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From Molecular Shape to Crystal Symmetry

Densest Packings of Radially Equilateral Molecules

Miloslav Torda

MACSMIN 2025

10 September 2025

diamond
Hartree Centre
Science & Technology Facilities Council
Imperial College London
ICNS
King Abdullah University of Science and Technology
University of Southampton

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Densest Packings of Hexagonal Molecules in Two Dimensions and Cuboctahedral Molecules in Three Dimensions

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Densest Packings of Cuboctahedral Molecules

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Densest Packings of Hexagonal Molecules in Two Dimensions

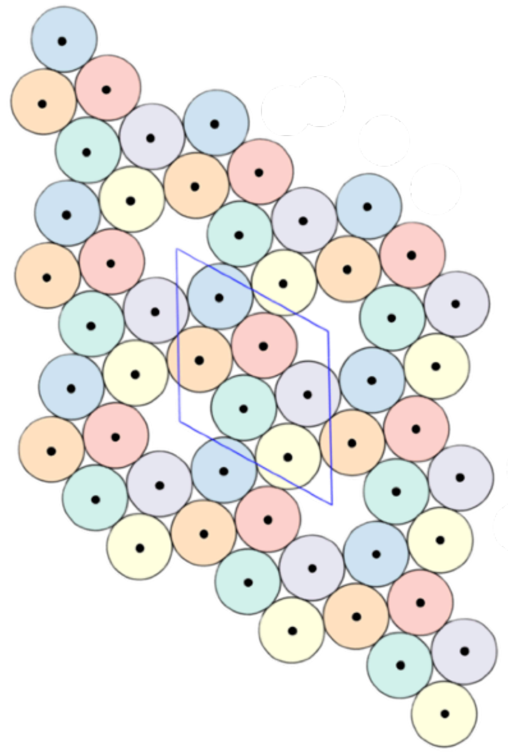
Chiral Interaction Energy Ground States

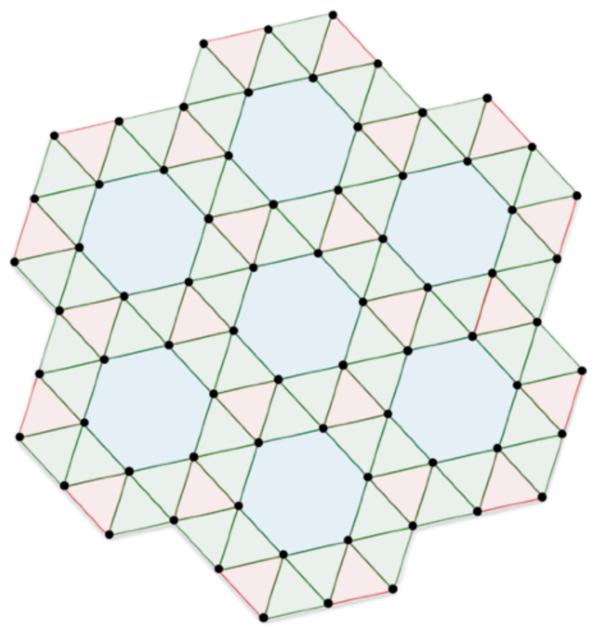
https://milotorda.net/blog/

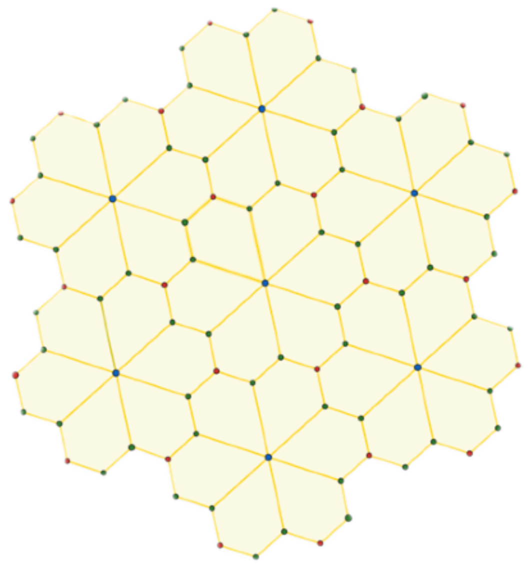
$$\rho\left(\mathscr{K}_{p6_{\mathbf{max}}}\right) = \frac{\sqrt{3}}{7}\pi = 0.7773425\ldots$$

Regular tessellation

Dual tessellation



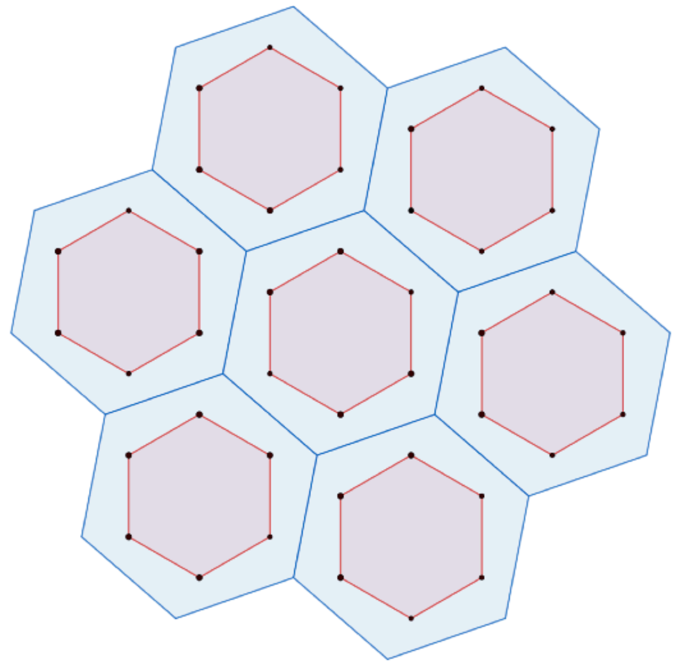


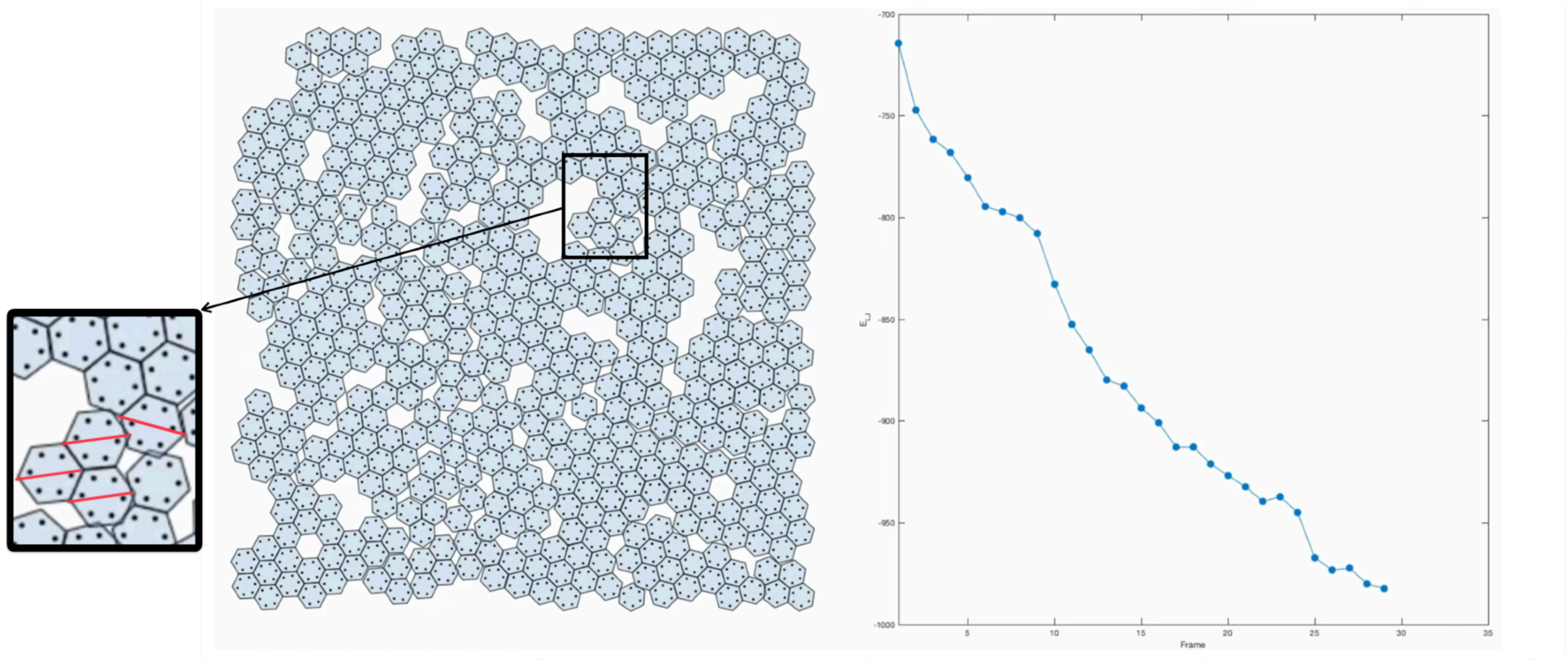


Densest $p6$ disc packing

Snub trihexagonal tiling

Floret pentagonal tiling





Lattice Energy and Sphere Packing

The link between the crystallization problem and the sphere packing problem has been highlighted by Heitmann and Radin in [129]. Indeed, if the interaction potential V is given by

$$V(r) = \begin{cases} +\infty & \text{if } 0 \leq r < 1, \\ -1 & \text{if } r = 1, \\ 0 & \text{if } r > 1, \end{cases} \tag{20}$$

then the particles can be considered as hard spheres of radius $1/2$. These spheres tend to touch due to the condition $V(1) = -1$. The crystallization problem is thus equivalent to the sphere packing, and one obtains that the solution is the hexagonal lattice in 2D, and either FCC or the other sphere packing solutions in 3D.

Subsequent works aimed at generalizing this result to potentials which are similar to (20), but are closer to physically realistic interactions. For instance, in [194], Radin considered a potential satisfying (20) for $r \in [0, 1]$, which is non-decreasing for $r \geq 1$, and tends to 0 fast enough as $r \to +\infty$. In a famous article [229], Theil dealt with smoother, more realistic potentials (which look like V_{LJ}), in dimension two. However, he still used restrictive hypotheses on V. This work has been extended to dimension three recently in [90], in which an additional three-body term is added, which favors particular angles between interatomic bonds. A similar strategy has been used in dimension $d = 2$ in [78, 169, 170], where the optimal lattice may be a square lattice. One can therefore consider that the problem is not completely understood in dimension two, and completely open in dimension three.

- Taking into account *monoatomic systems.*
- We are considering *molecular systems— multi-atomic systems.*

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The crystallization conjecture: a review

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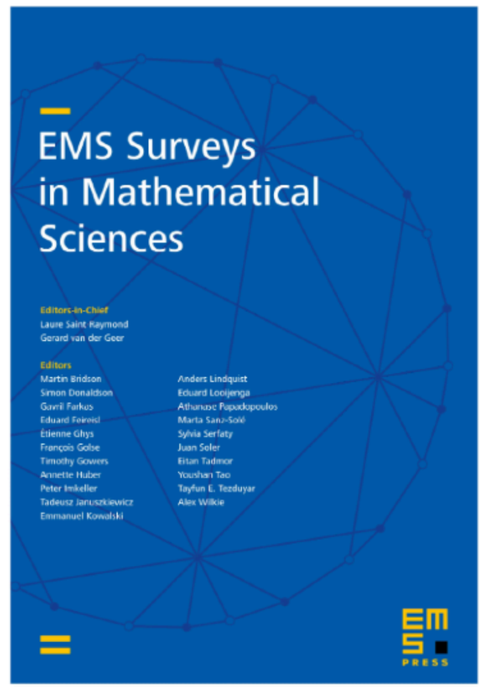
Mathieu Lewin
Université de Cergy-Pontoise, France



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Abstract

In this article we describe the *crystallization conjecture*. It states that, in appropriate physical conditions, interacting particles always place themselves into periodic configurations, breaking thereby the natural translation-invariance of the system. This famous problem is still largely open. Mathematically, it amounts to studying the minima of a real-valued function defined on $\mathbb{R}^{3N}$ where N is the number of particles, which tends to infinity. We review the existing literature and mention several related open problems, of which many have not been thoroughly studied.

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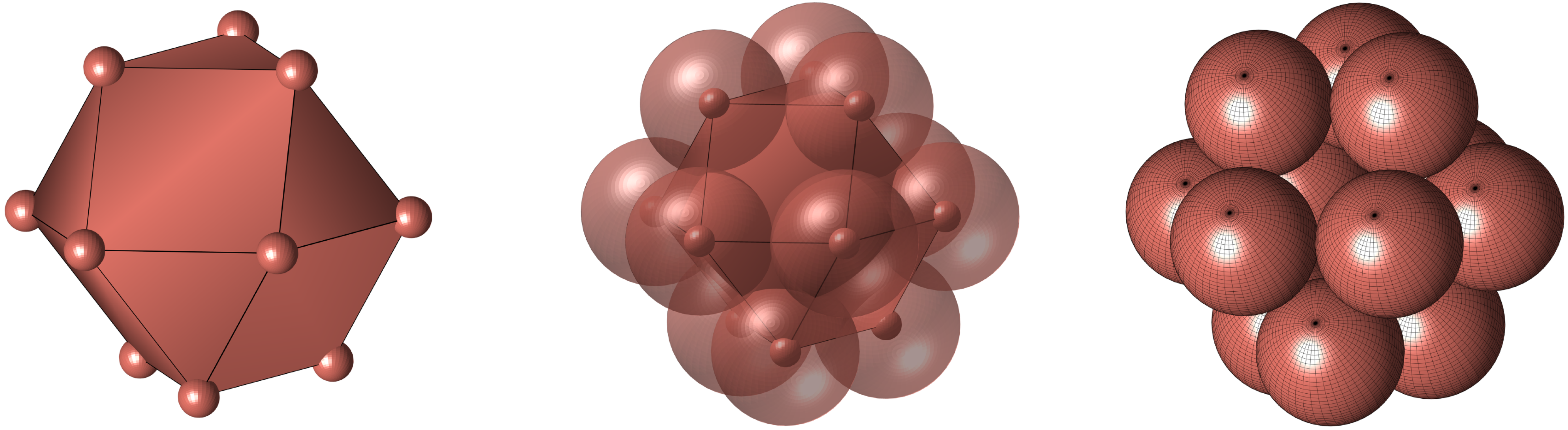
Mathematics Subject Classification

82-XX 11-XX 35-XX 49-XX

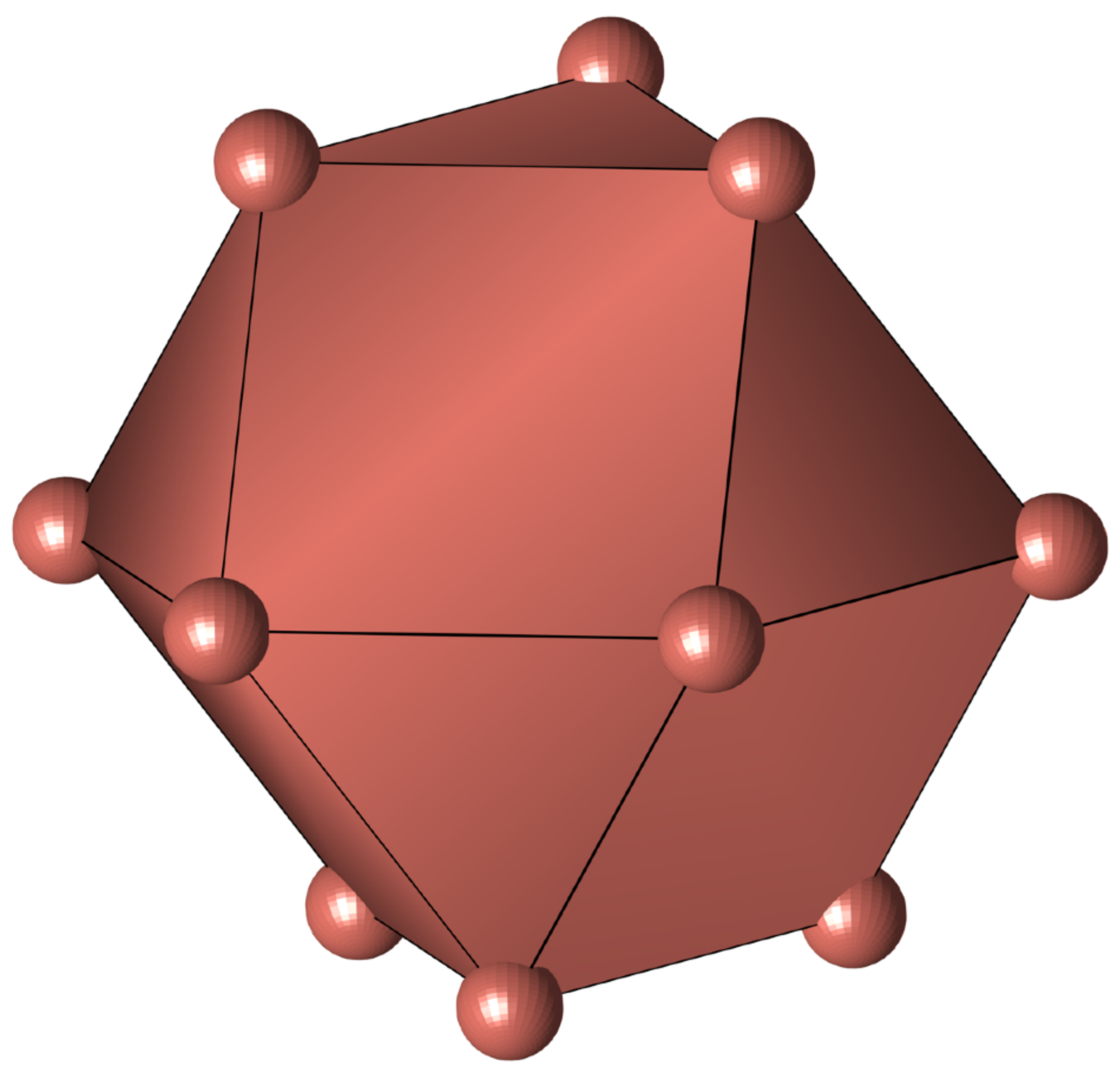
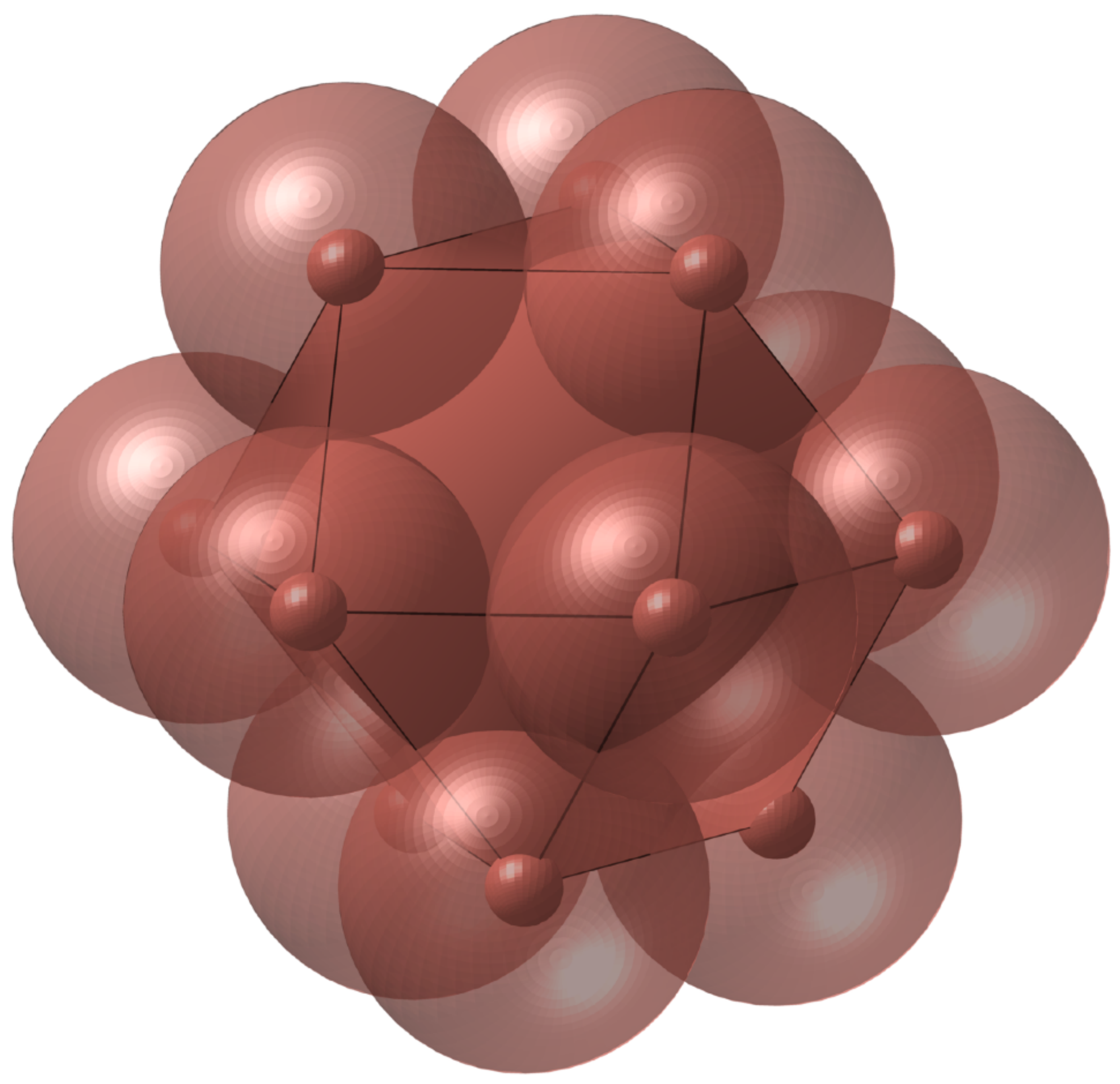
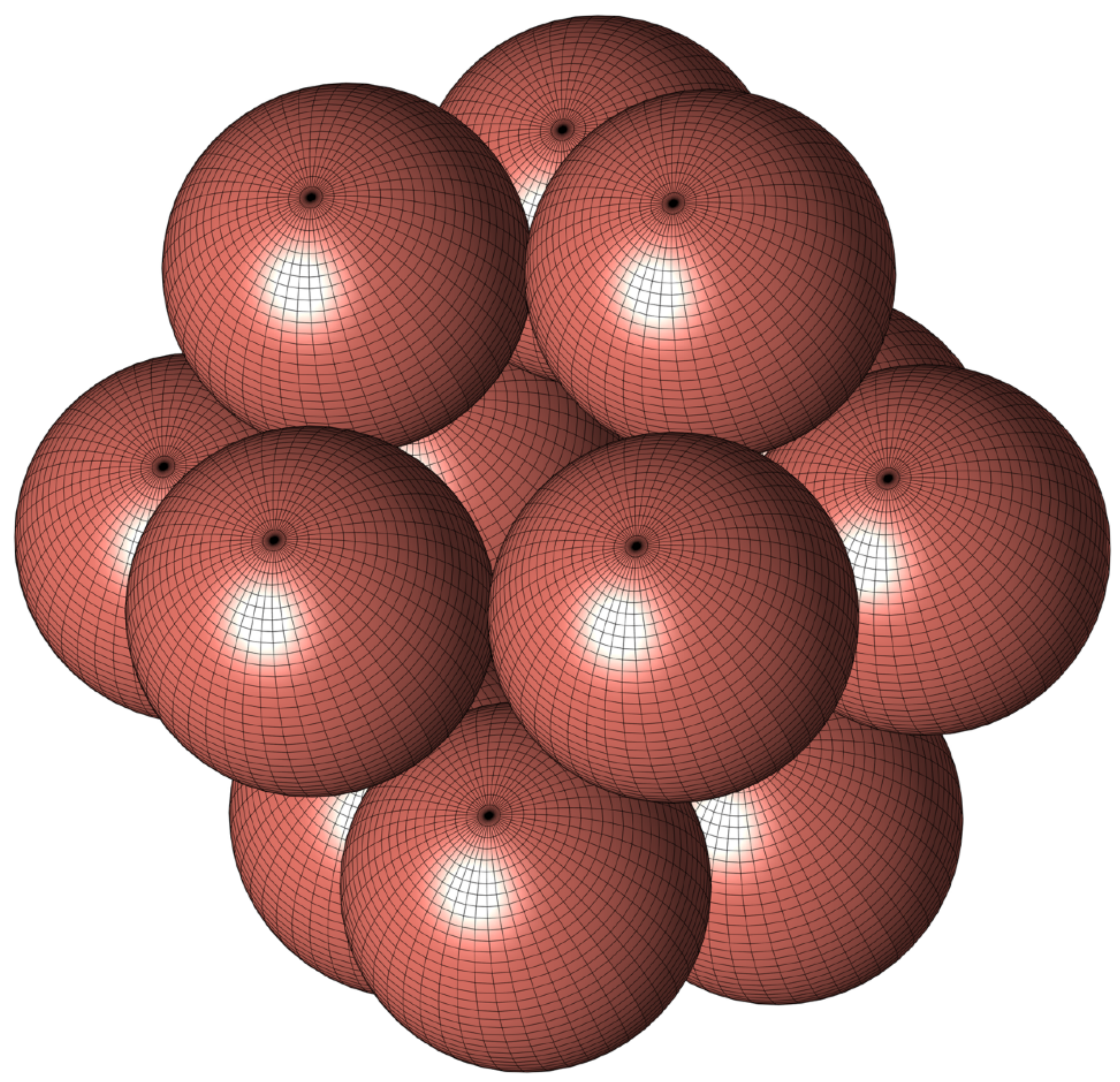
Cuboctahedral Molecule Model

