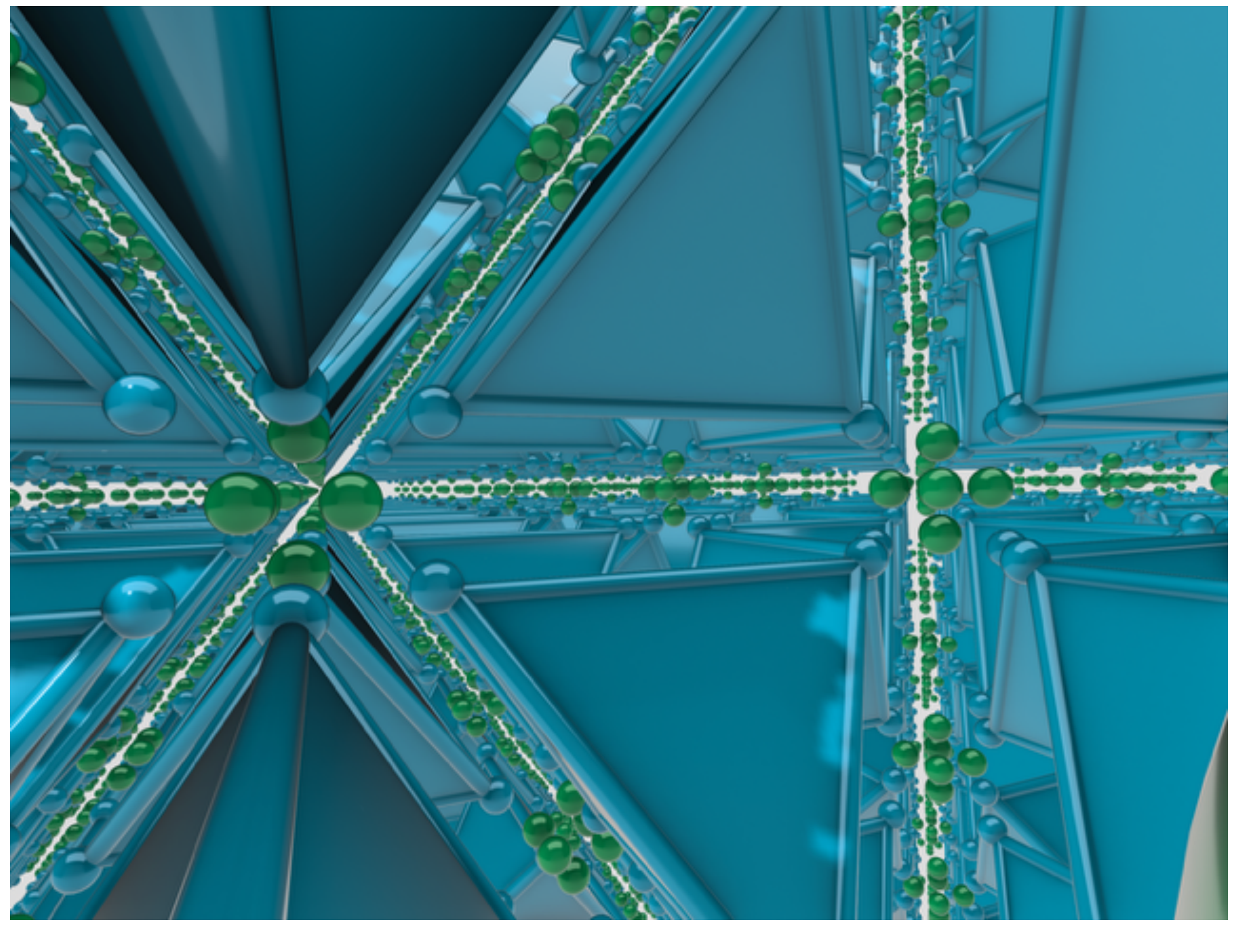
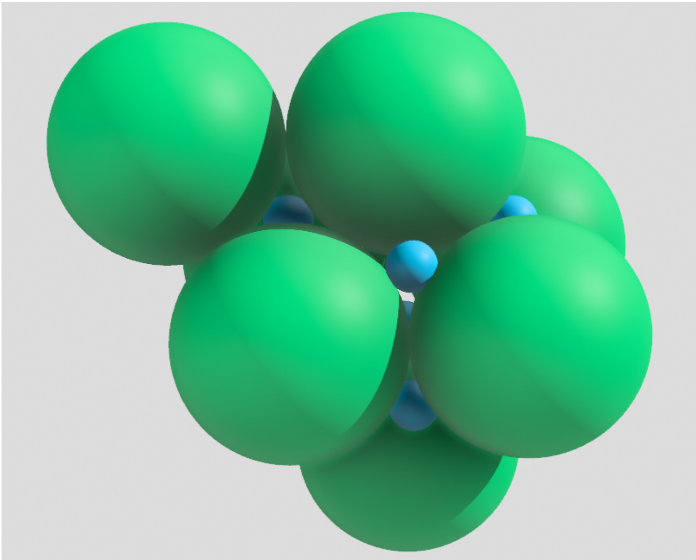