- *Molecule* a rigid collection of hard spheres



Cuboctahedral Molecule Model

- *Molecule* a rigid collection of hard spheres
- Place 12 equal spheres on vertices of one cuboctahedron

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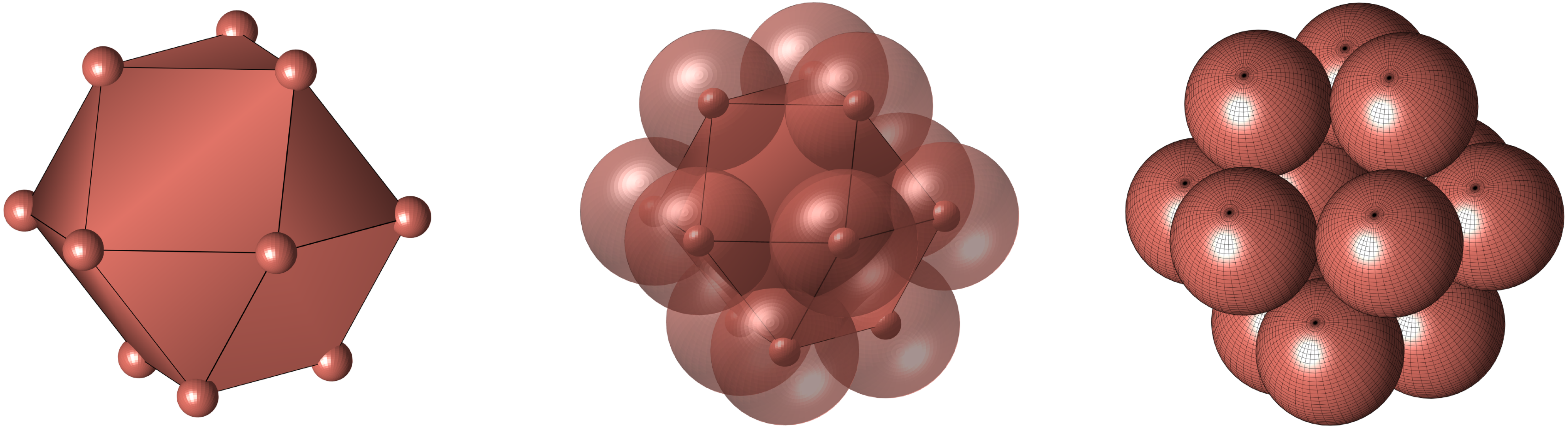
- Question: What is its densest packing molecules with this geometry?



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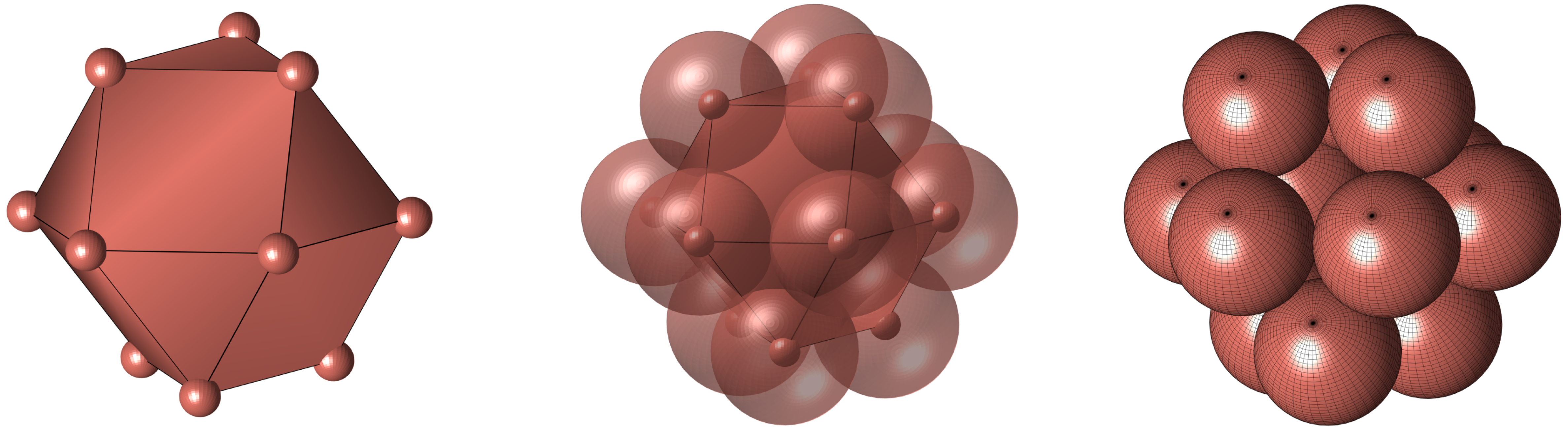

Possible candidate but *is it the densest packing?*

Divide and Conquer

- Start with simpler molecules

Divide and Conquer

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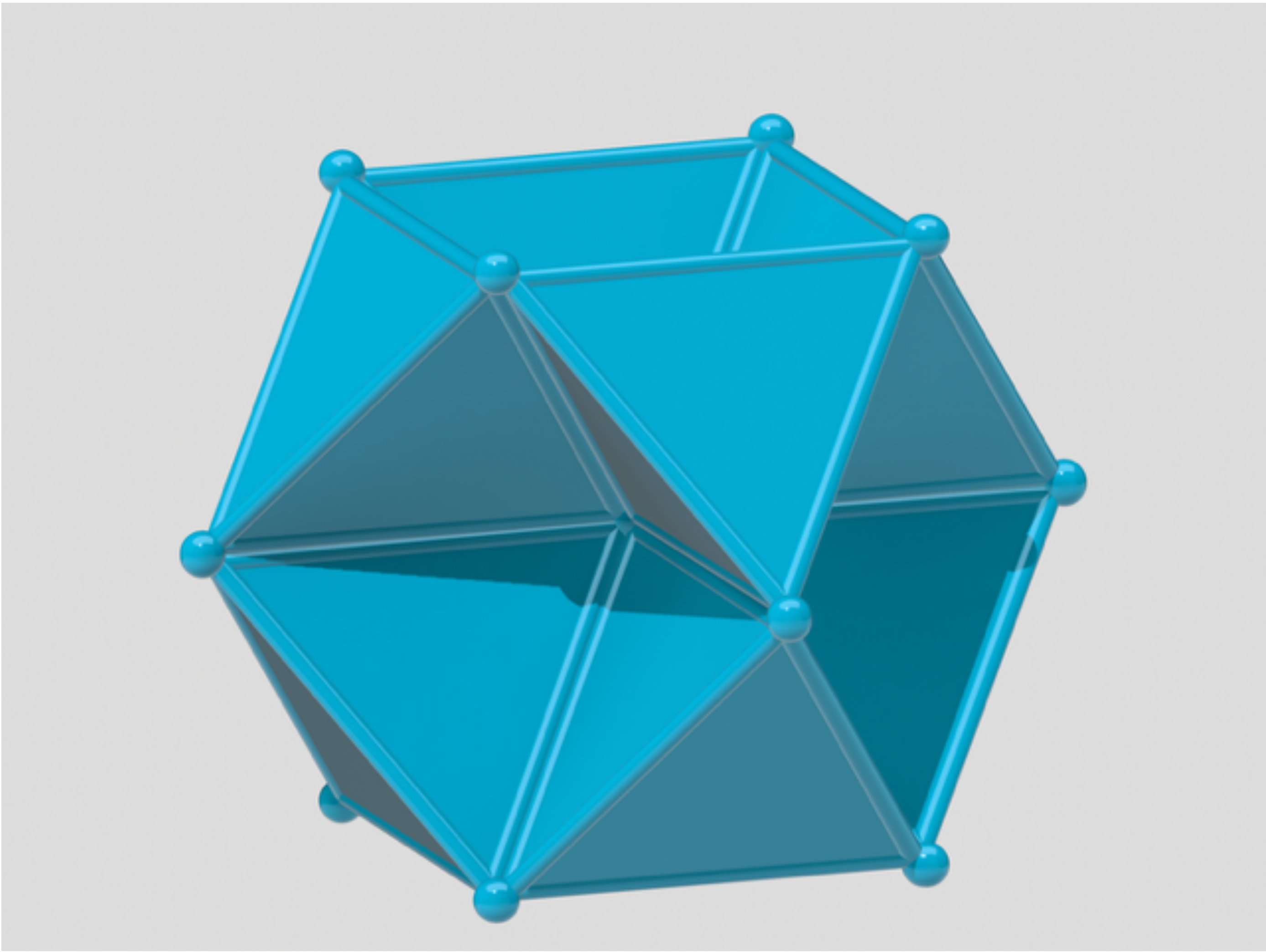
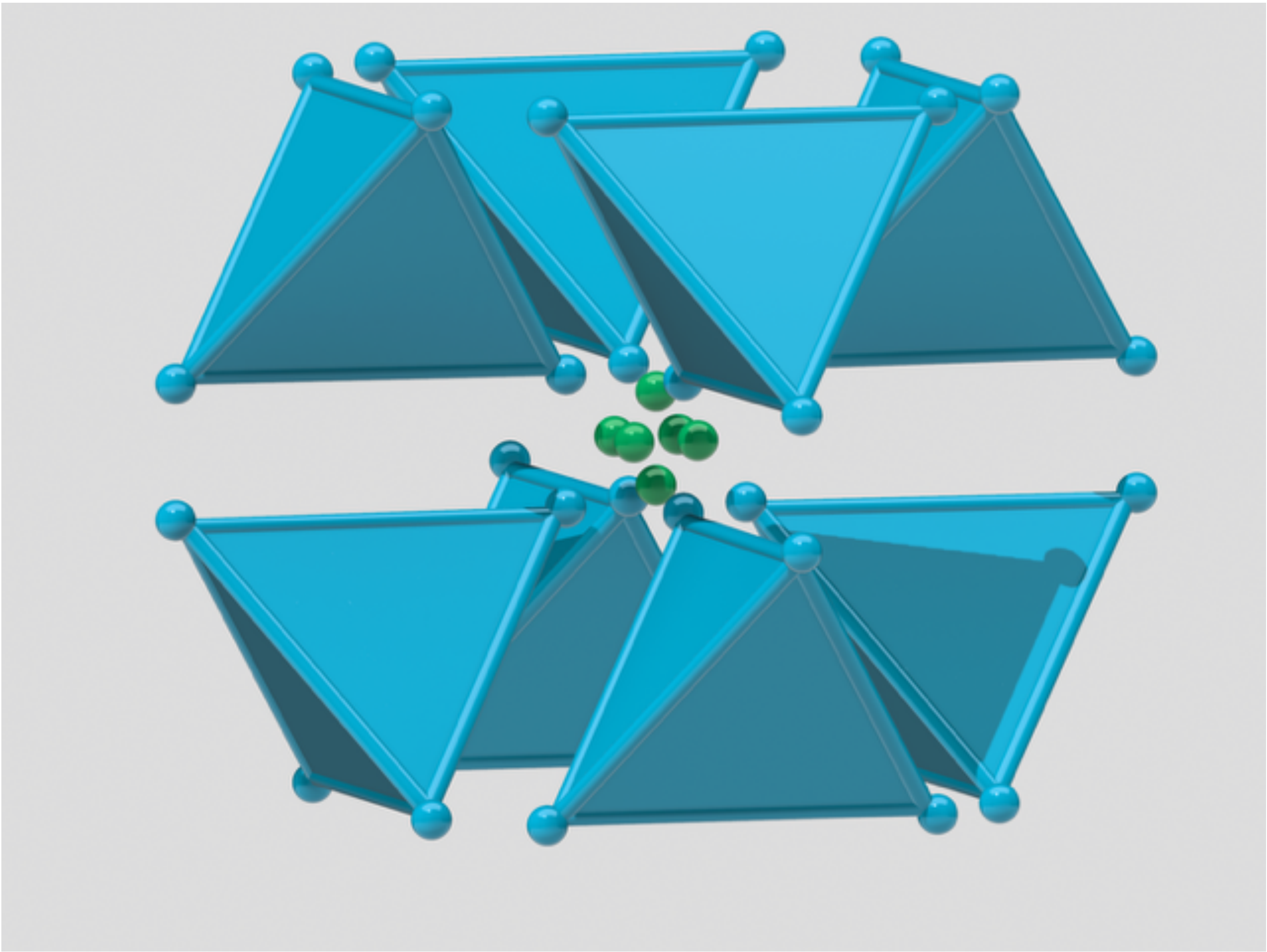
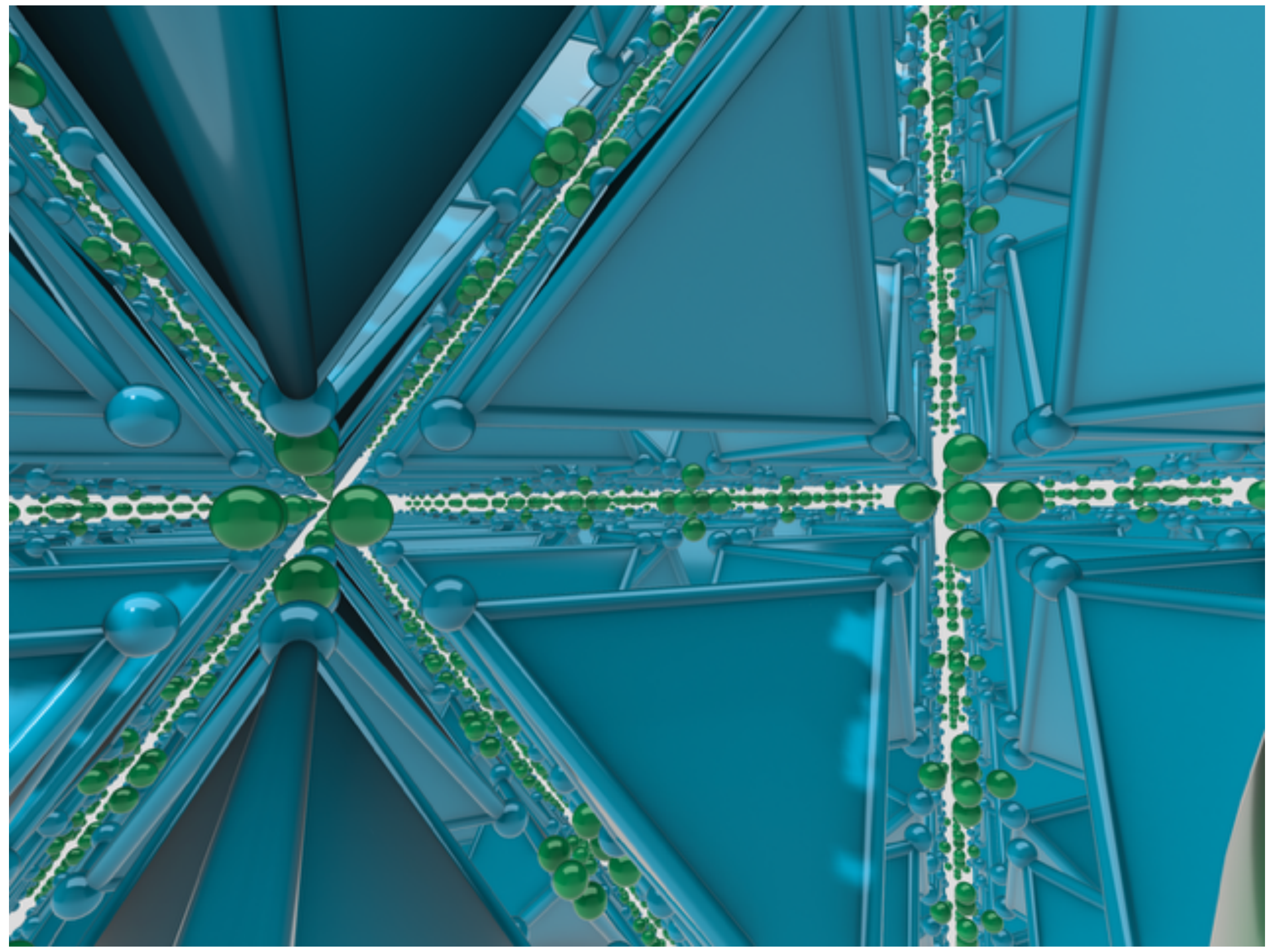
- Tetrahedral / octahedral molecules

Octatetrahedron



Tetrahedral framework- tetrahedra builds blocks and octahedral hollows





Divide and Conquer

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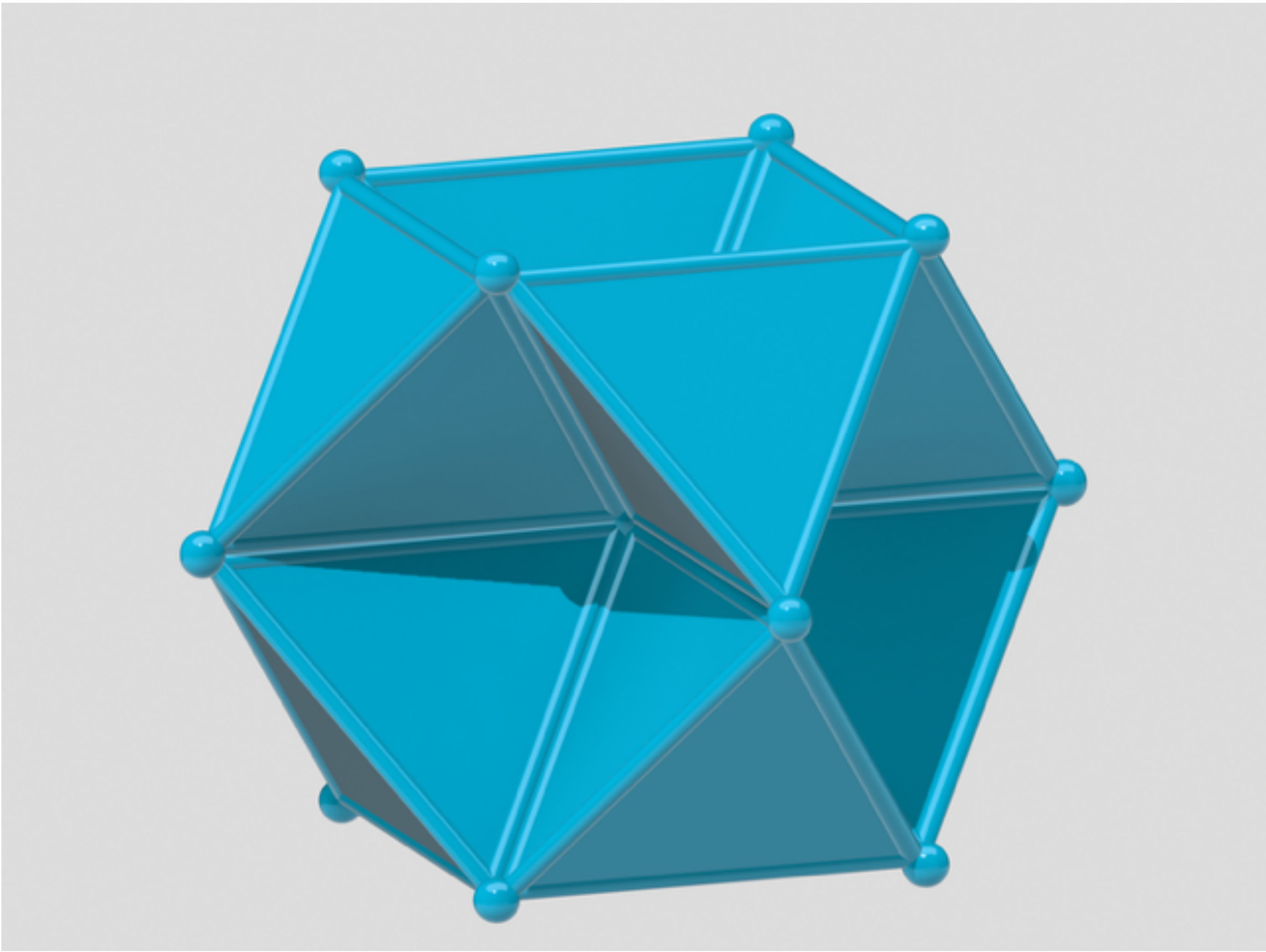

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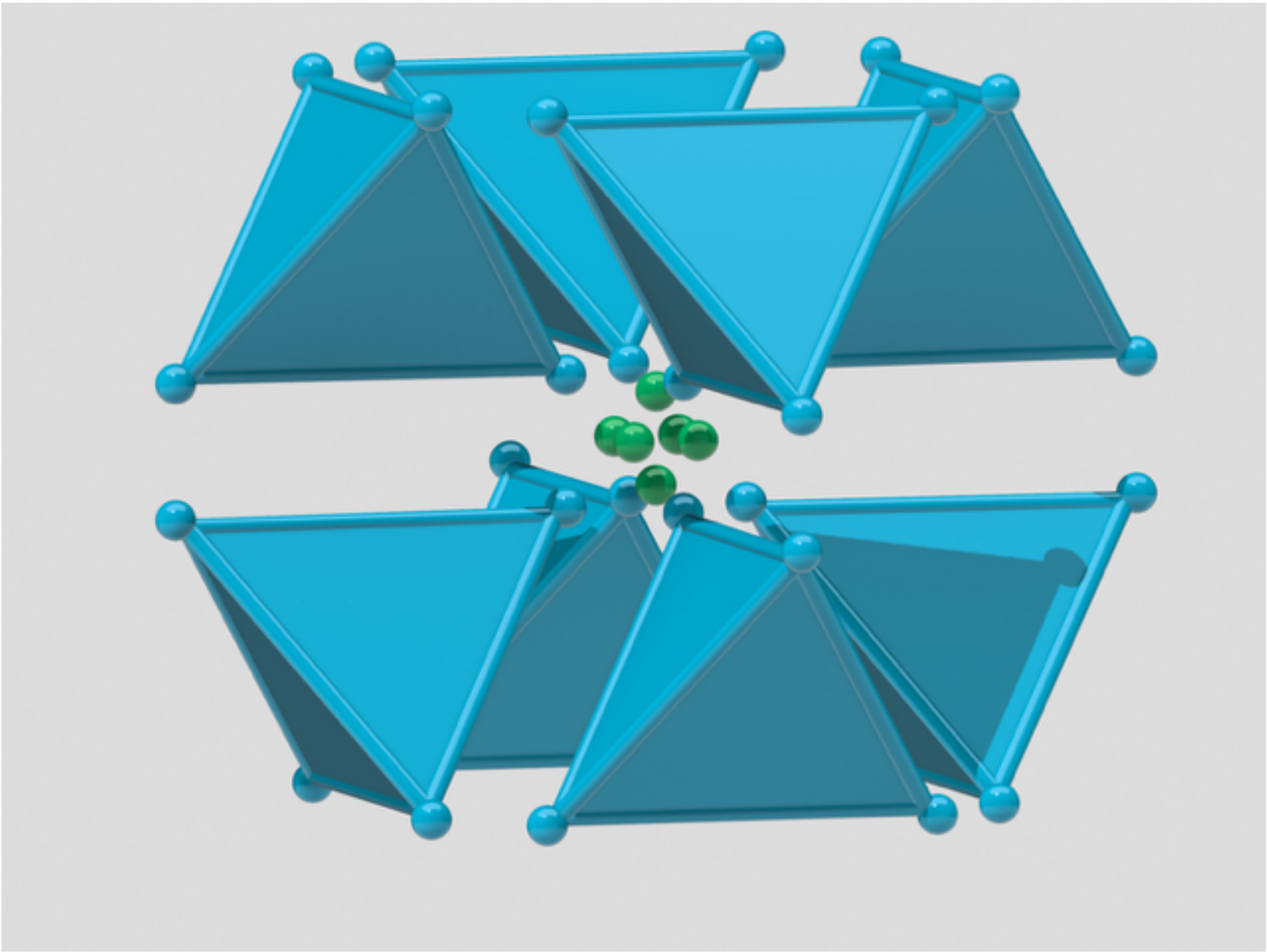

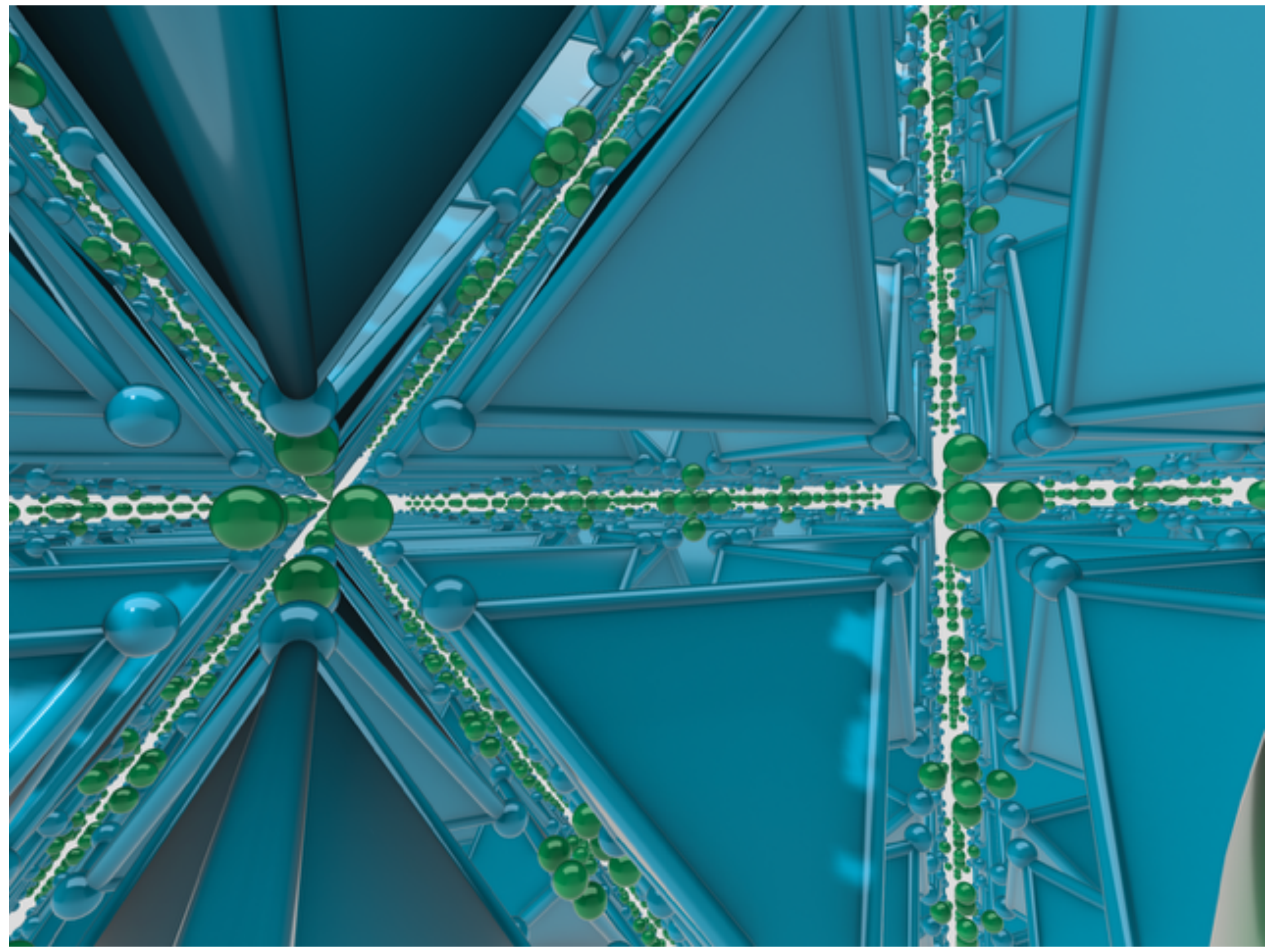

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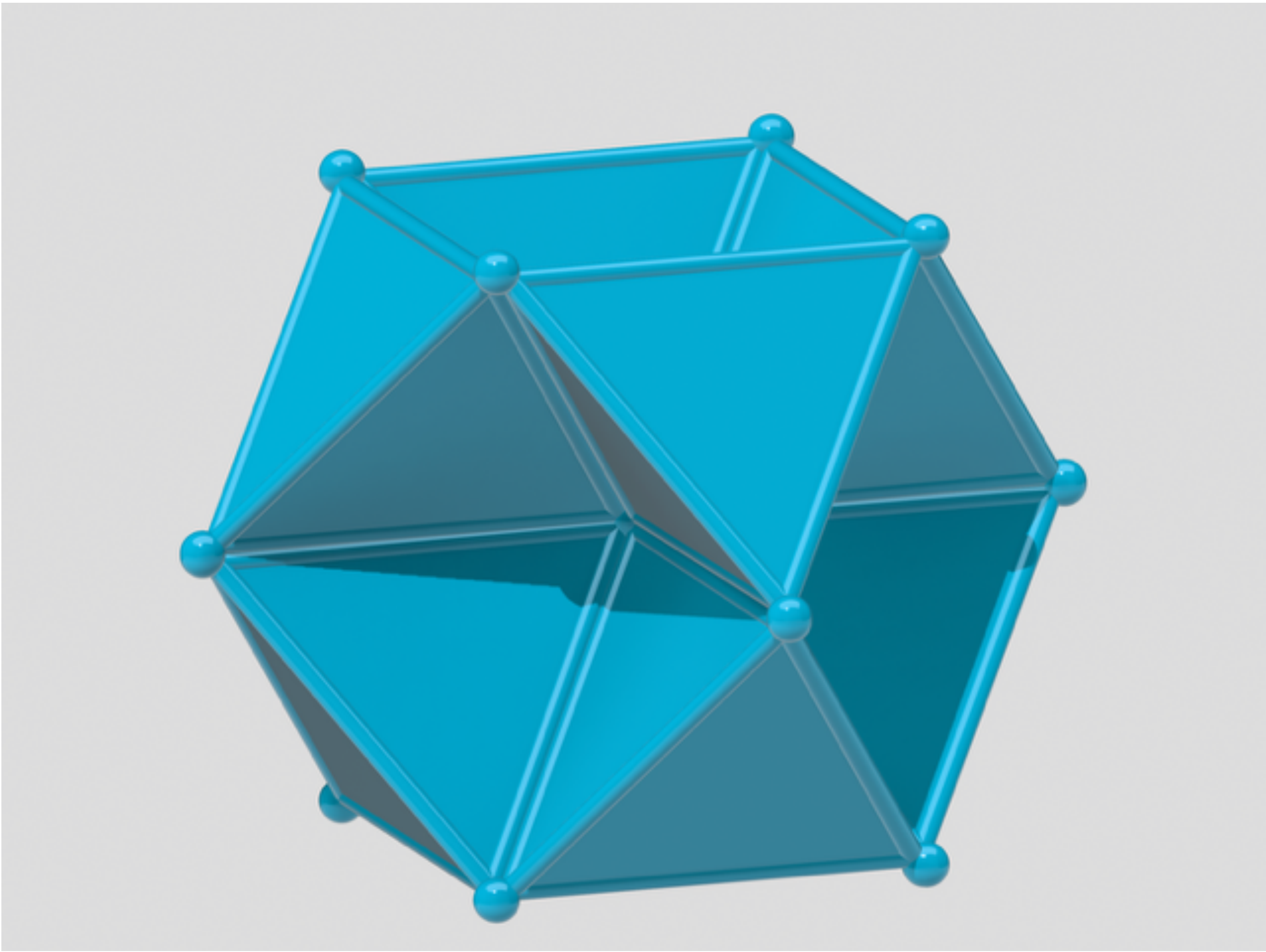

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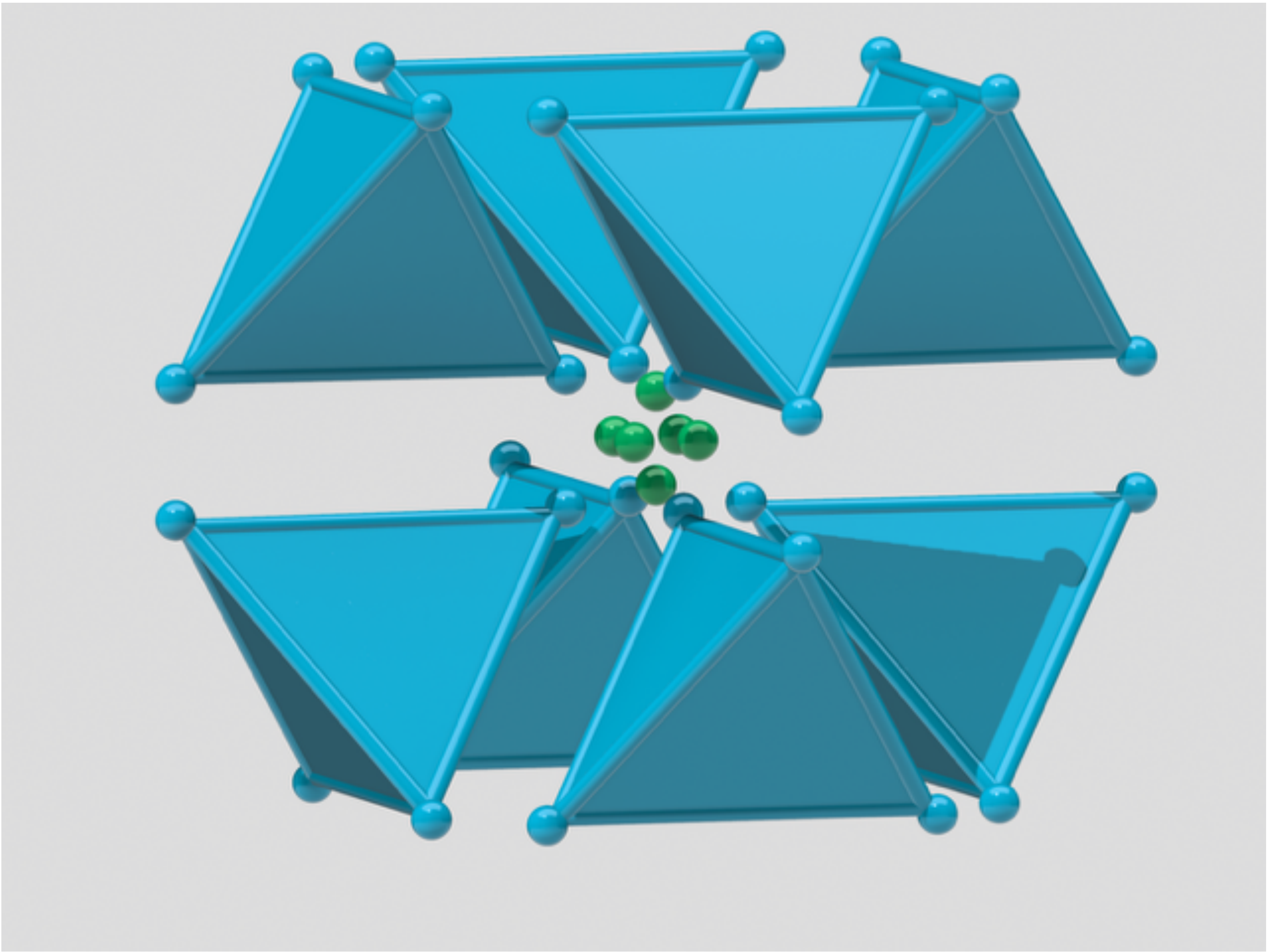

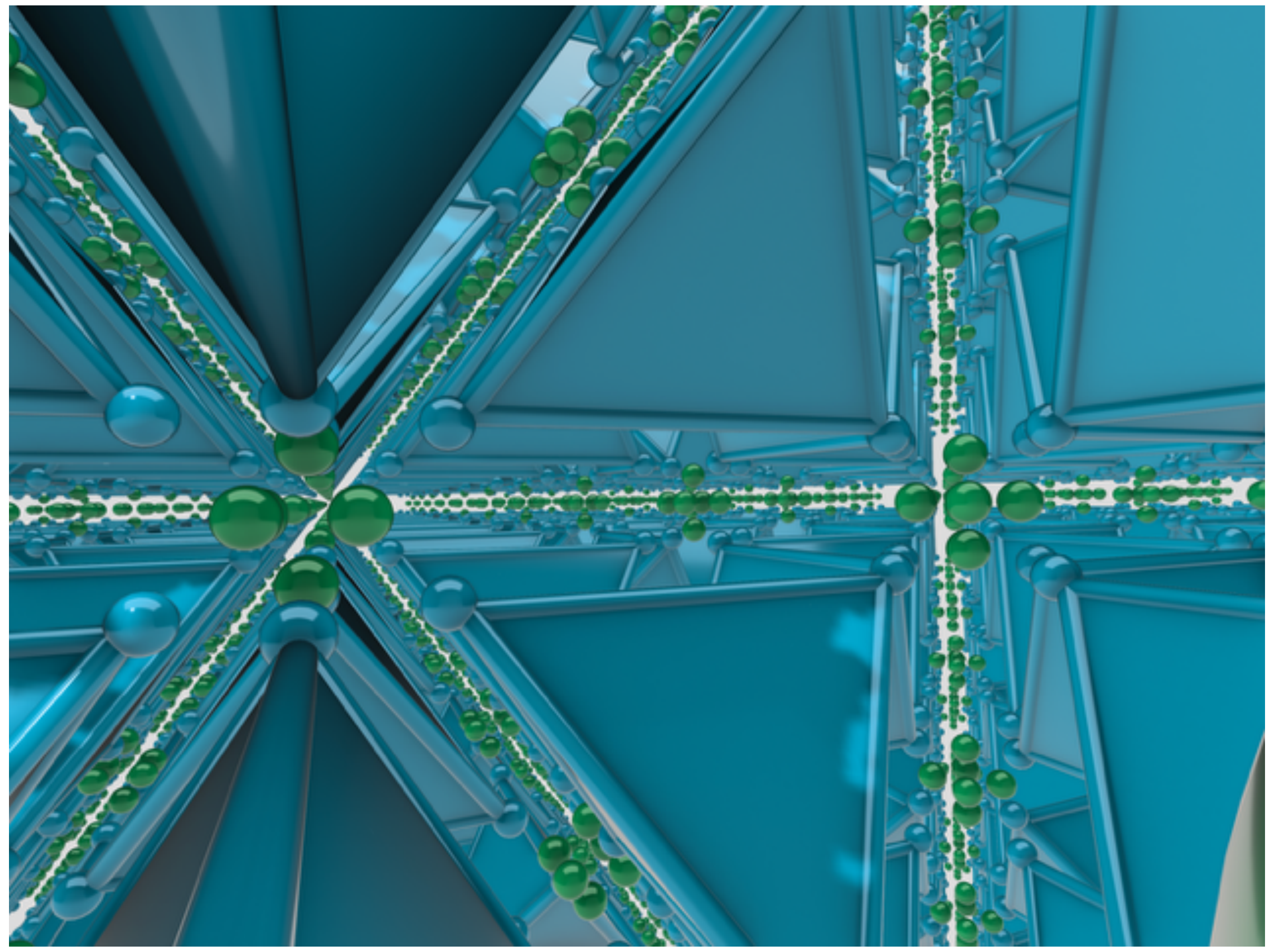

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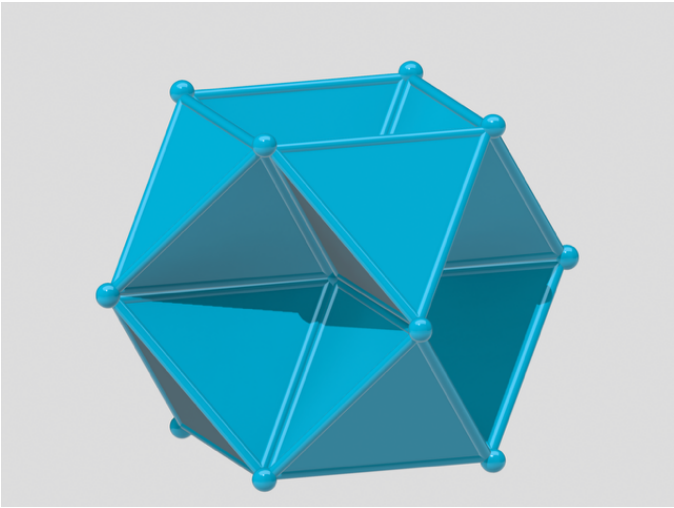
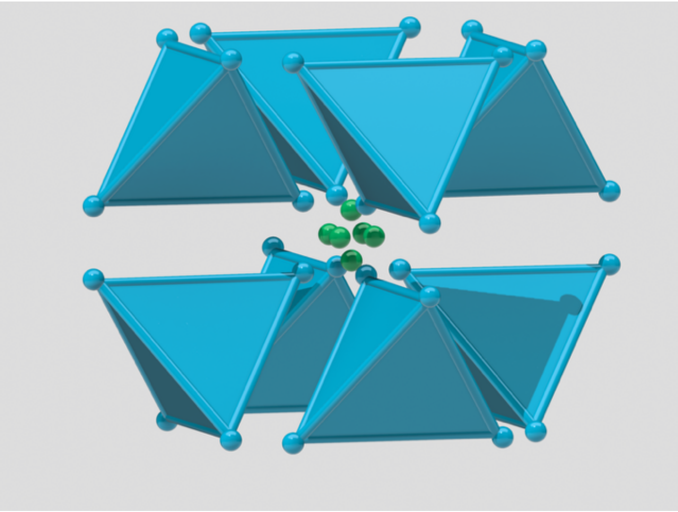
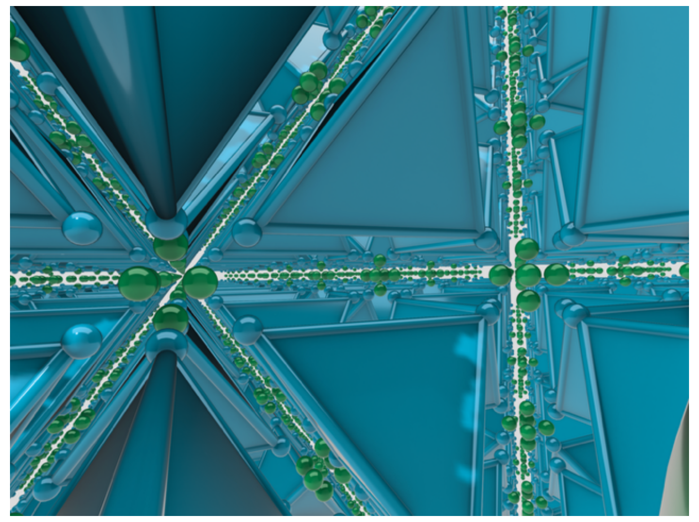