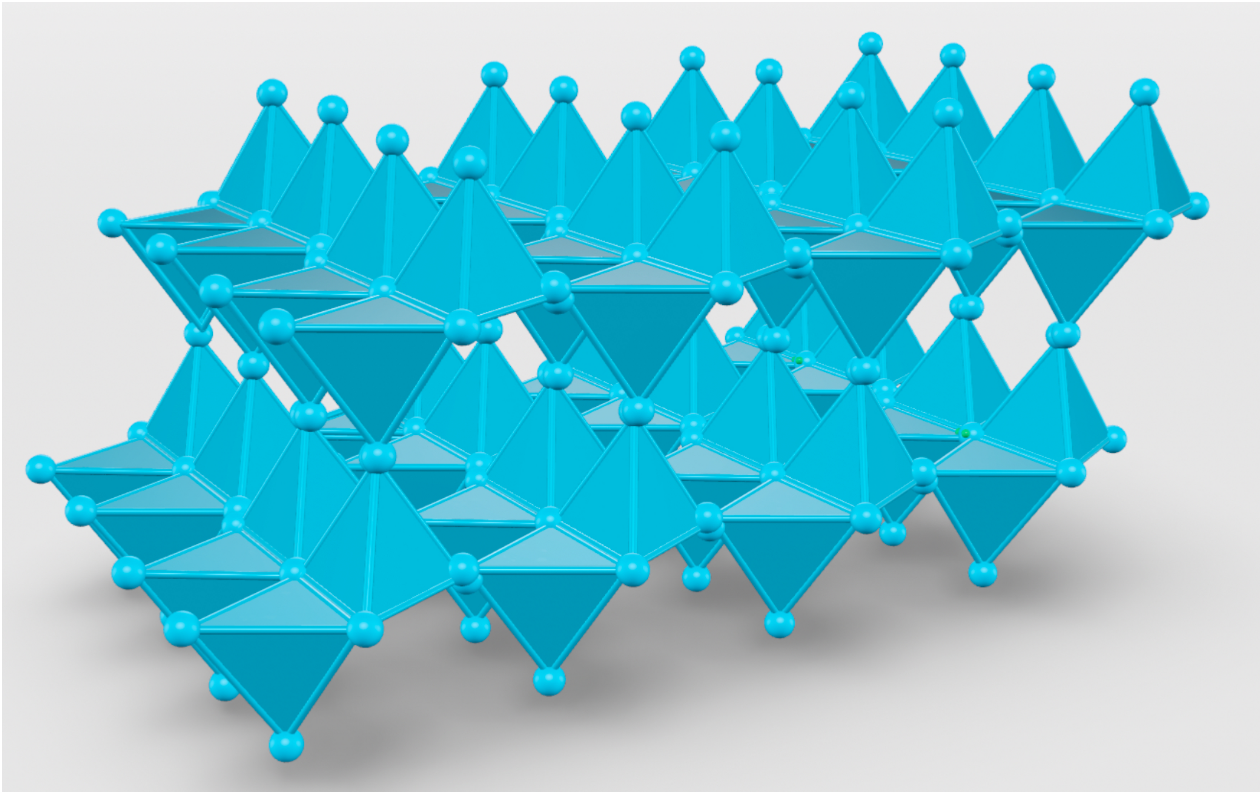


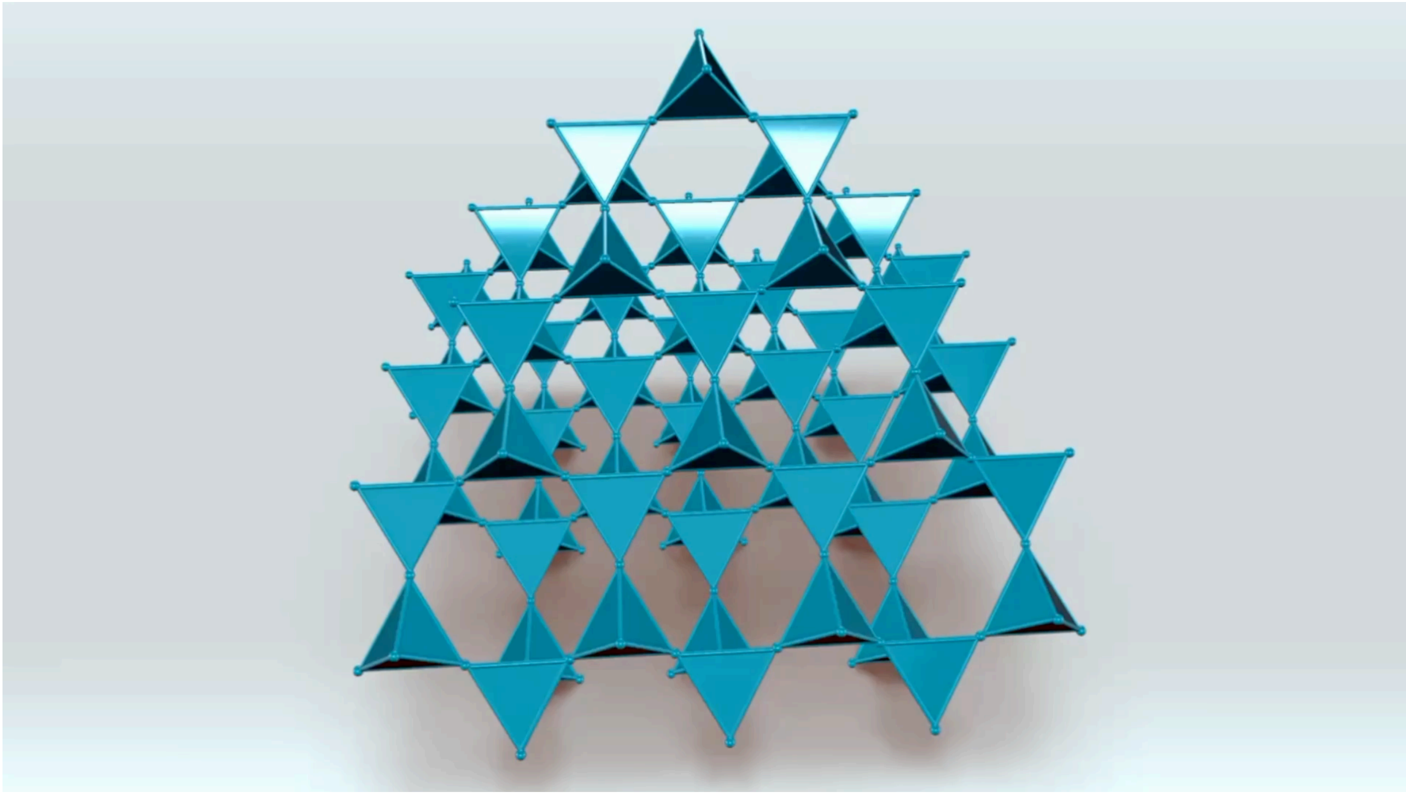




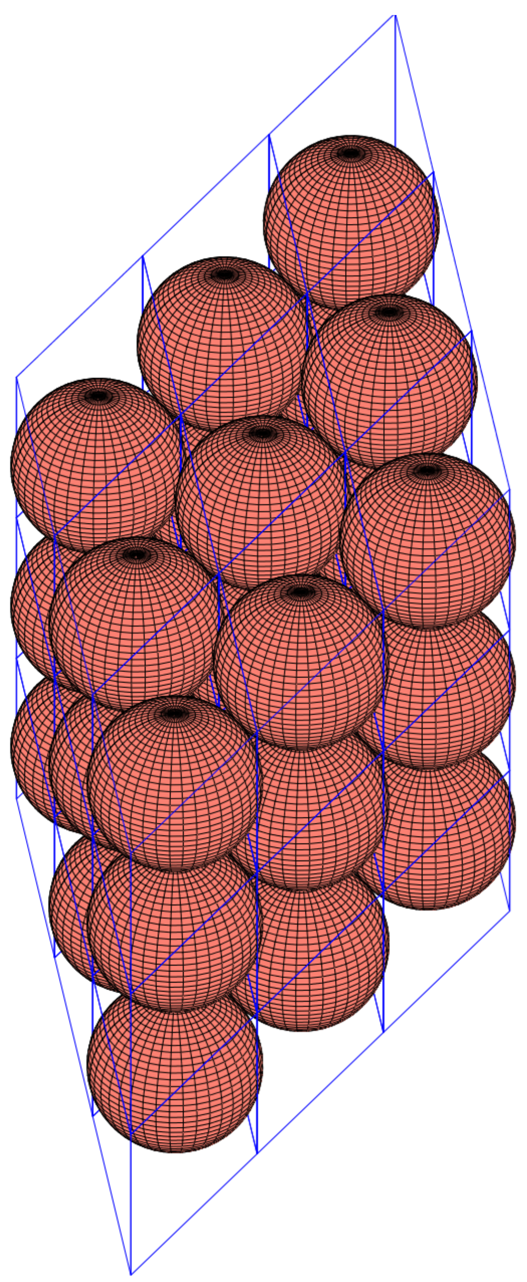








Face Centered Cubic Packing of Spheres



Lattice packing of spheres with density of $\dfrac{\pi}{\sqrt{18}}$

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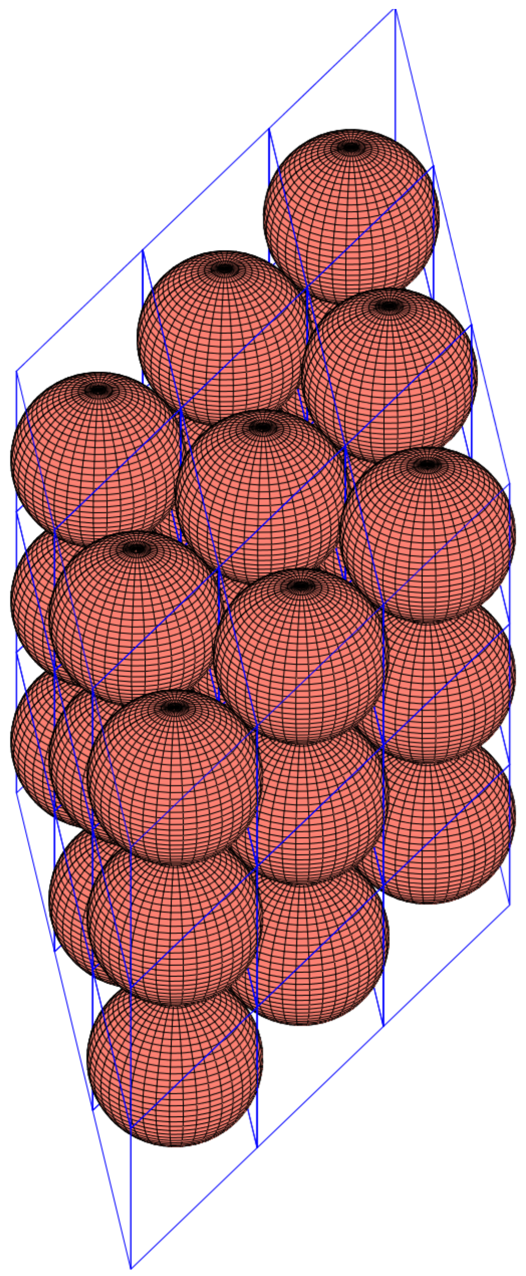

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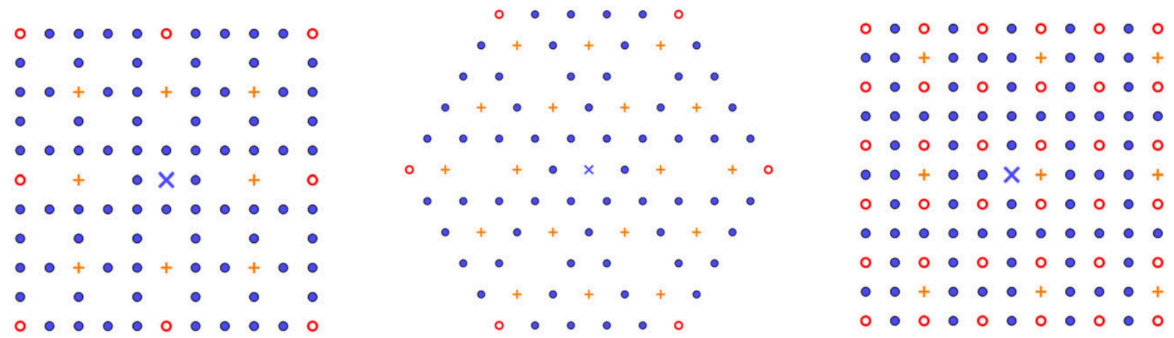

FIGURE 2. Mathematical examples of periodic array of defects performed on a patch of the square lattice $\mathbb{Z}^2$ (left and right) and the triangular lattice A_2 (middle). The cross blue times represents the origin O of $\mathbb{R}^2$. The points marked by blue point are the original points of the lattice, whereas the points marked by orange plus and red point are substitutional defects of charge $1 - a_k$ for some $a_k \in \mathbb{R}^*\backslash\{1\}$ and some $k \in K_: = \{2, 3, 4, 5\}$. The missing lattice points are the vacancy defects. The patch on the right contains two shifted periodic arrays of defects (color figure online)

Under certain assumptions, if the minimal energy is achieved by a lattice structure, some of its sub-lattices also remain minimizers of this energy[1].