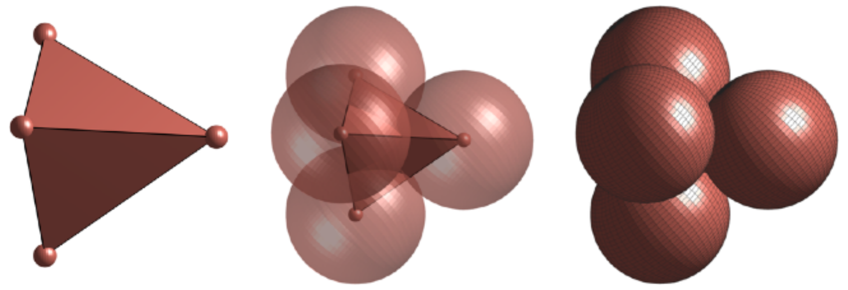
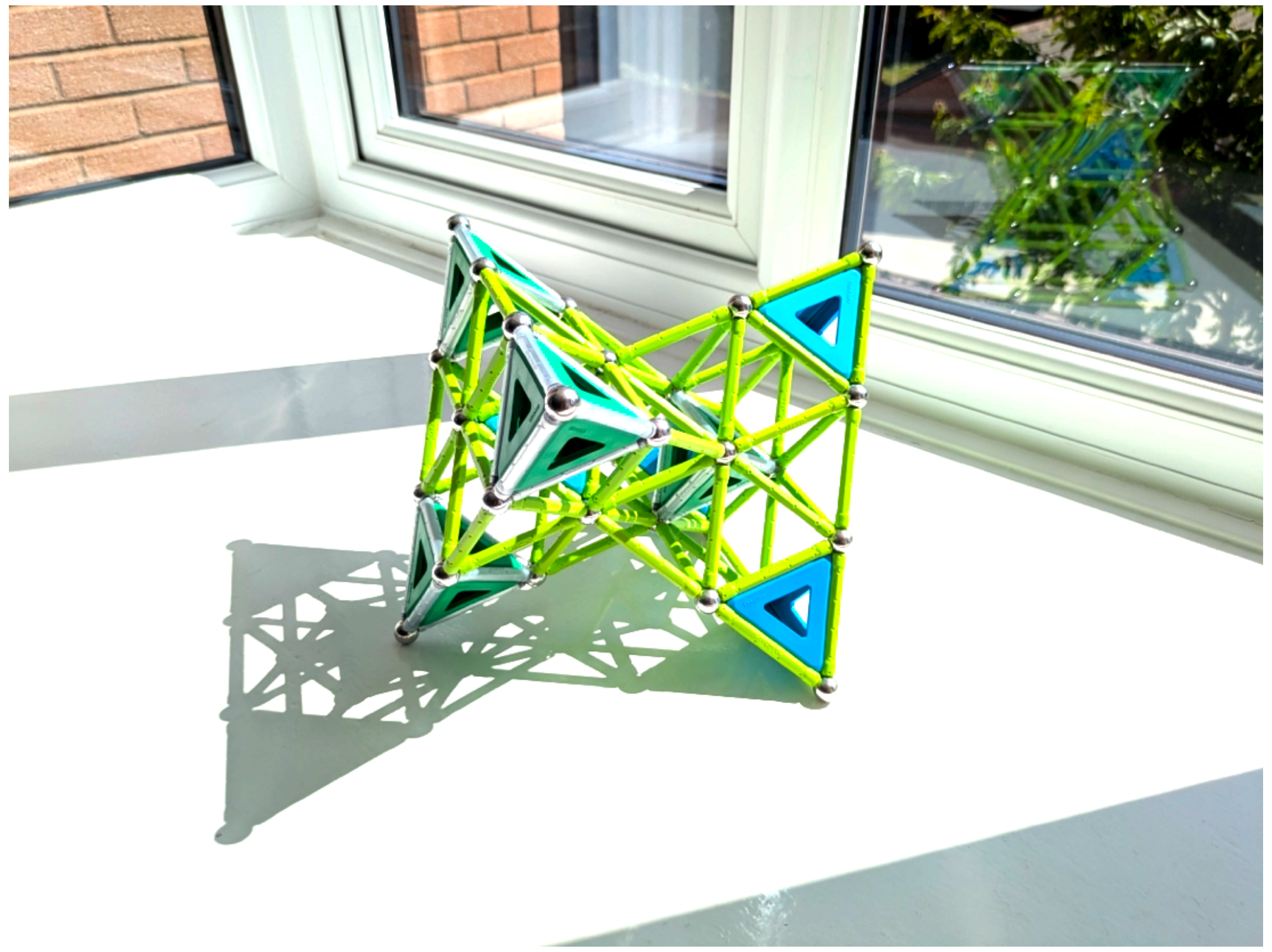

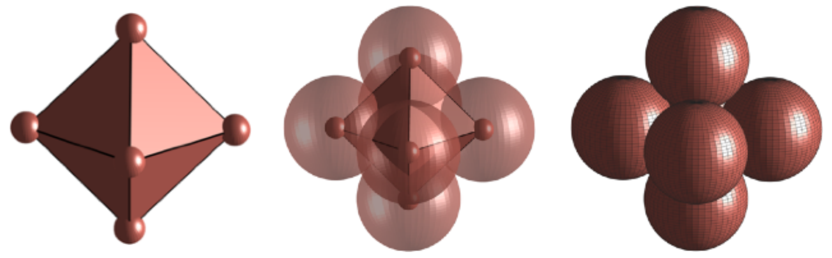
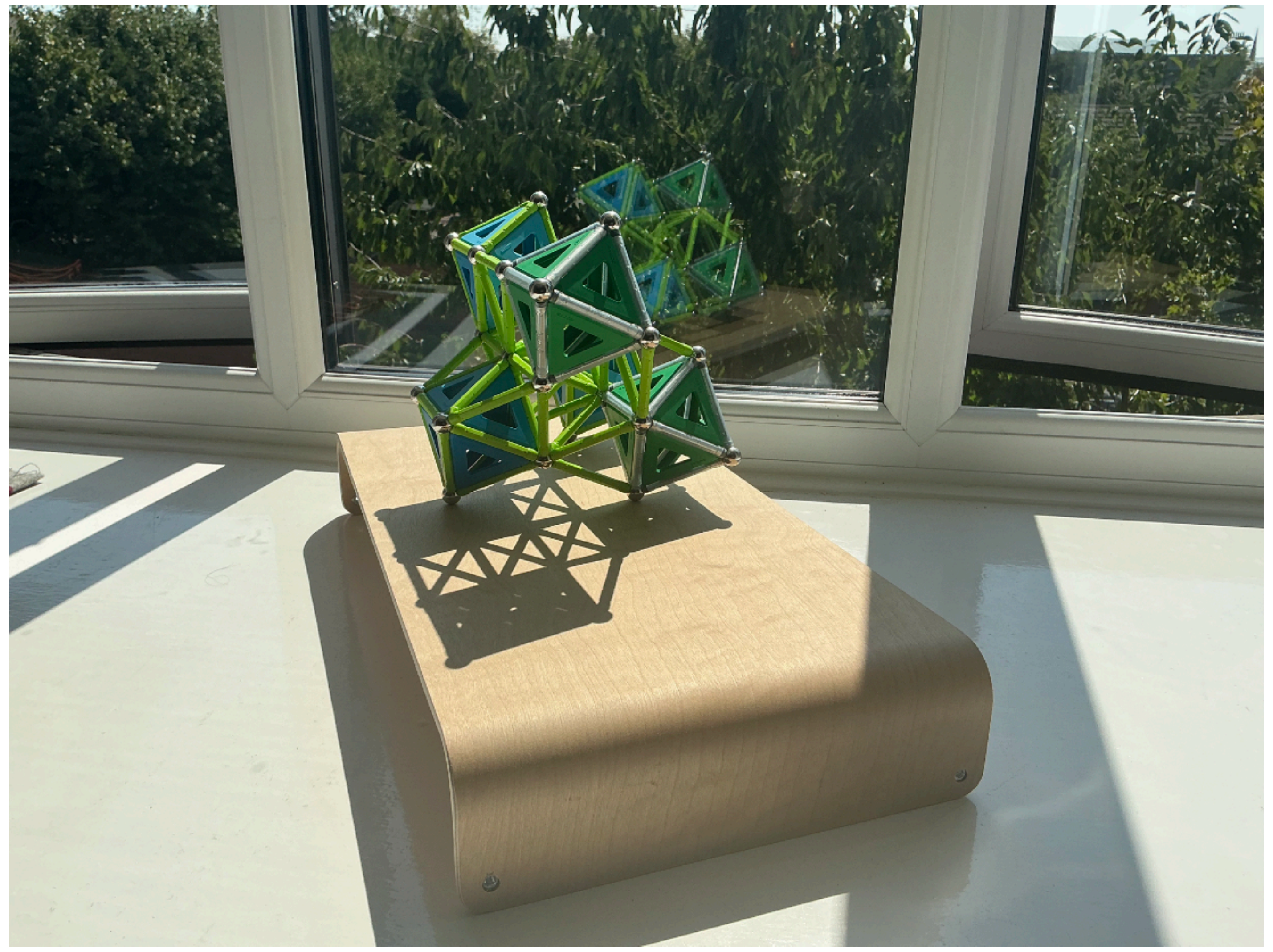

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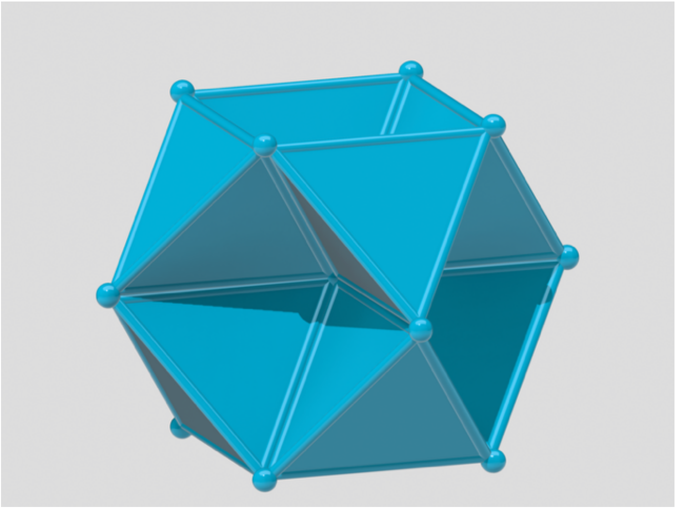
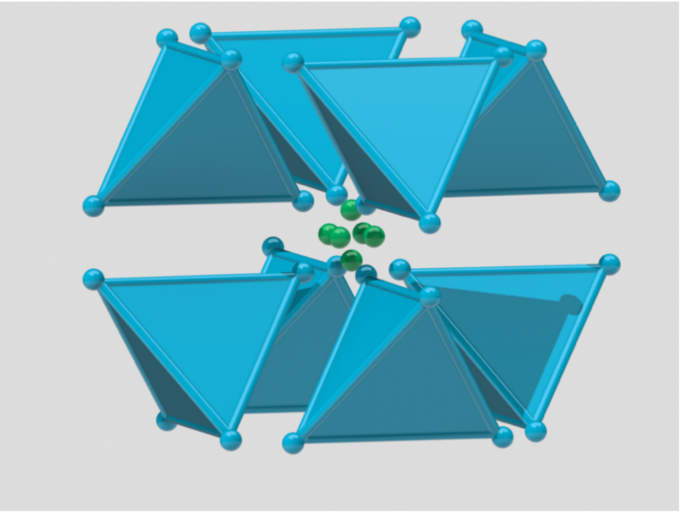
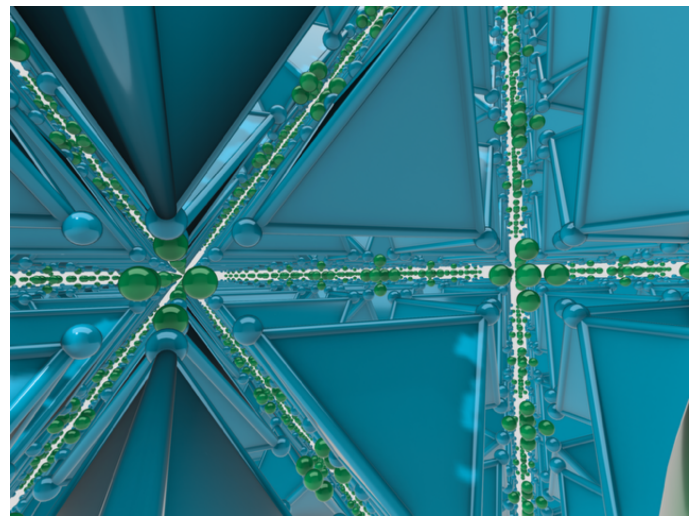

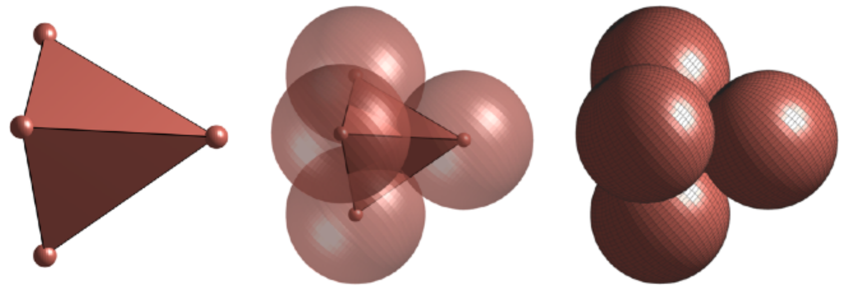
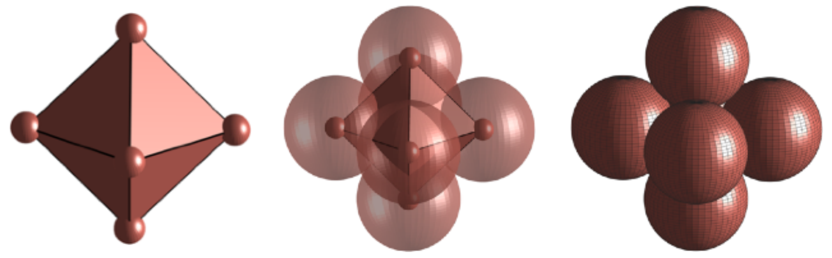

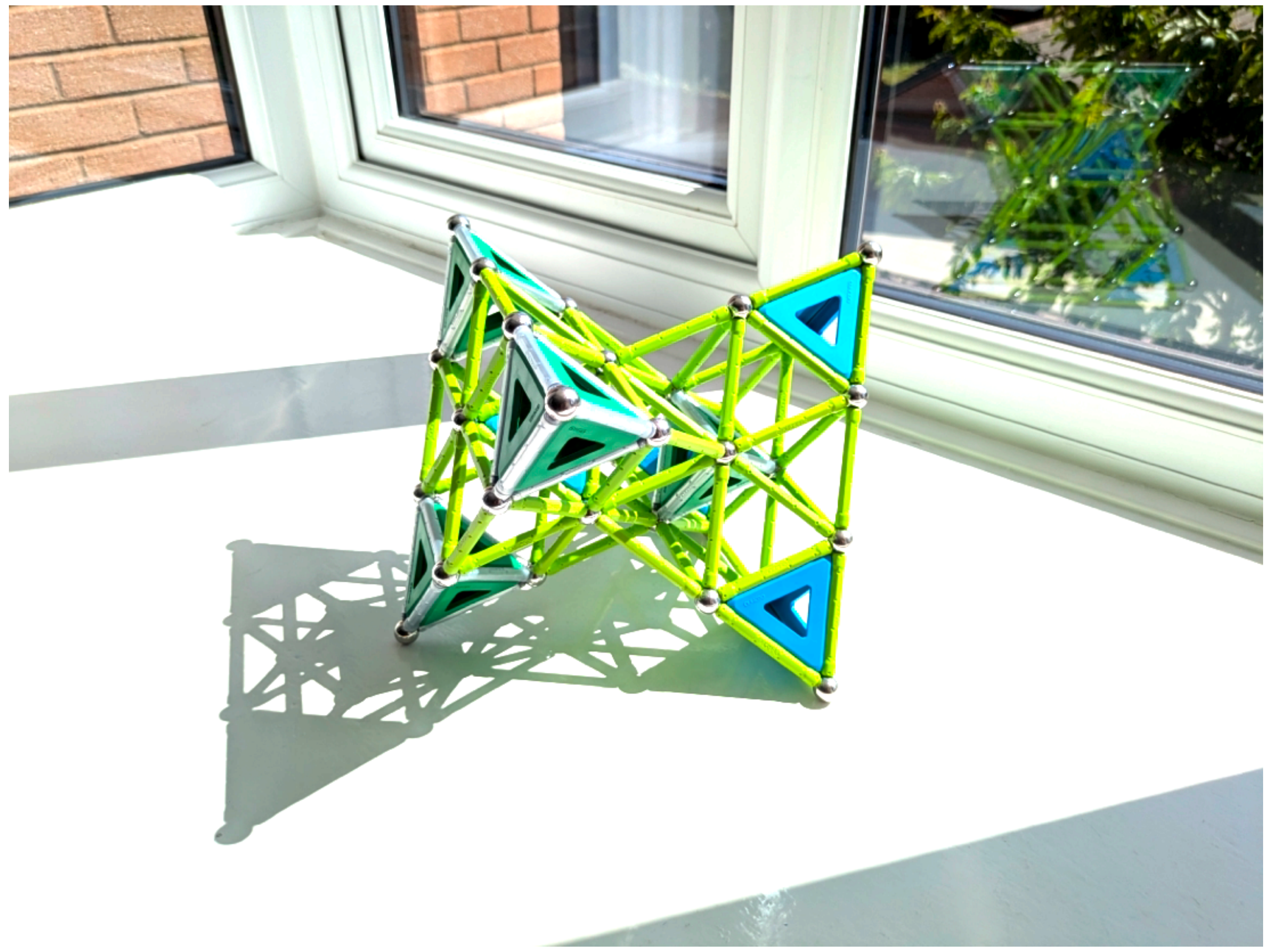
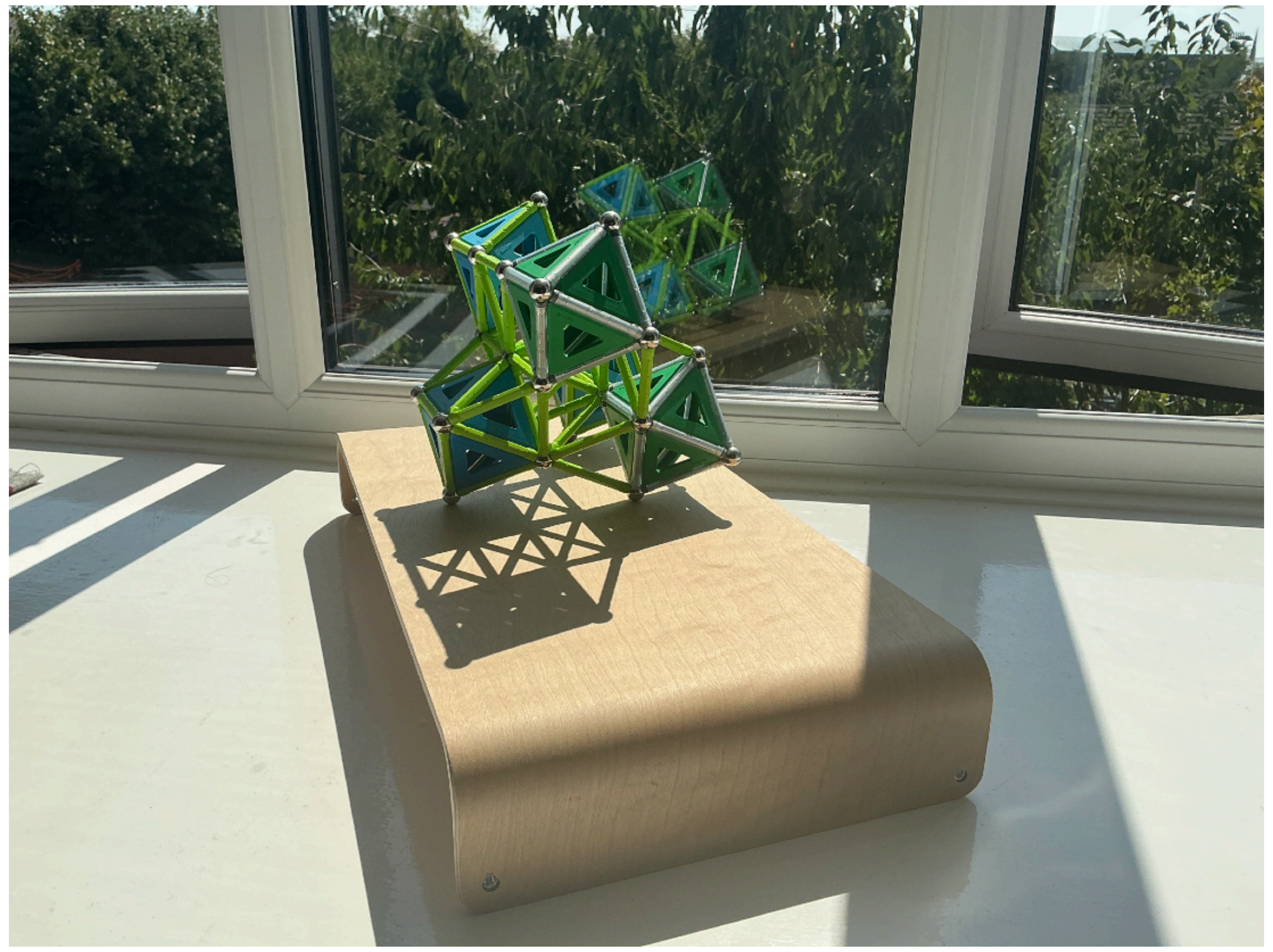

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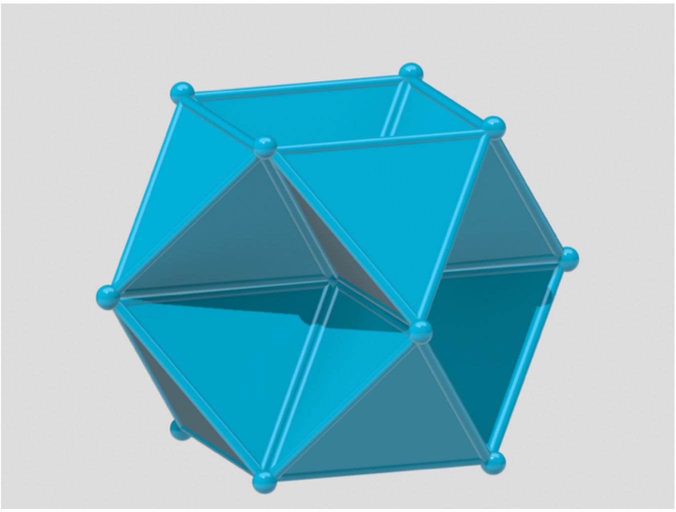

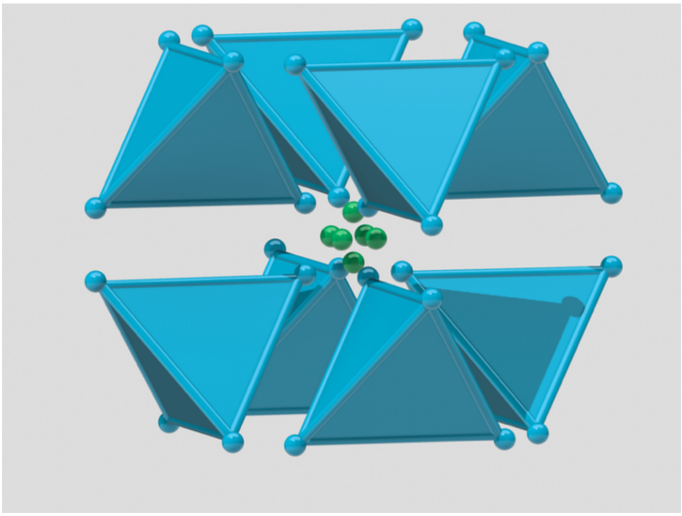

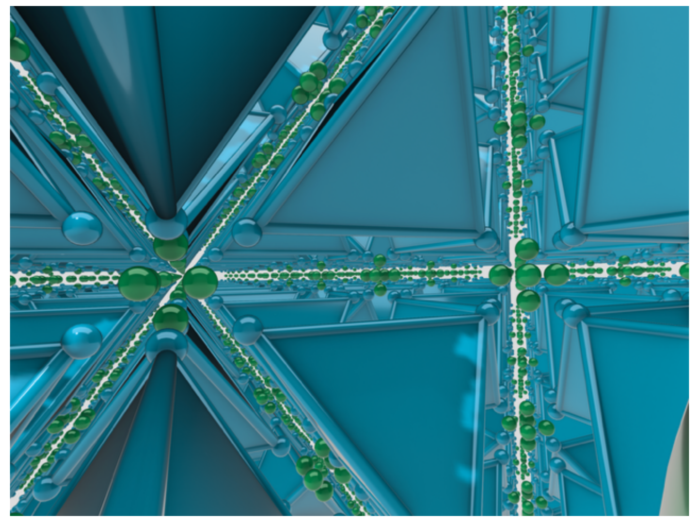

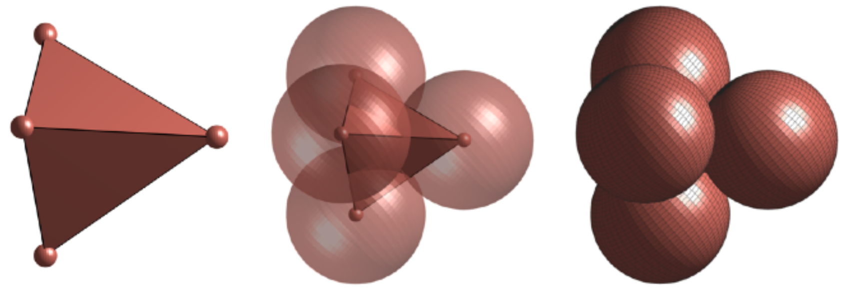

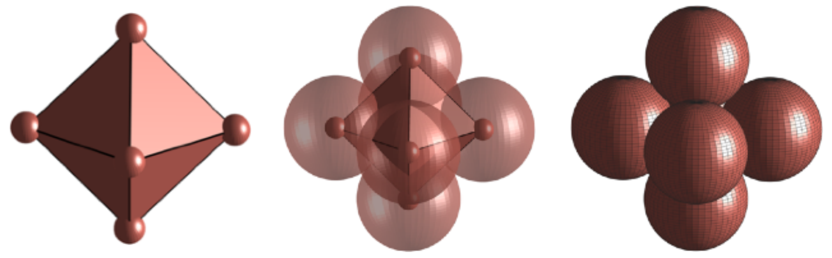

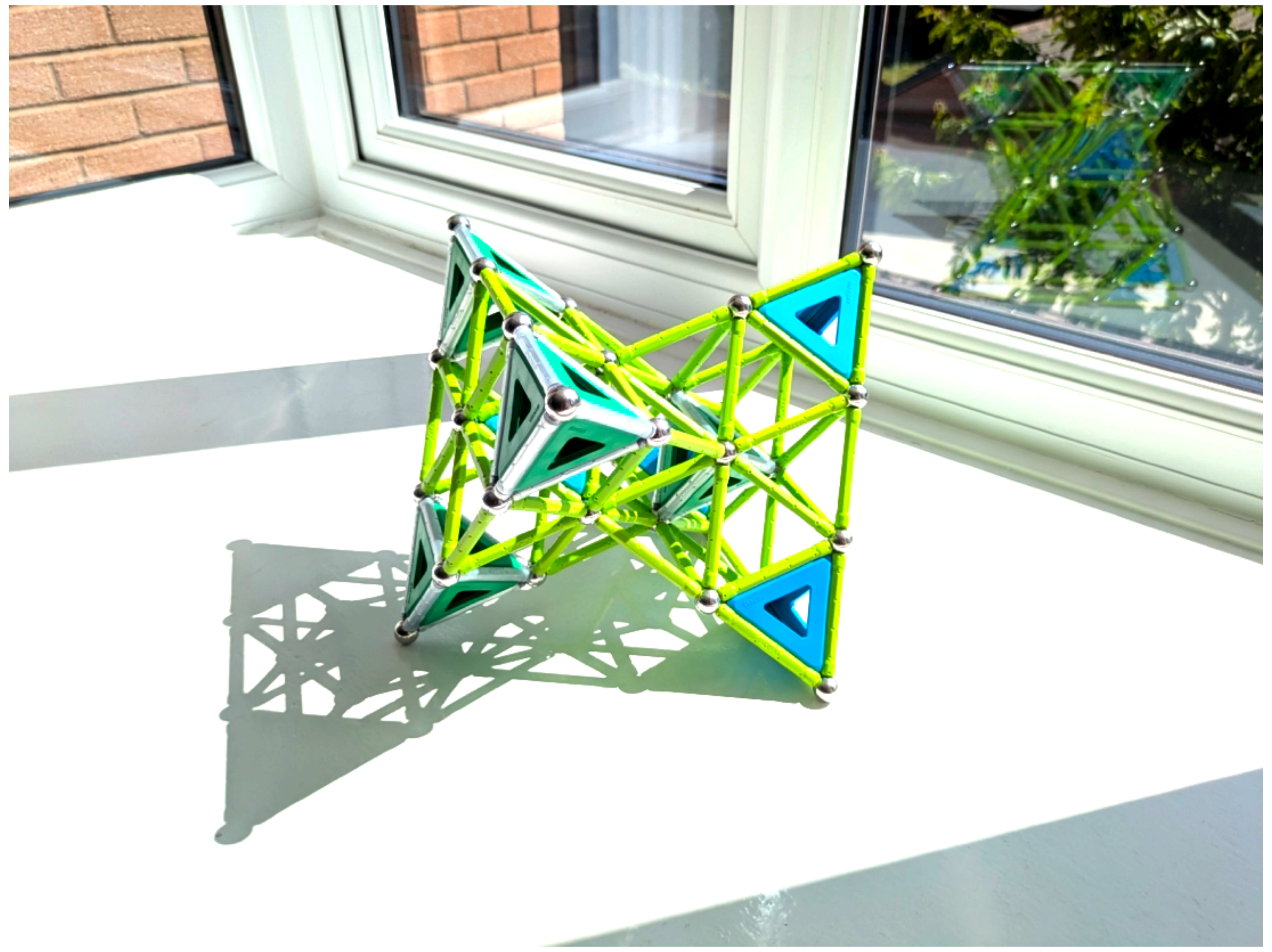

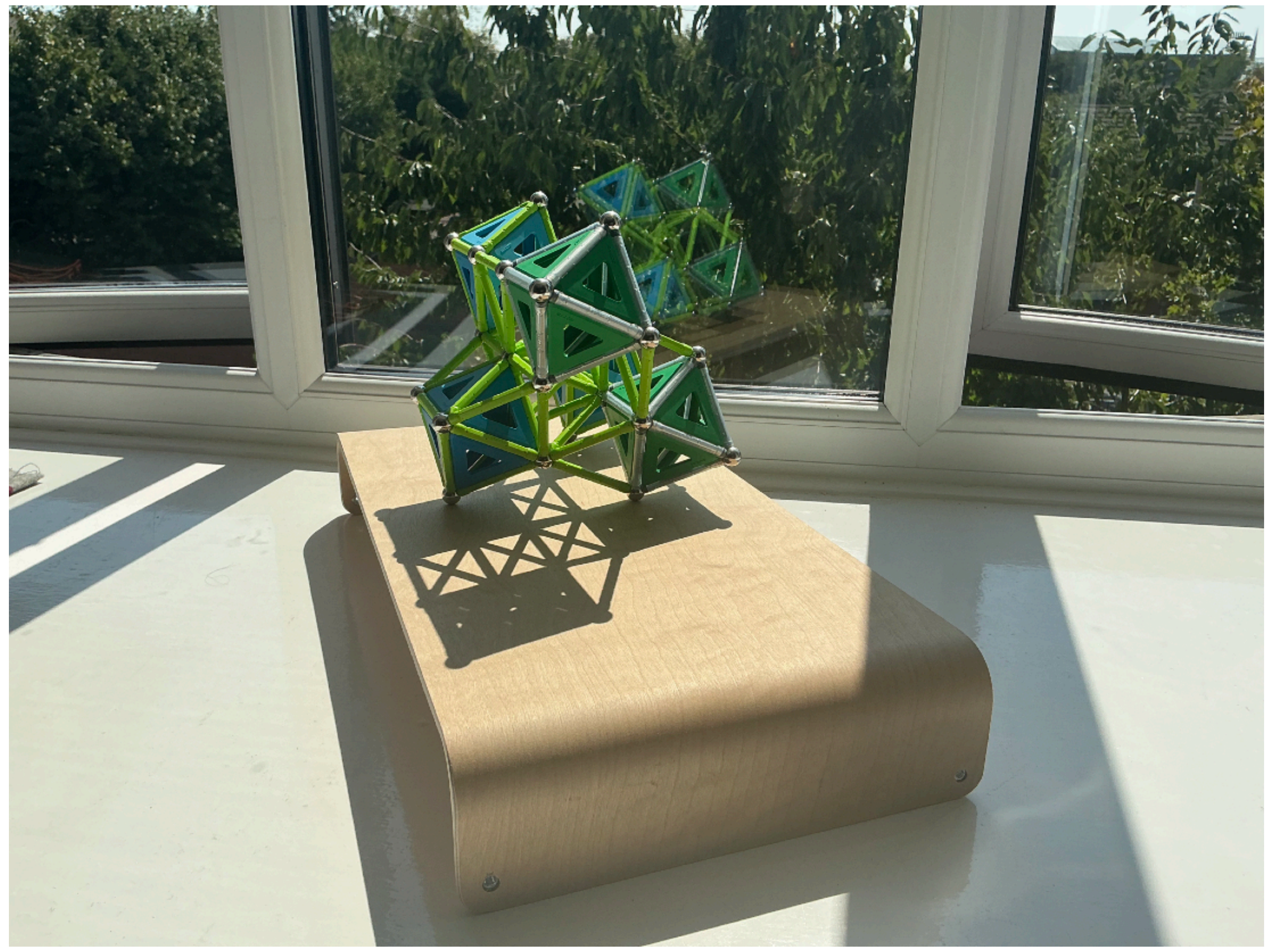

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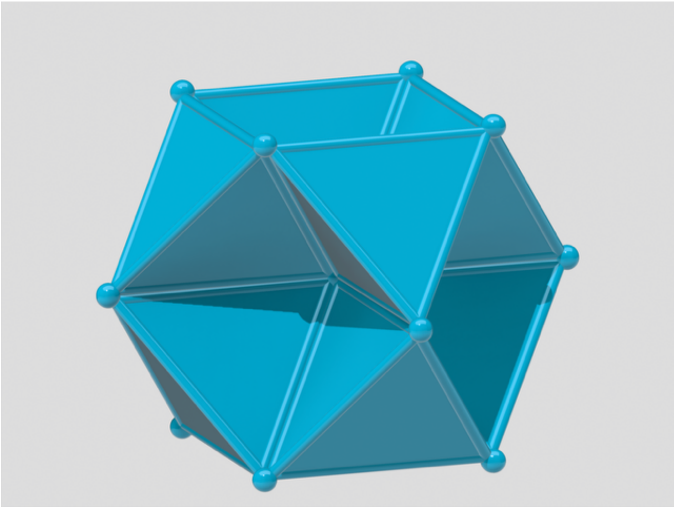