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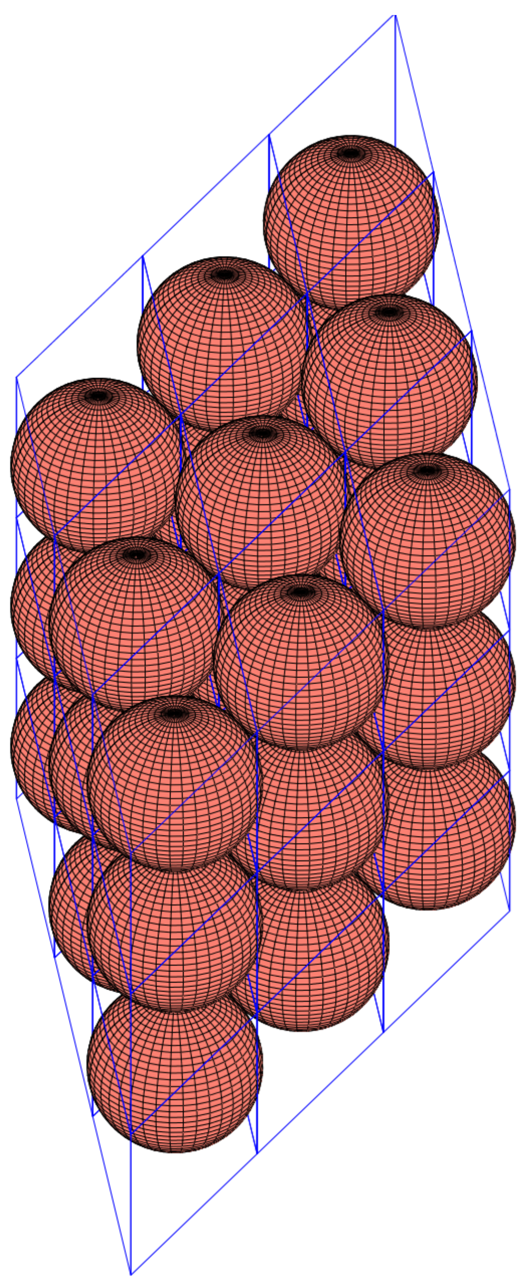
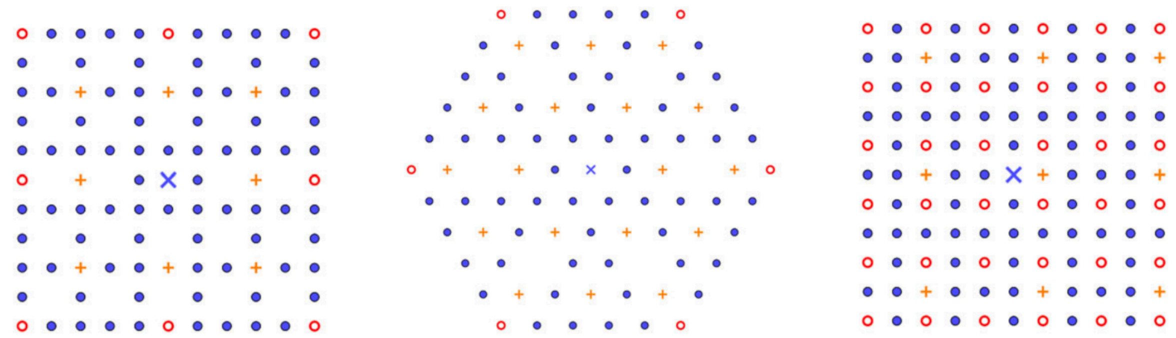


Lattice packing of spheres with density of $\dfrac{\pi}{\sqrt{18}}$

The Face Centred Cubic lattice with quadratic form[2]. $X^2 + Y^2 + Z^2 + XY$



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2. K. L. Fields. (1979). Stable, fragile and absolutely symmetric quadratic forms. Mathematika, 26(1), 76-79.

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