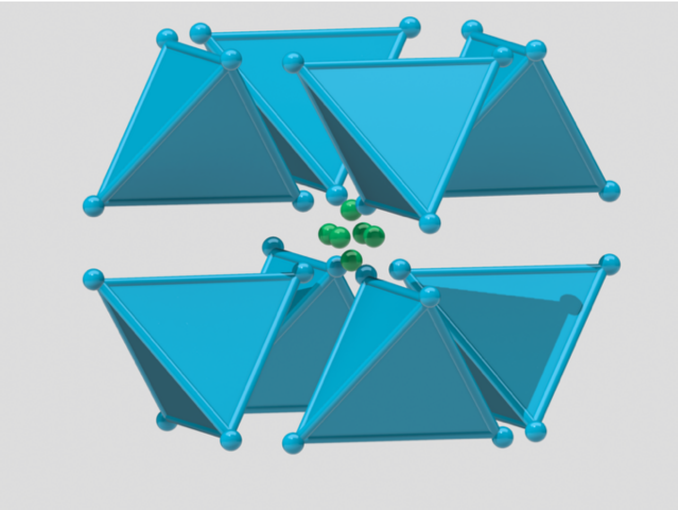

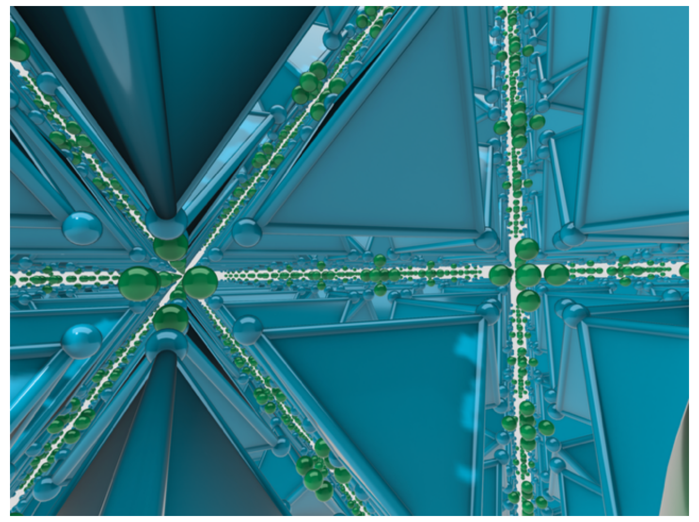

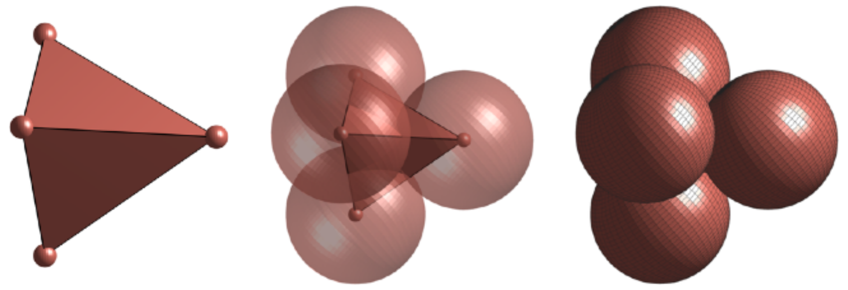

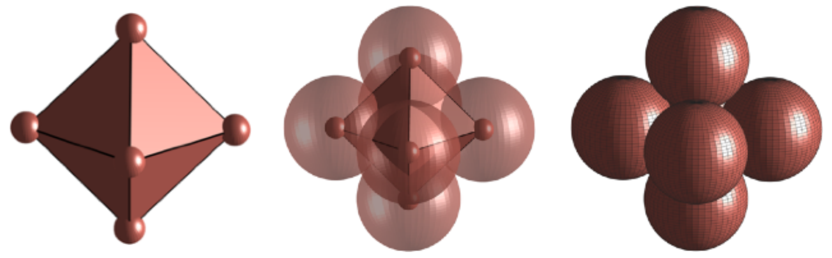

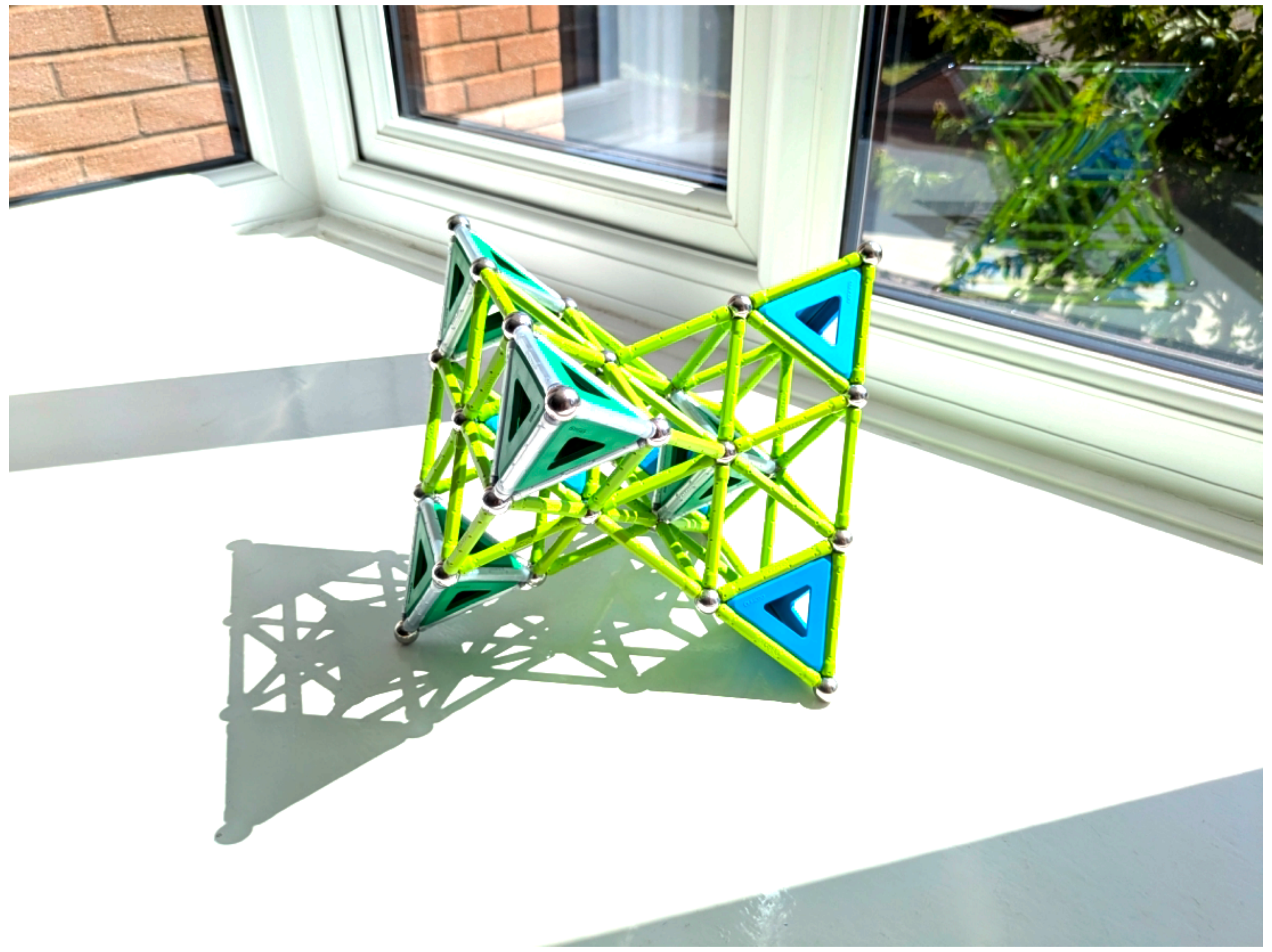

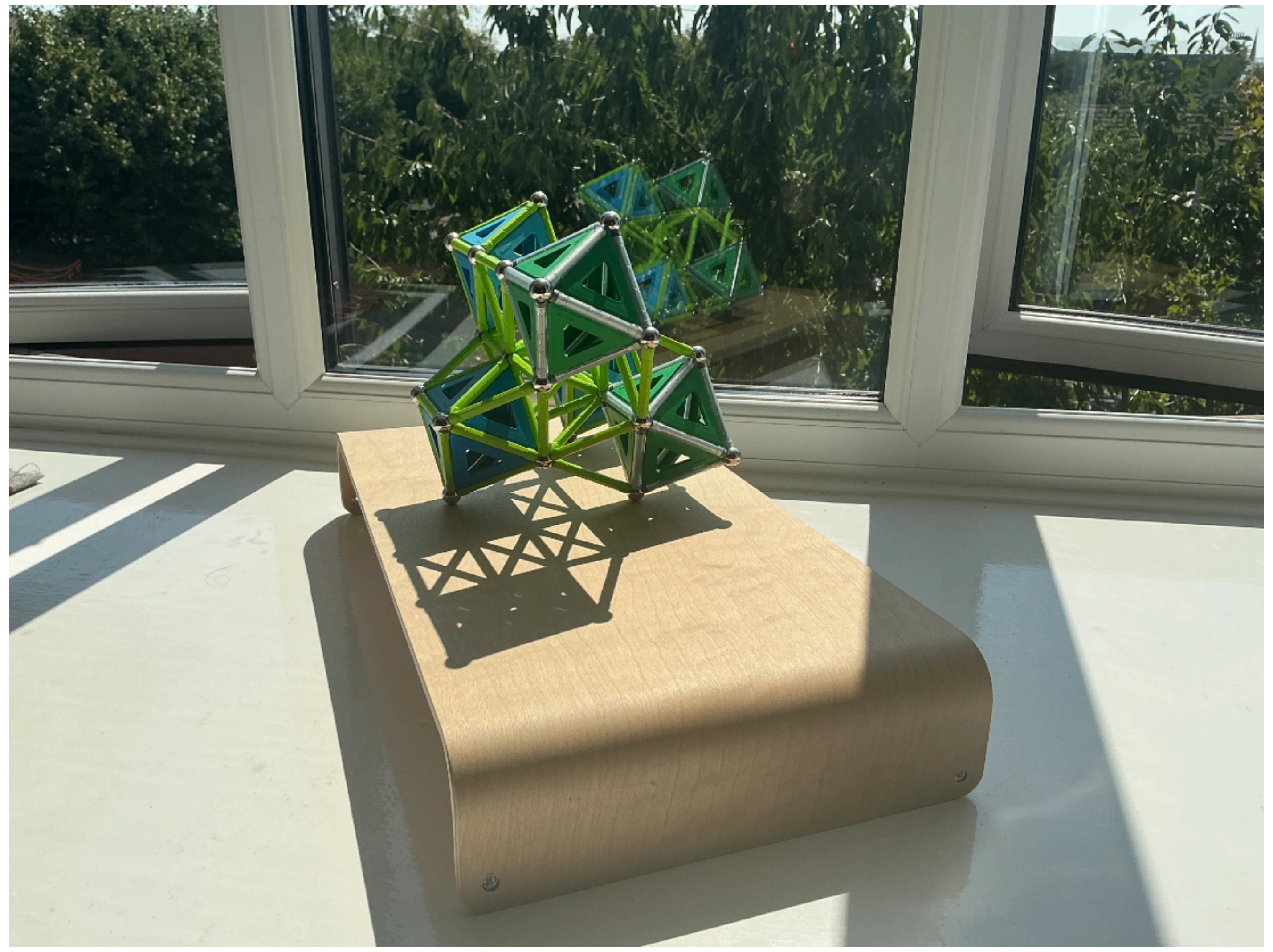

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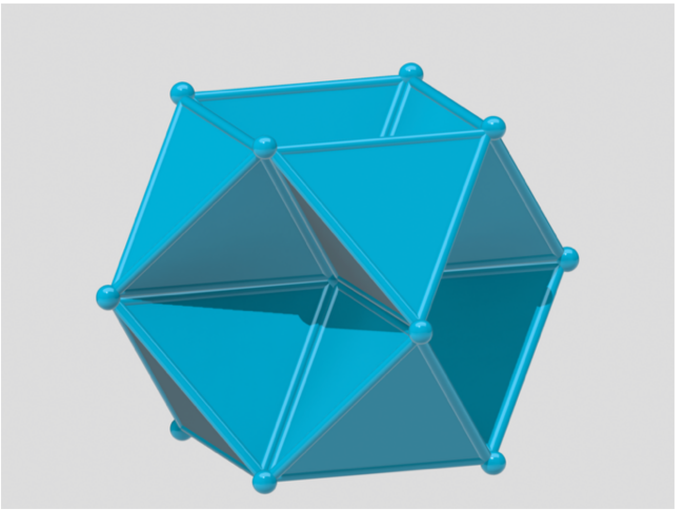
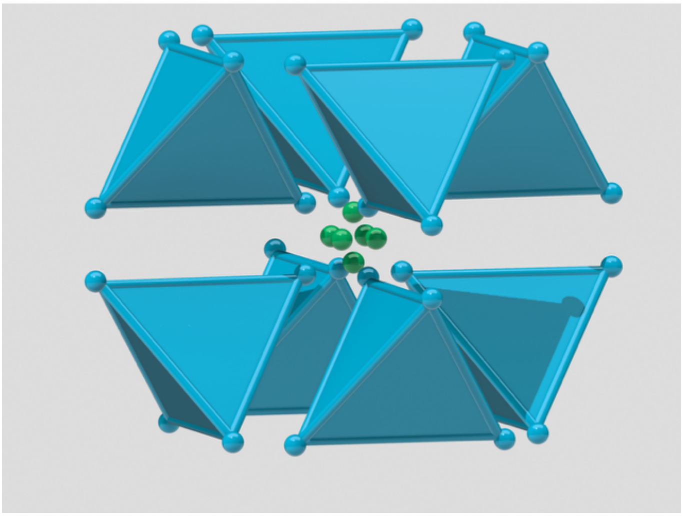
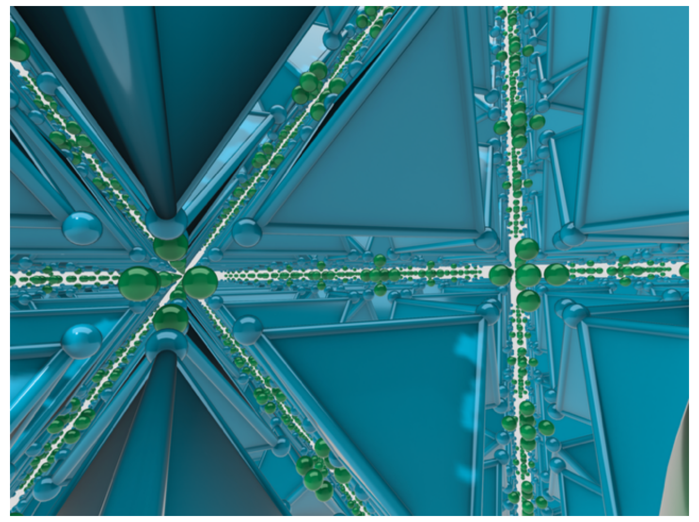
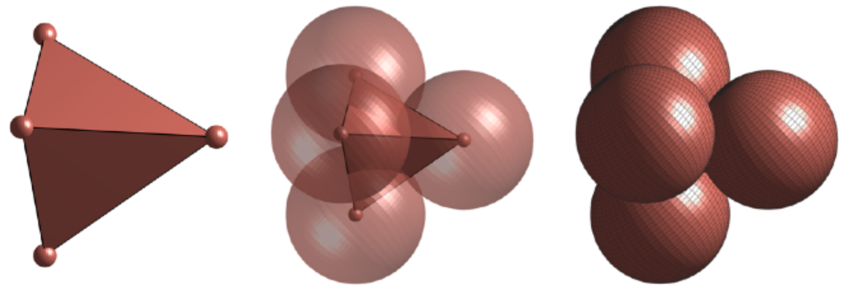
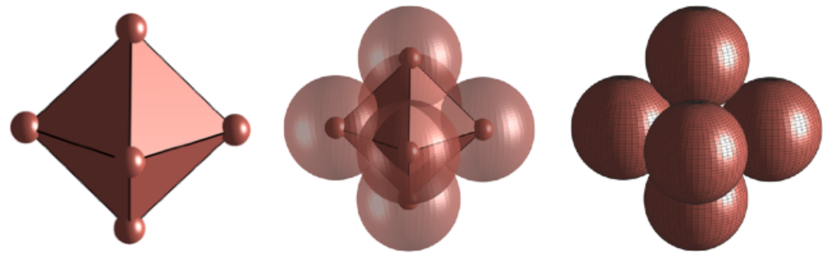
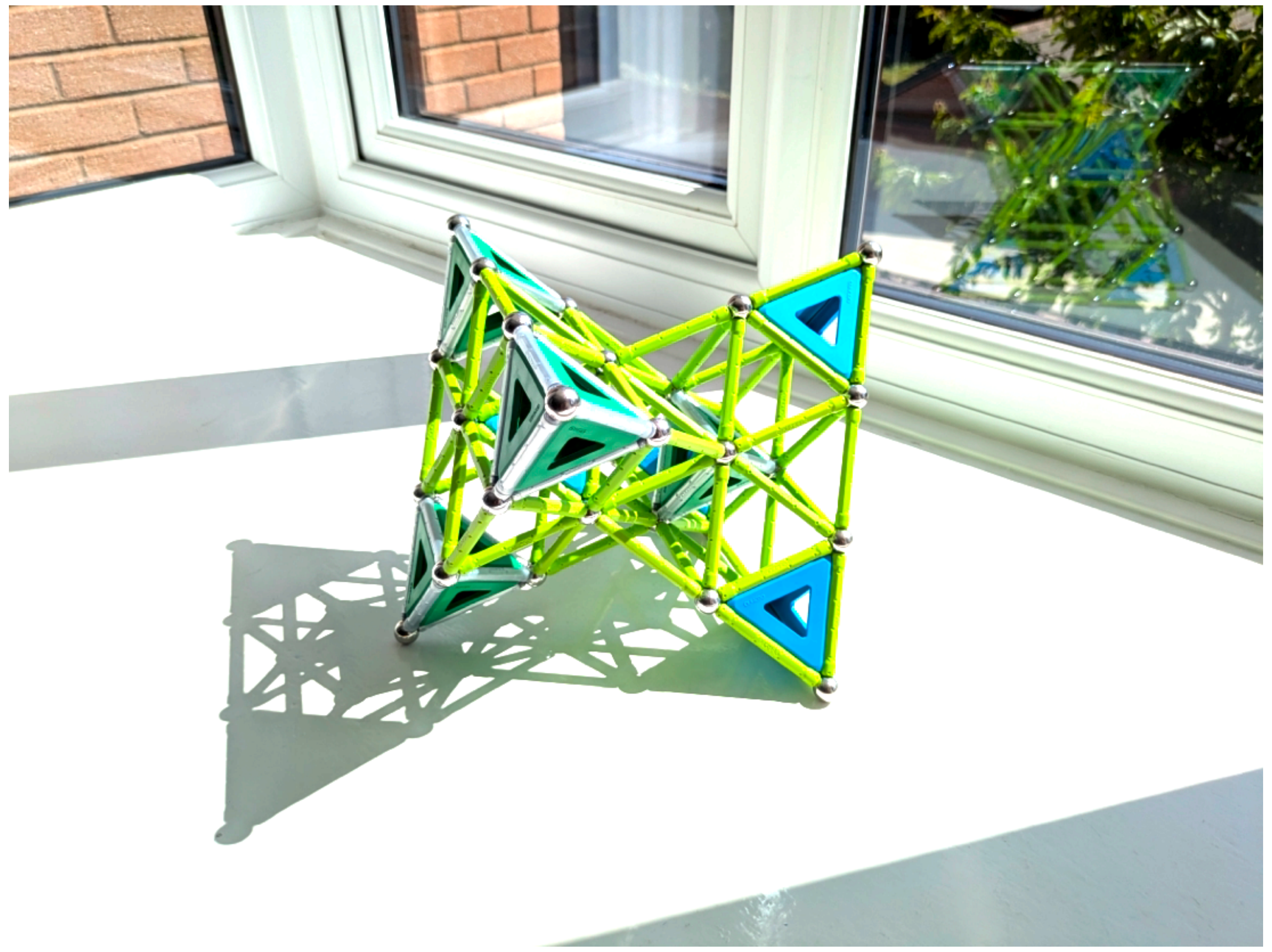
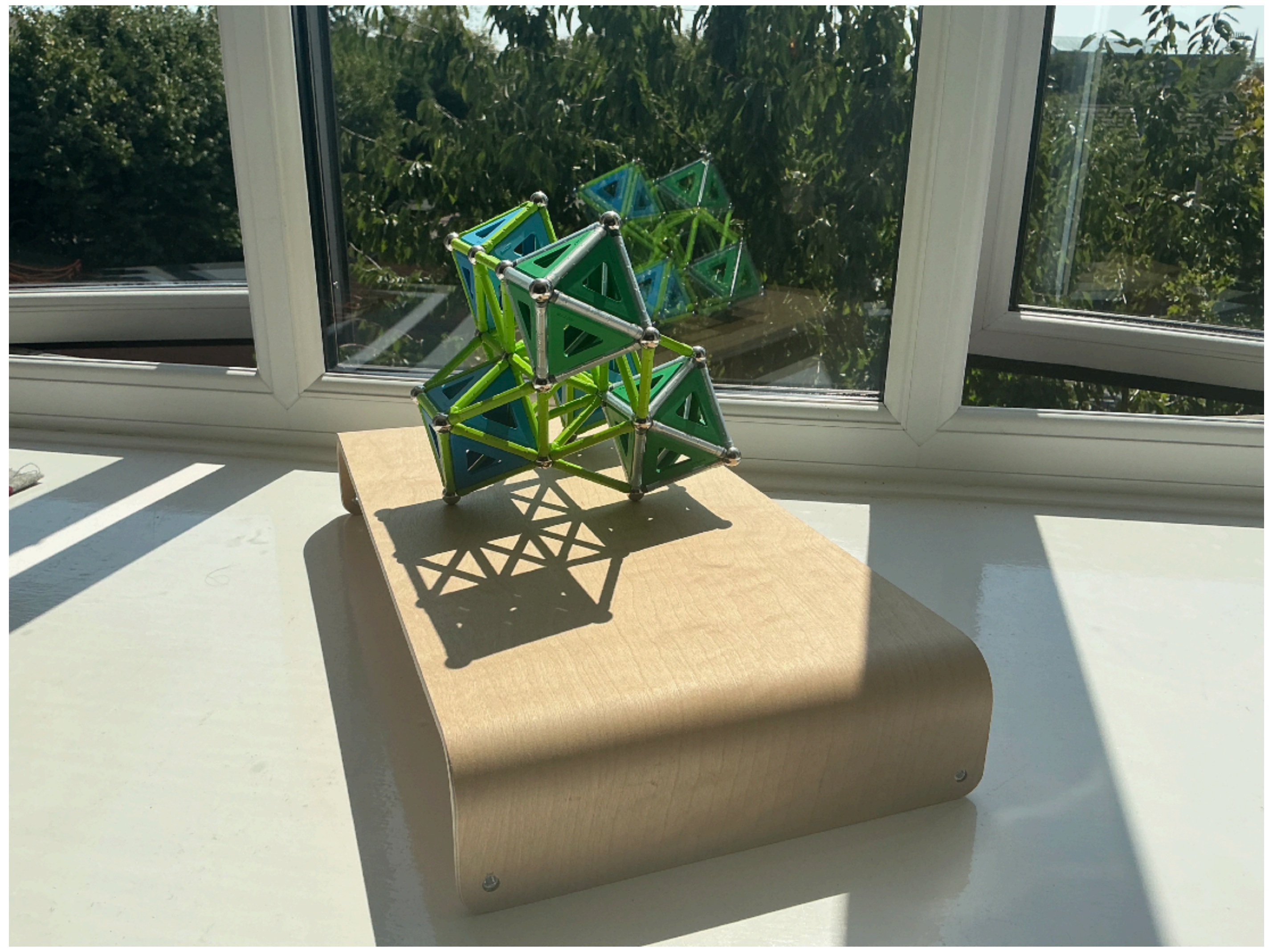

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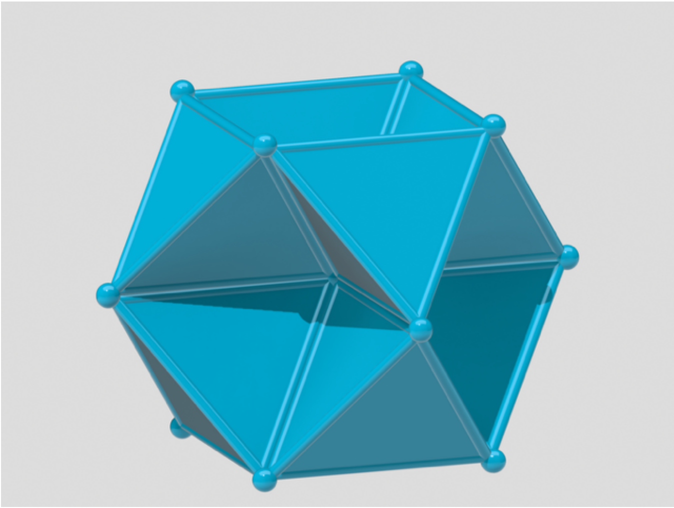
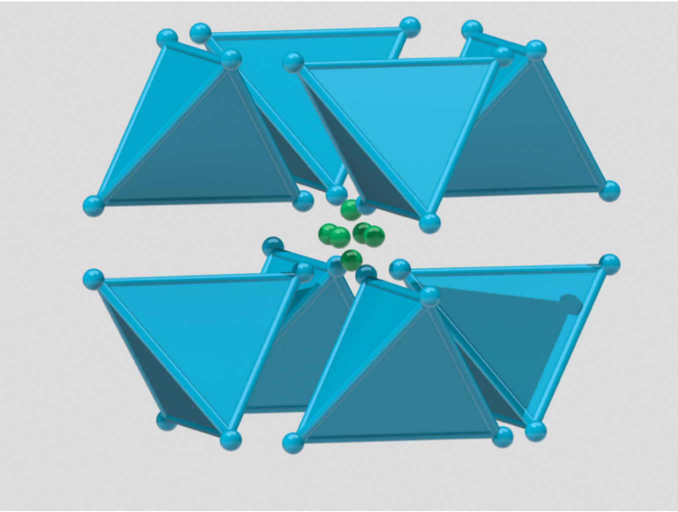
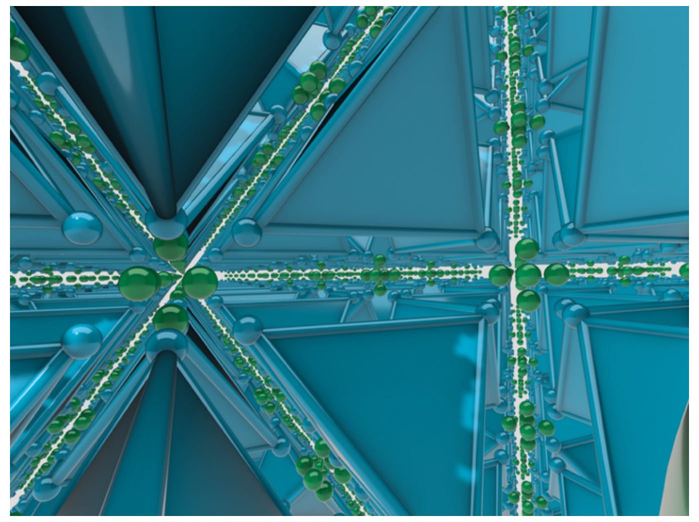
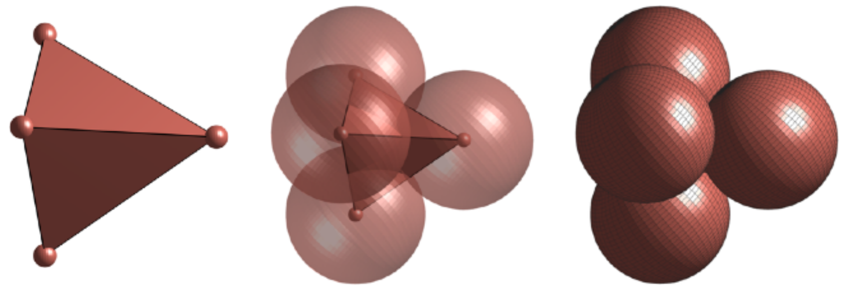
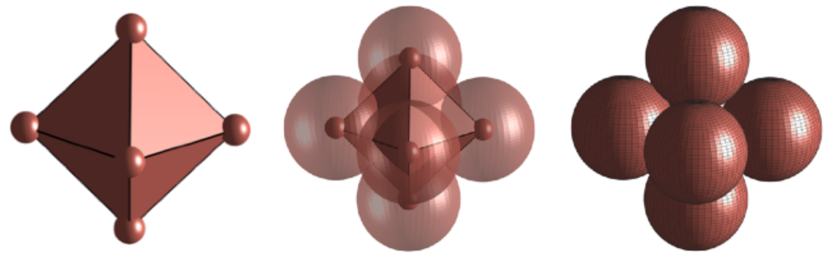
  - Proved to be correct by Thomas Hales in 2005

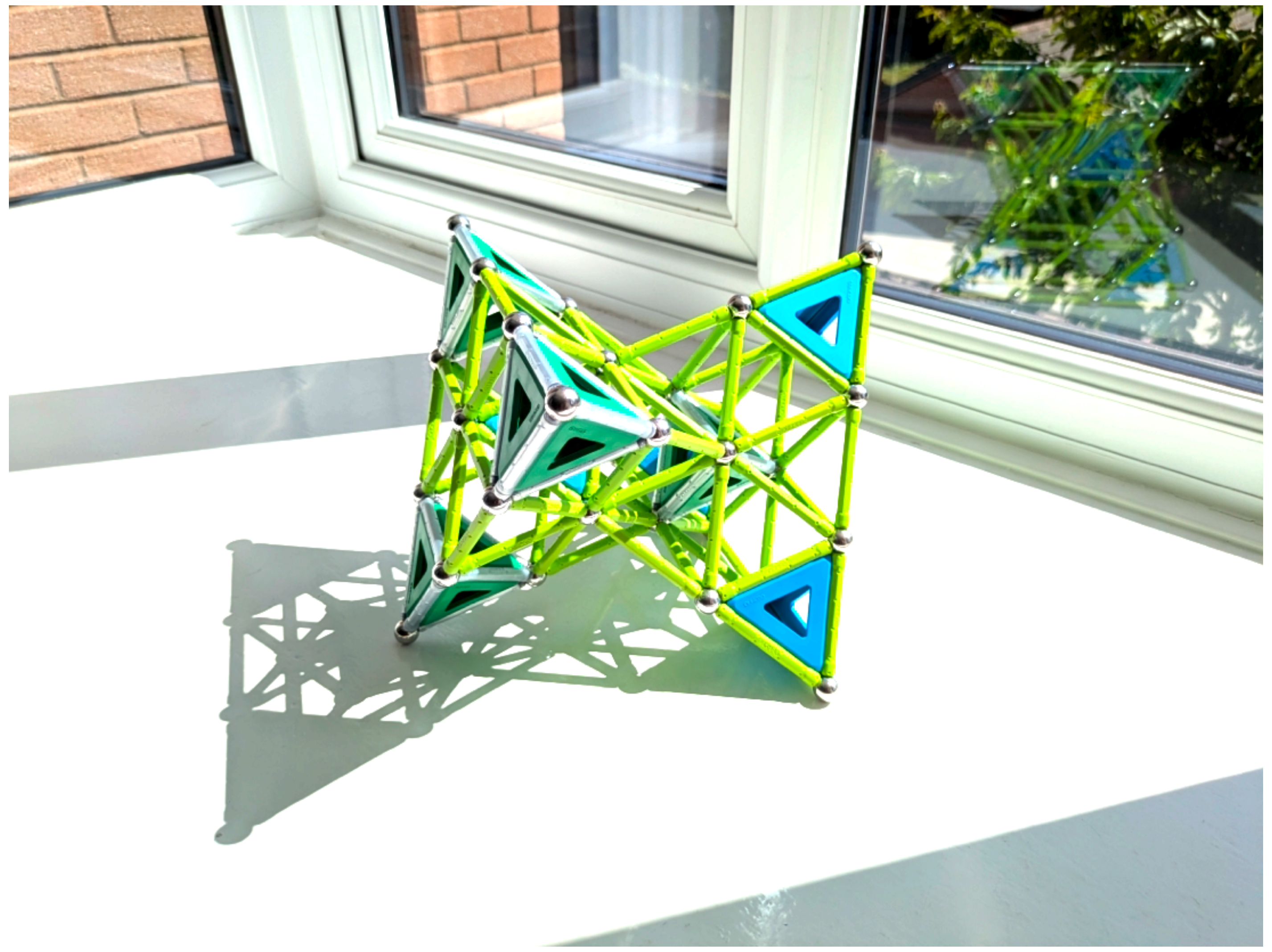


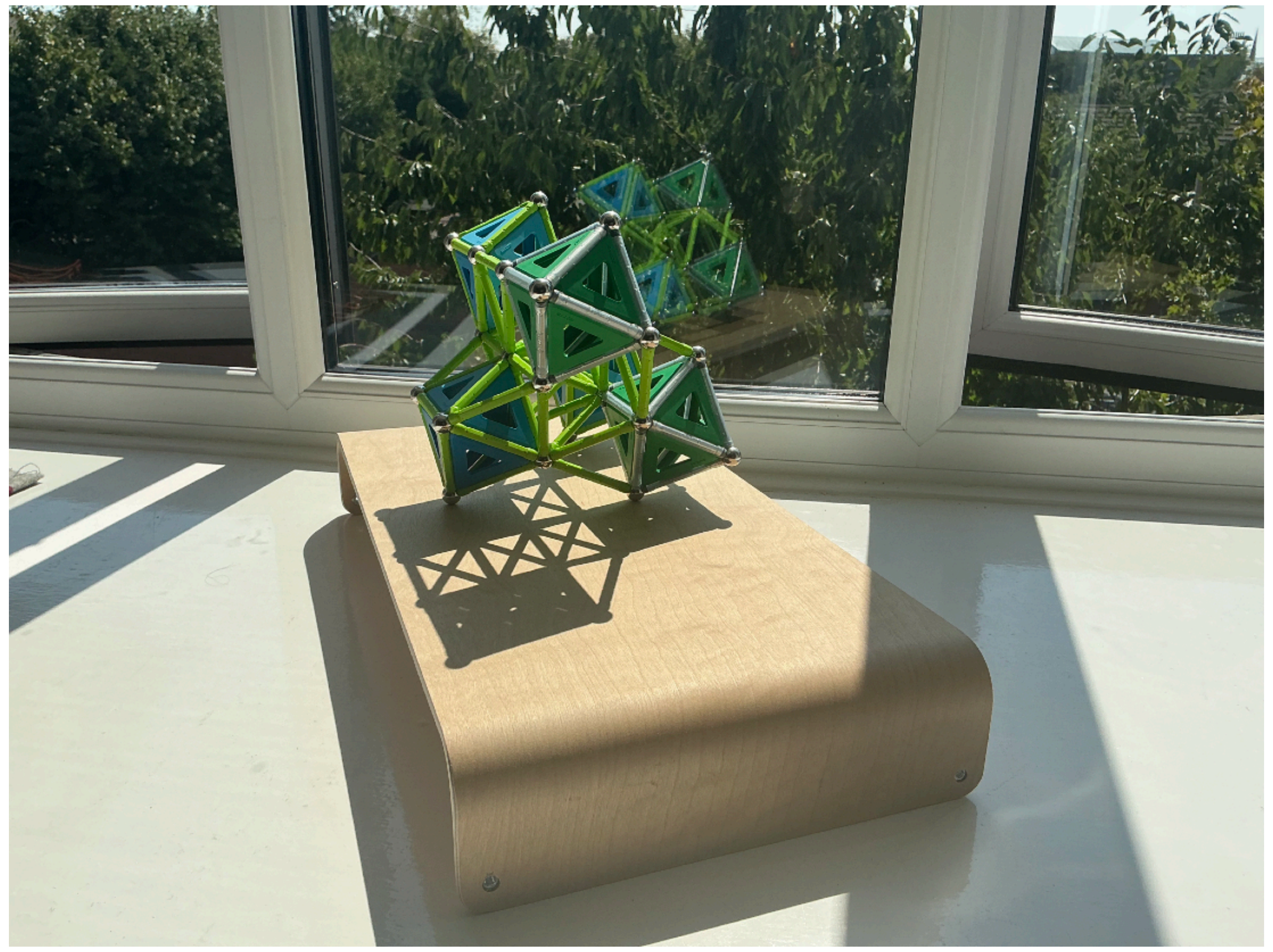












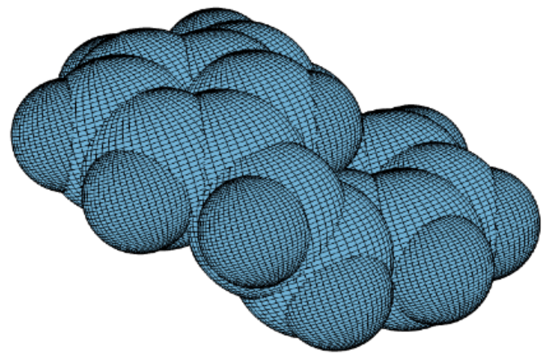
Proved by Thomas Hales in 2005 Hales, T. C. (2005). A proof of the Kepler conjecture. *Annals of mathematics*, 1065-1185.

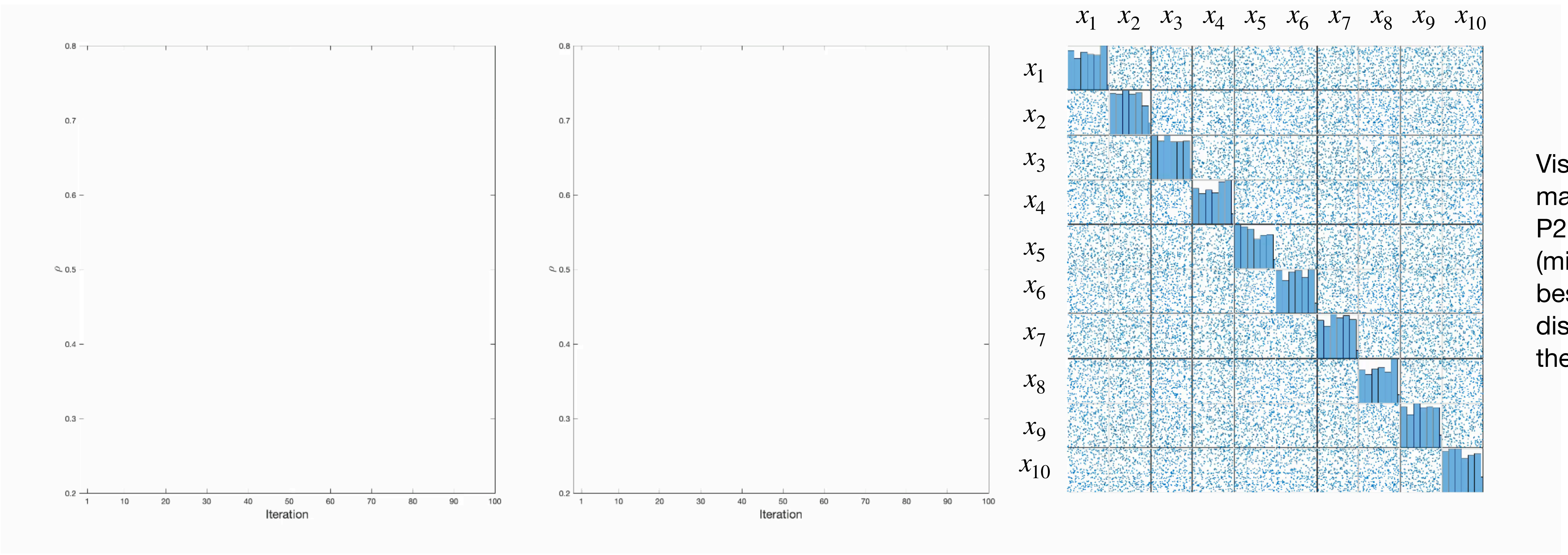
Close-Packings of Volumetric Models of Molecules

Packing MCYPDE in Space Group $P2_1$

Space-filling / Spacefill
Visualisation Style

Spheres with Van der Waals radii





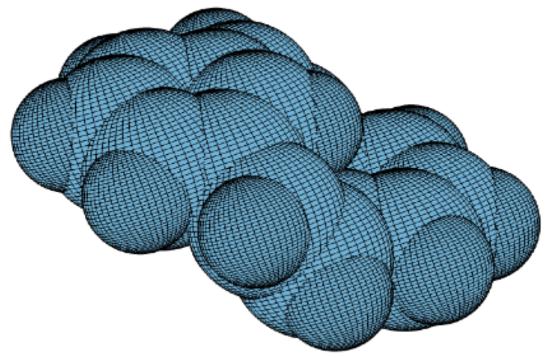
Visualization of the MCYPDE packing maximization run for the space group $P2_1$ (Left) Maximum packing density; (middle) average packing density of N-best packings at $i-th$ iteration; (right) distribution of the packing generation at the iteration.

§ M. Torda, J. Y. Goulermas, R. Púček and V. Kurlin, *Entropic Trust Region for Densest Crystallographic Symmetry Group Packings*, SIAM Journal on Scientific Computing, (2023).

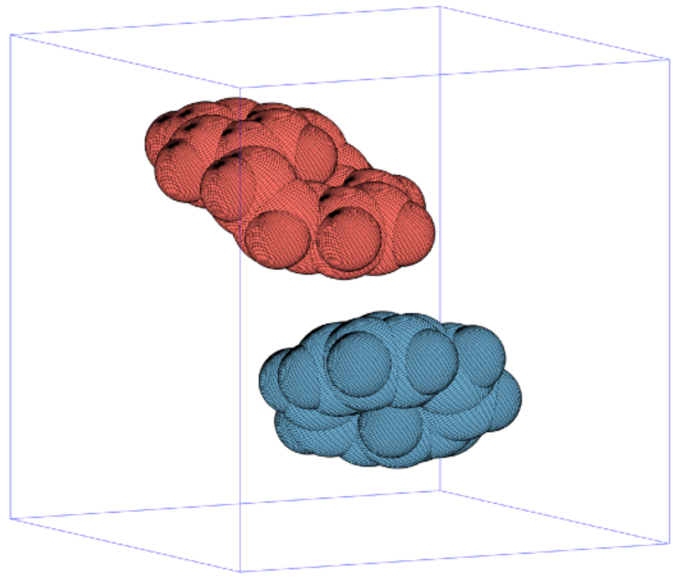
Close-Packings of Volumetric Models of Molecules

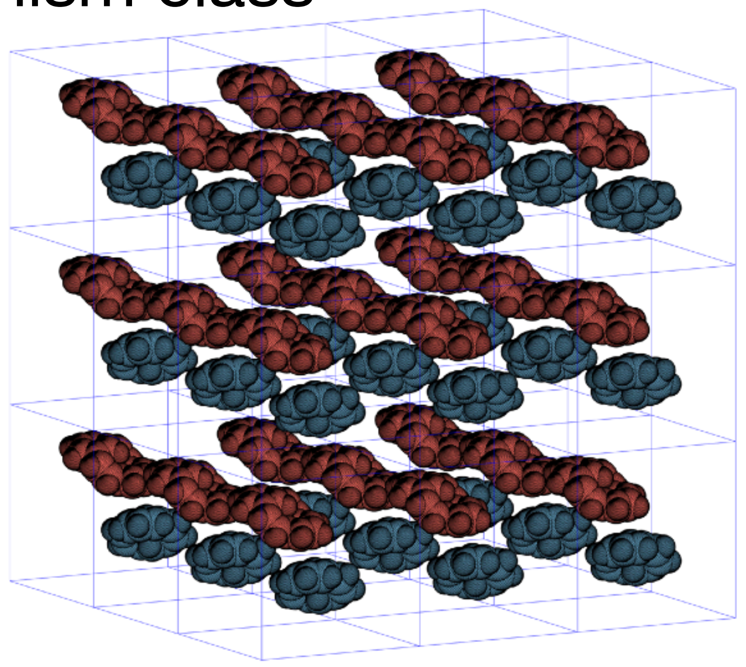
Space-filling / Spacefill Visualisation Style

Spheres with Van der Waals radii

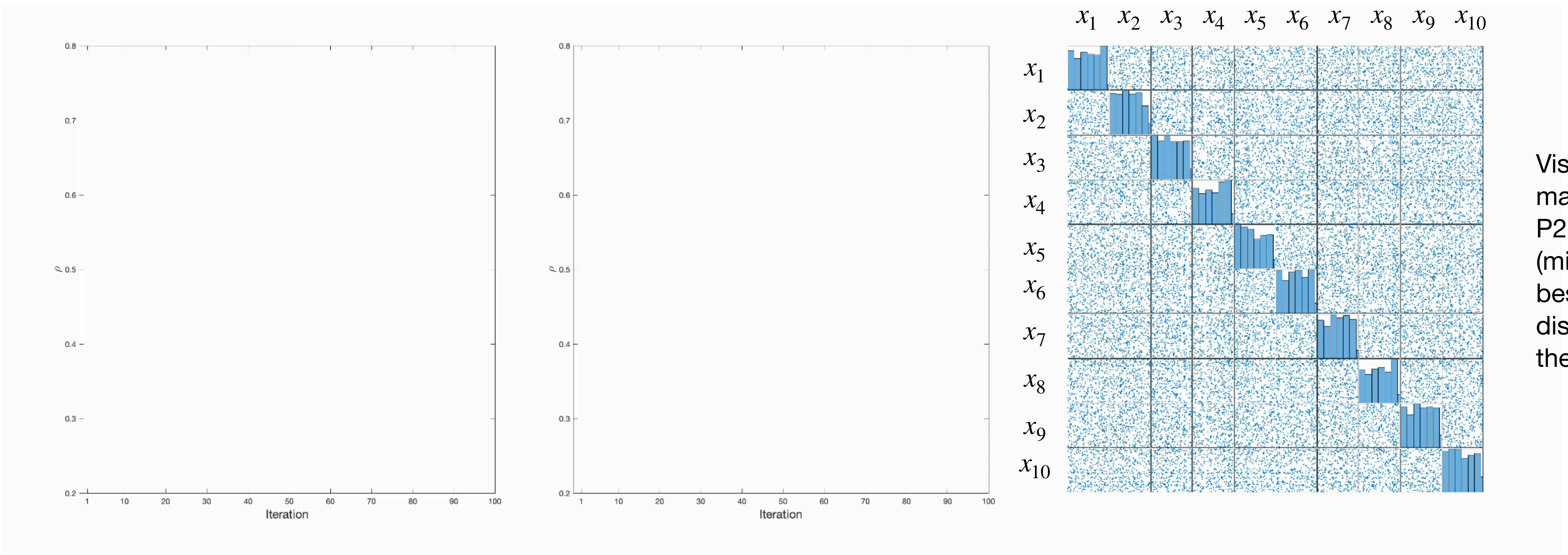


Fix the space group isomorphism class





Packing MCYPDE in Space Group $P2_1$



Visualization of the MCYPDE packing maximization run for the space group $P2_1$ (Left) Maximum packing density; (middle) average packing density of N-best packings at $i - th$ iteration; (right) distribution of the packing generation at the iteration.

- Non-linear non-convex optimisation problem

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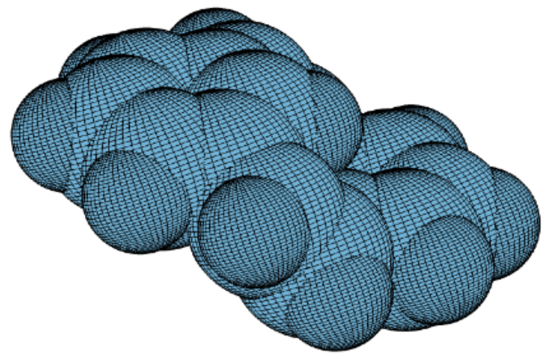
Close-Packings of Volumetric Models of Molecules

Space-filling / Spacefill
Visualisation Style

Spheres with Van der Waals radii



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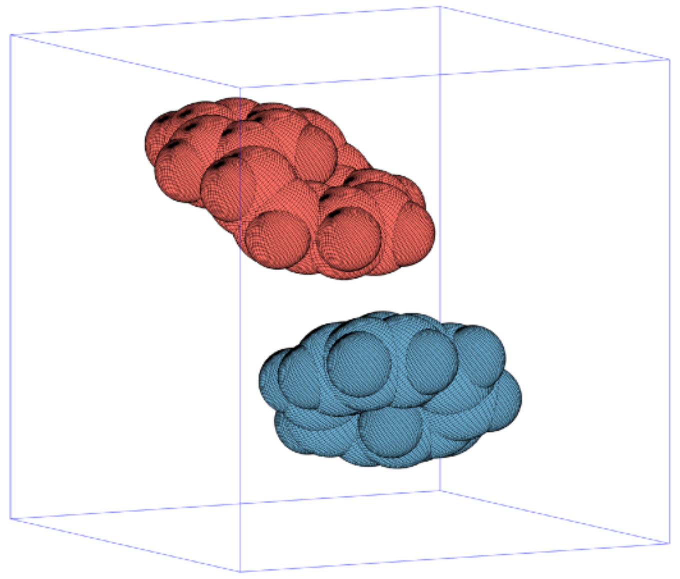
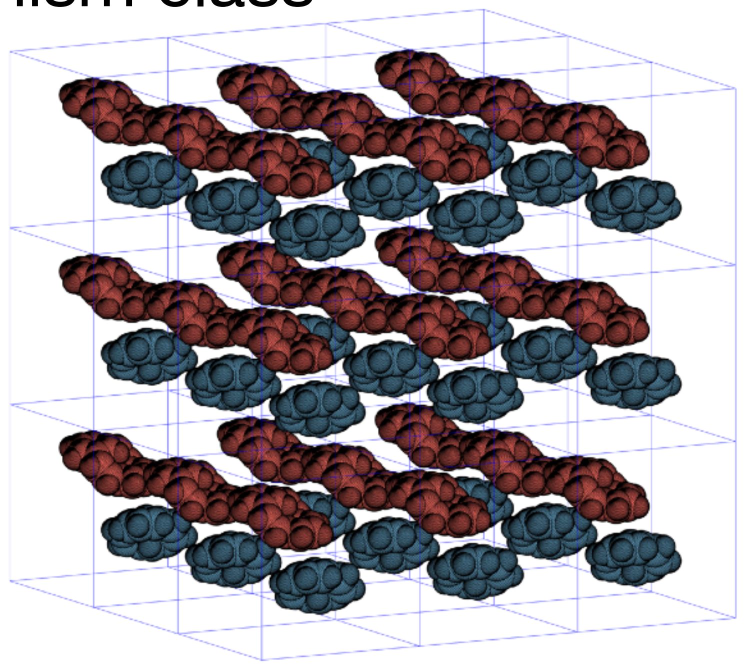
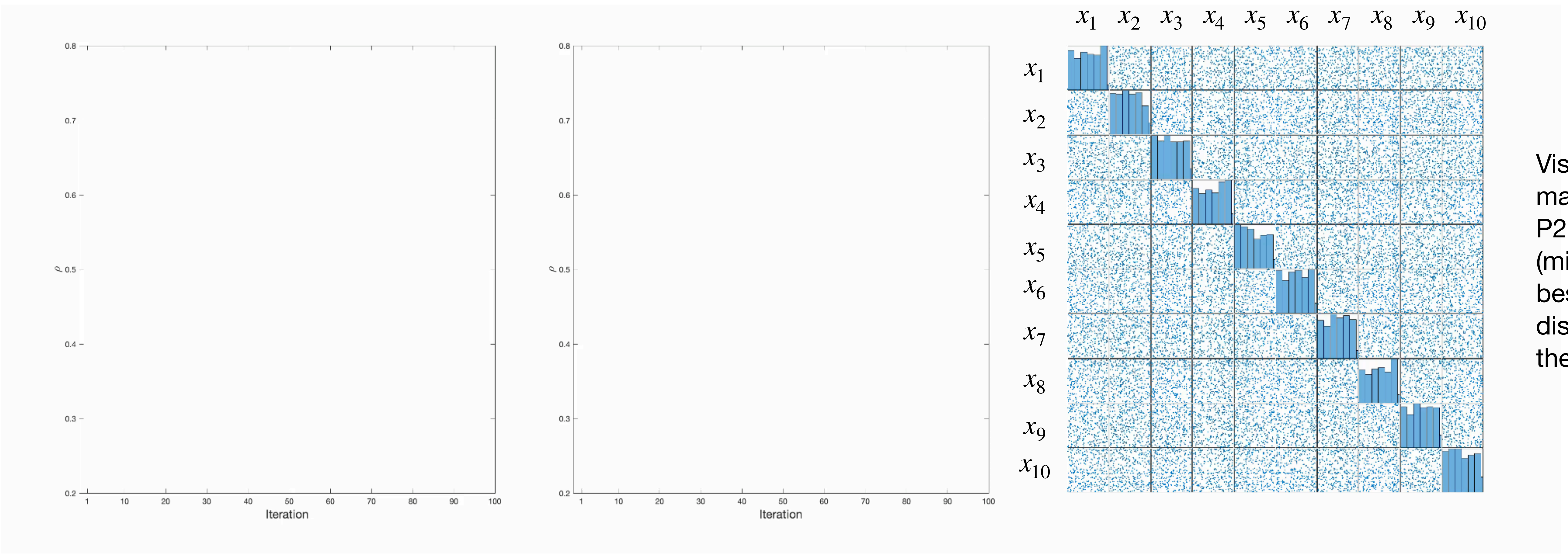




Packing MCYPDE in Space Group $P2_1$



Visualization of the MCYPDE packing maximization run for the space group $P2_1$ (Left) Maximum packing density; (middle) average packing density of N-best packings at $i-th$ iteration; (right) distribution of the packing generation at the iteration.

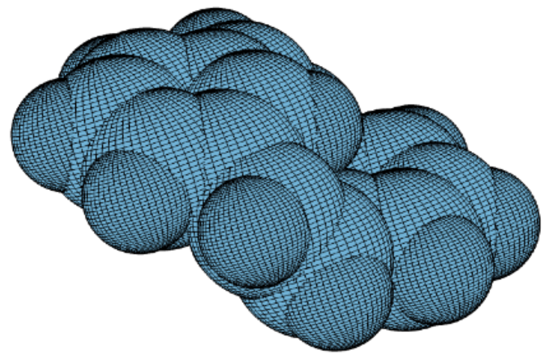
- Non-linear non-convex optimisation problem
  - Solve it via a modified version of the Entropic Trust Region Crystallographic Packing Algorithm

§ M. Torda, J. Y. Goulermas, R. Púček and V. Kurlin, *Entropic Trust Region for Densest Crystallographic Symmetry Group Packings*, SIAM Journal on Scientific Computing, (2023).

Close-Packings of Volumetric Models of Molecules

Space-filling / Spacefill
Visualisation Style

Spheres with Van der Waals radii



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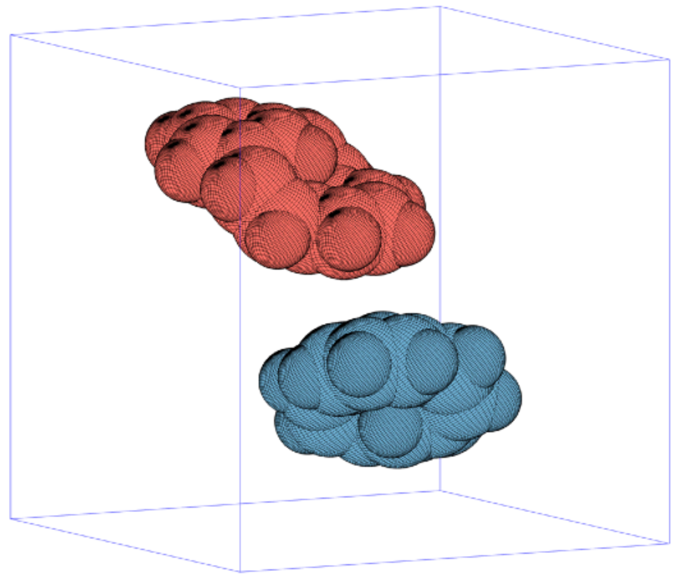
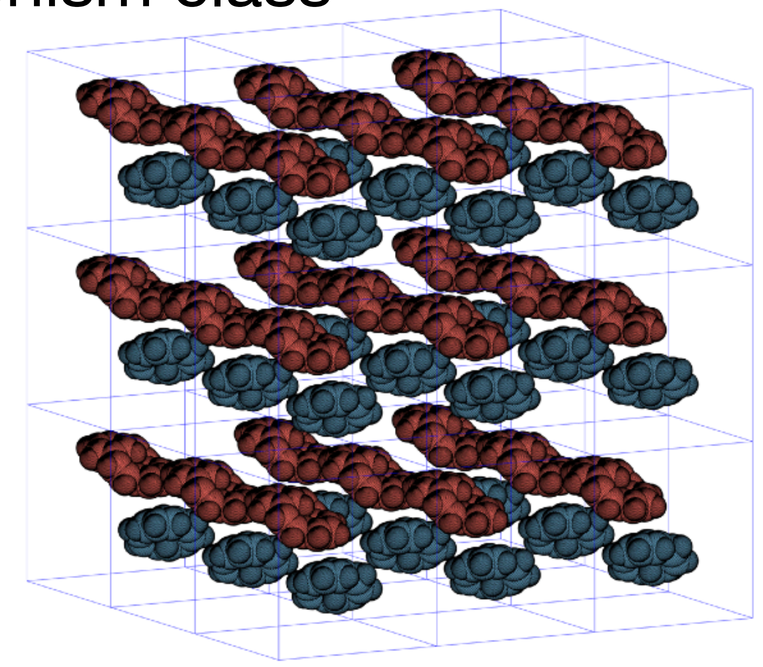
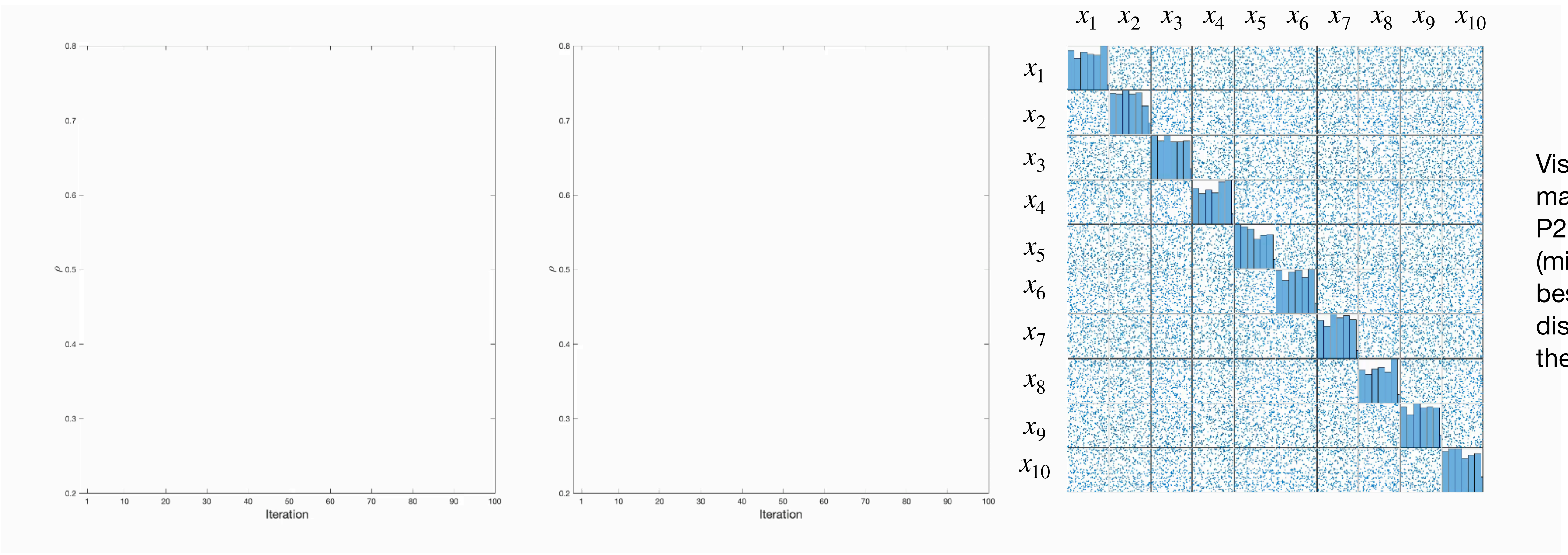




Packing MCYPDE in Space Group $P2_1$



Visualization of the MCYPDE packing maximization run for the space group $P2_1$ (Left) Maximum packing density; (middle) average packing density of N-best packings at $i-th$ iteration; (right) distribution of the packing generation at the iteration.

- Non-linear non-convex optimisation problem
  - Solve it via a modified version of the Entropic Trust Region Crystallographic Packing Algorithm
    - Information-geometry based global search method

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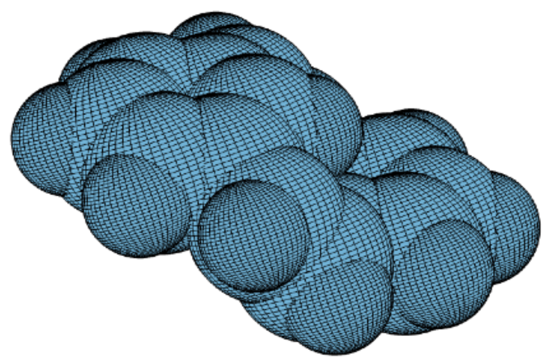
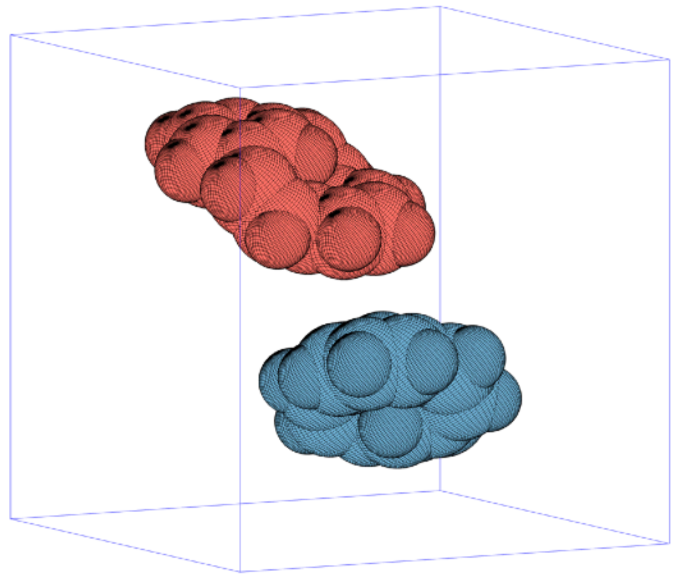
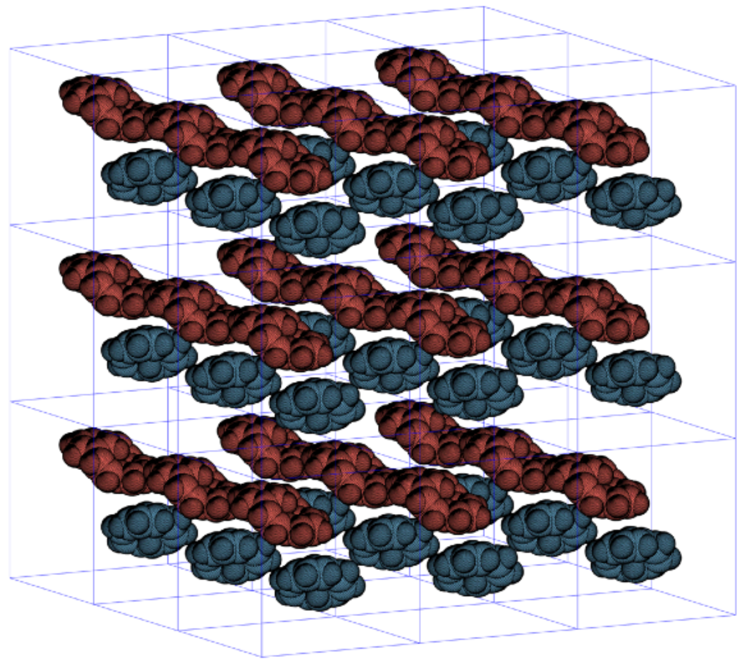
Close-Packings of Volumetric Models of Molecules

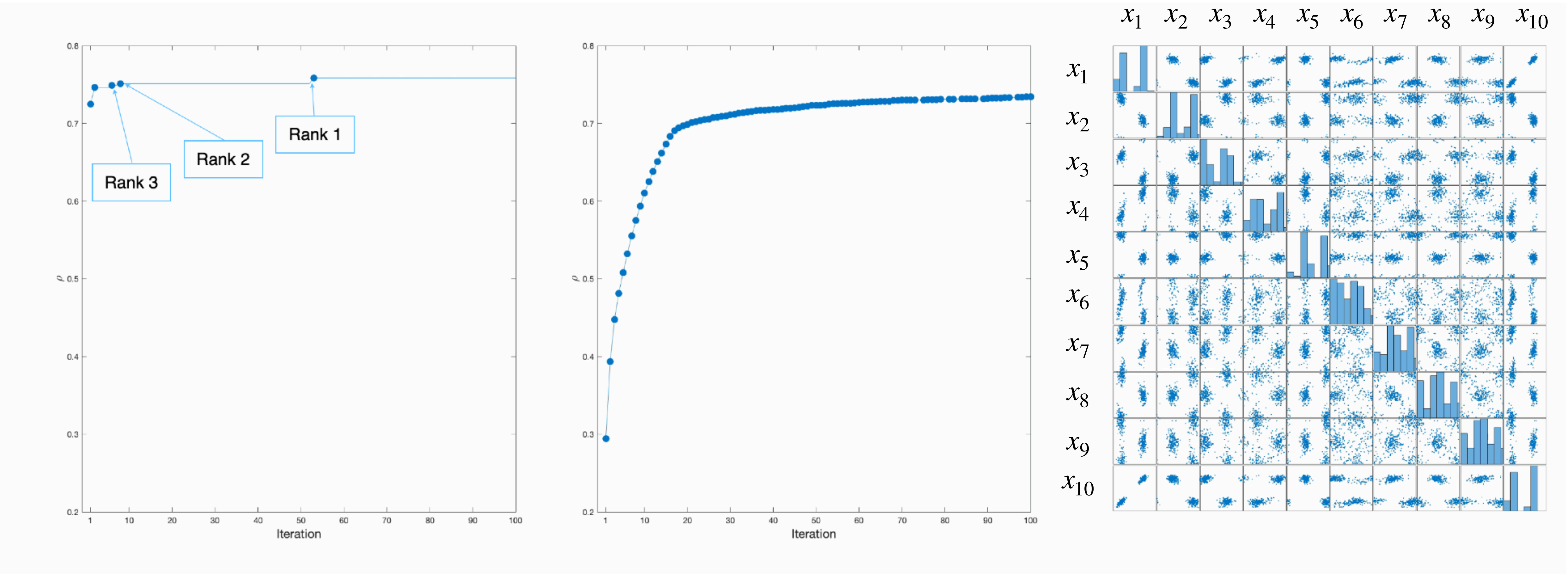
Packing MCYPDE in Space Group $P2_1$

Molecule as a collection of Van der Waals spheres



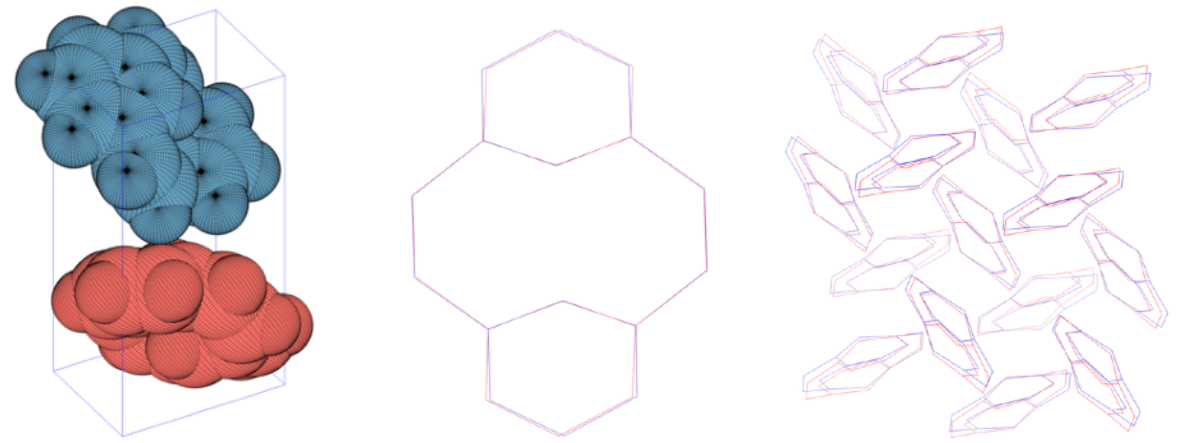






Visualization of the MCYPDE packing maximization run for the space group $P2_1$ (Left) Maximum packing density; (middle) average packing density of N-best packings at $i-th$ iteration; (right) distribution of the packing generation at the iteration.

Reference	Comparison	Molecules in Common	ρ
Ground state	Rank 1	30 out of 30	0.7584
Ground state	Rank 2	8 out of 30	0.7514
Ground state	Rank 3	10 out of 30	0.7510



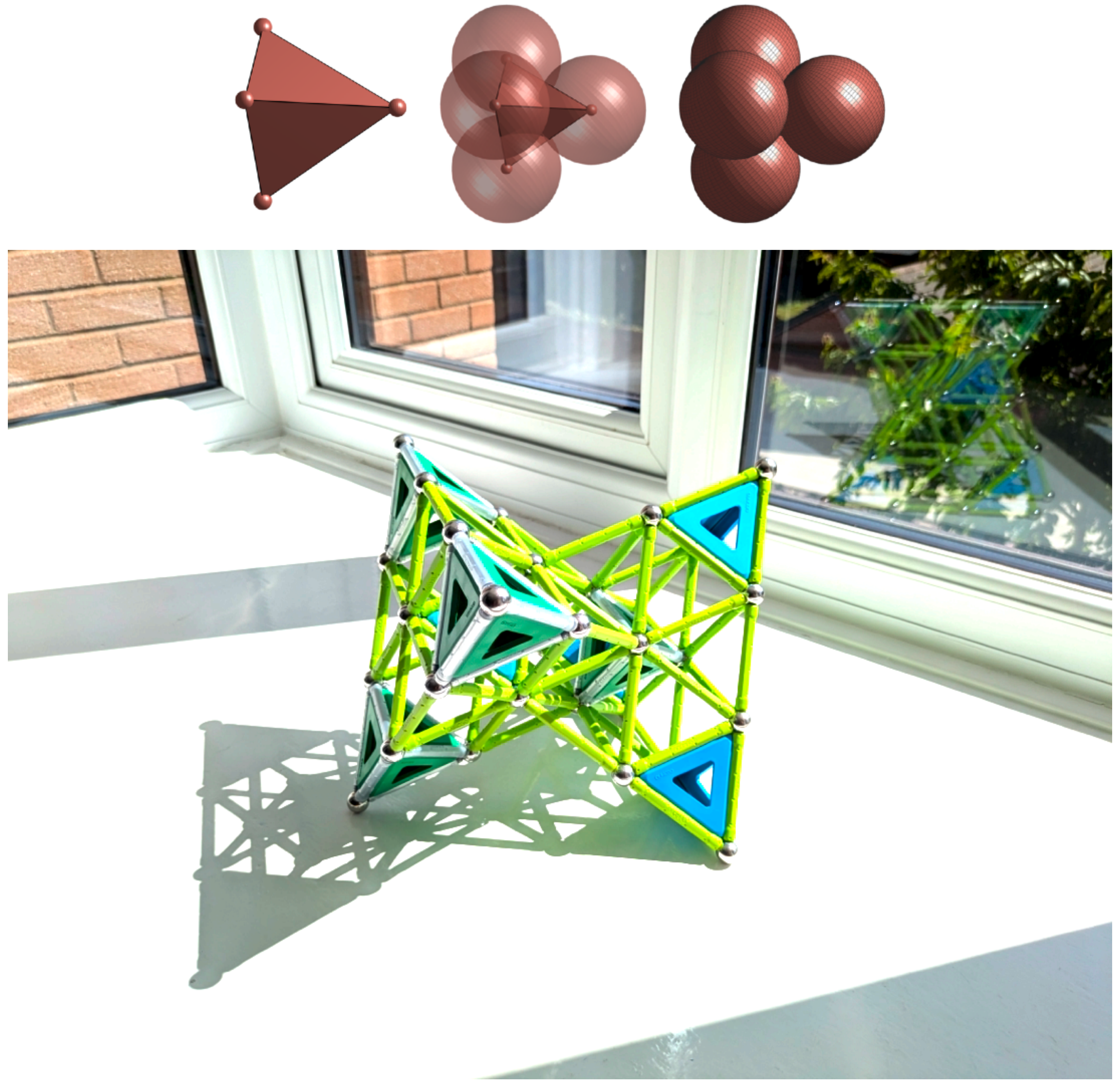
Visualization of the packing match to the CSP lowest energy structure (Left) A single unit cell displayed in a space-filling representation, where colors indicate symmetry operations modulo lattice translations. (Middle and right) Overlay in a wireframe representation: the global energy minimum (blue) and the matching packing (red). (Middle) Asymmetric unit of the configuration; (right) a 15-molecule cluster.

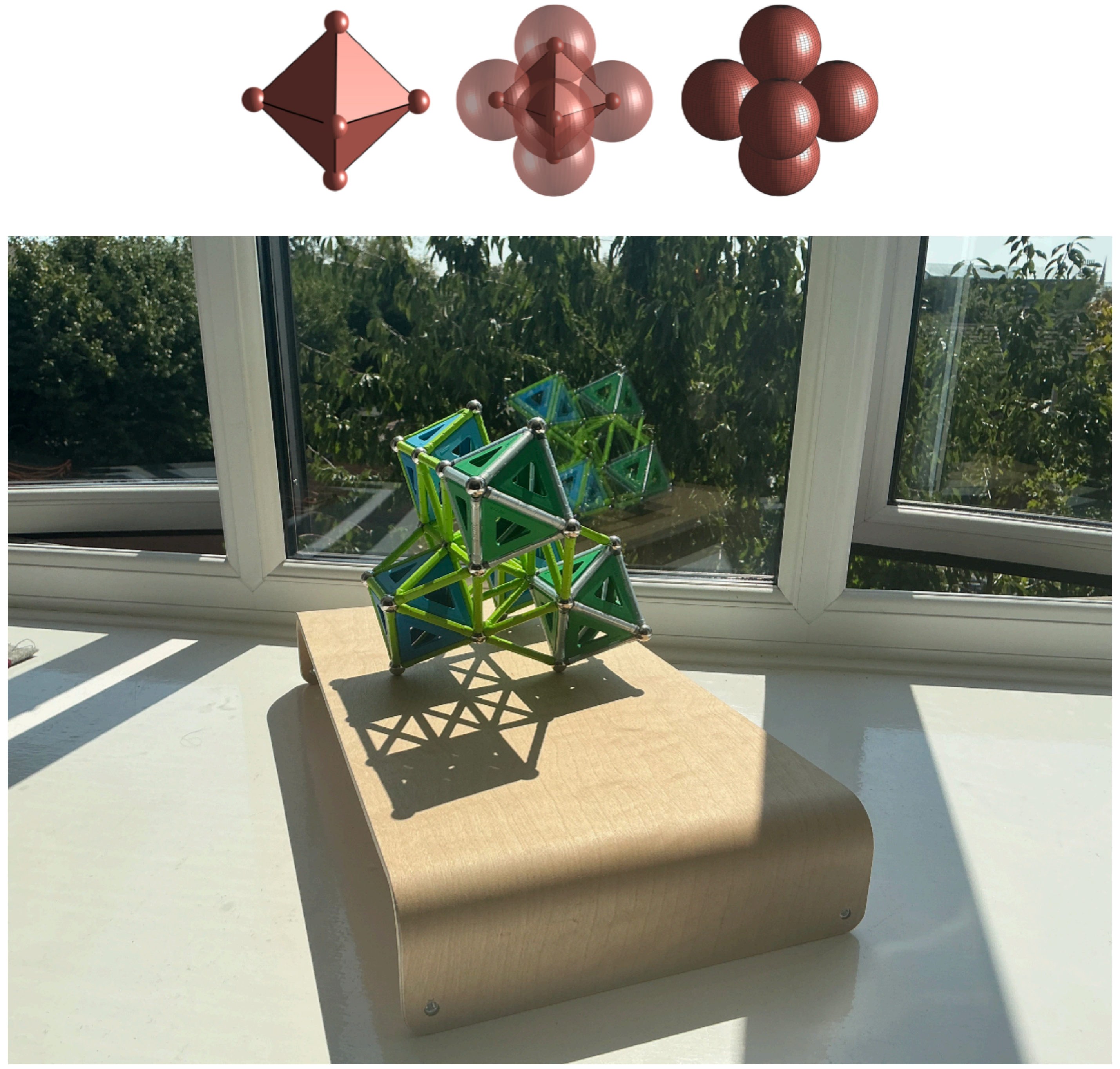
x_7 x_6

§ M. Torda, J. Y. Goulermas, R. Púček and V. Kurlin, *Entropic Trust Region for Densest Crystallographic Symmetry Group Packings*, SIAM Journal on Scientific Computing, (2023).

Which space group to search first?

Symmetries of the tetrahedral and octahedral molecule packing models

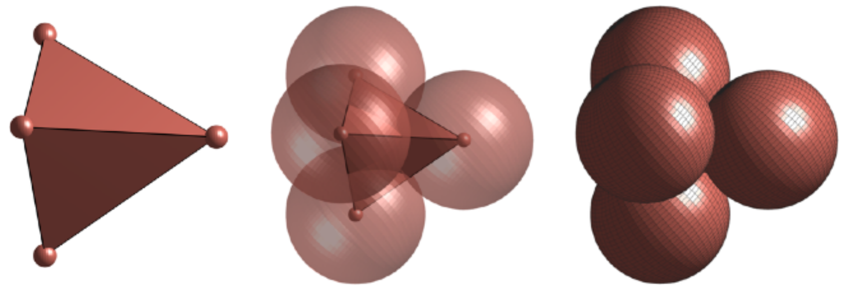


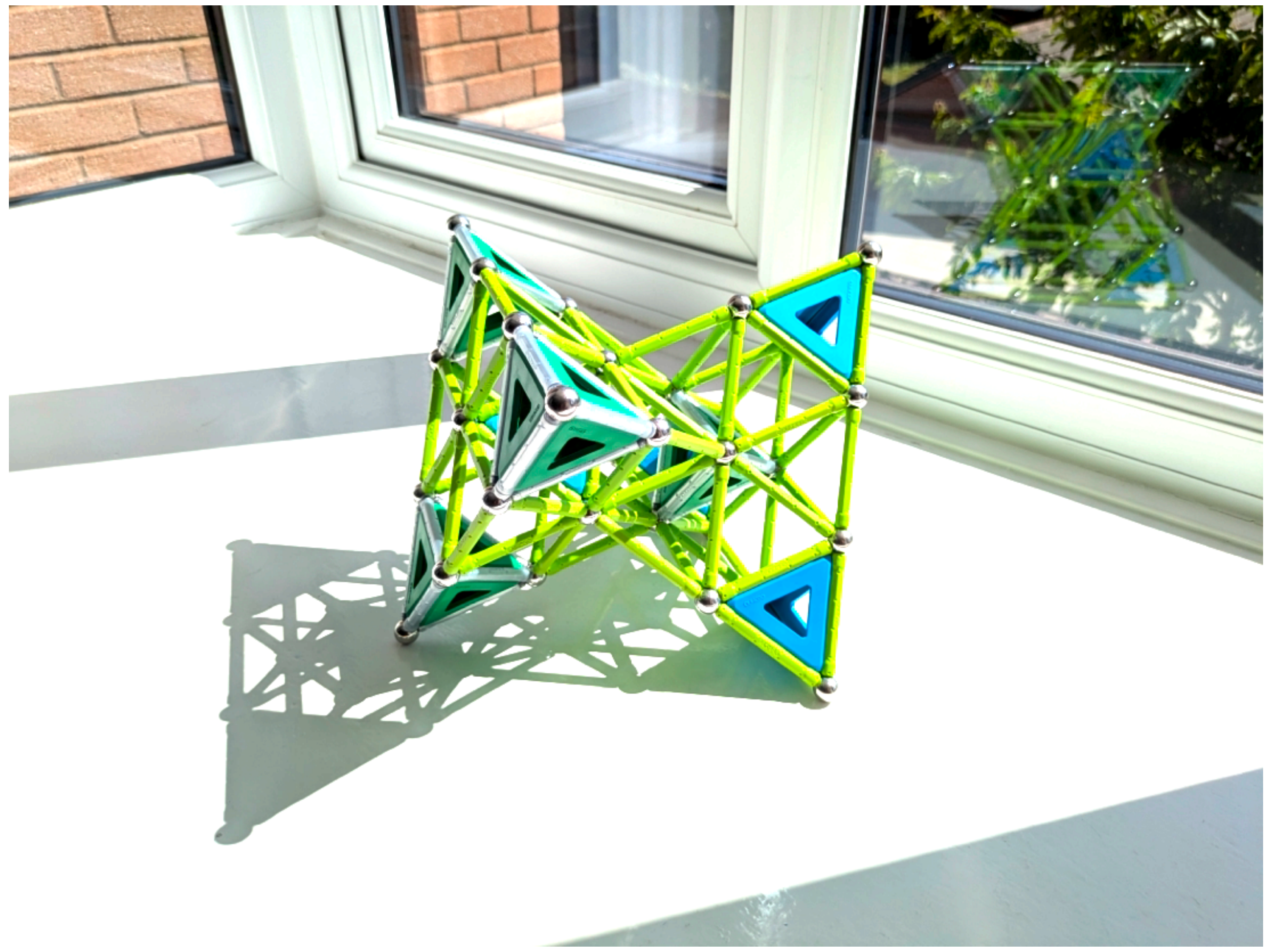


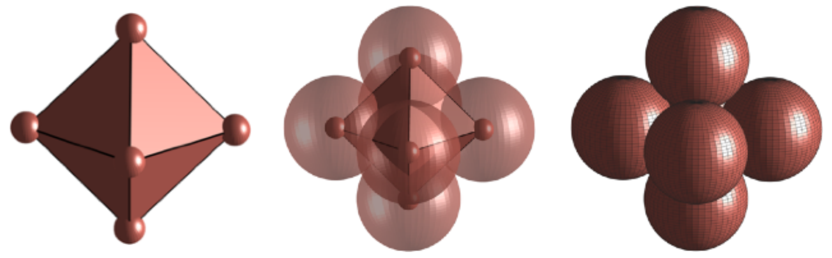
Which space group to search first?

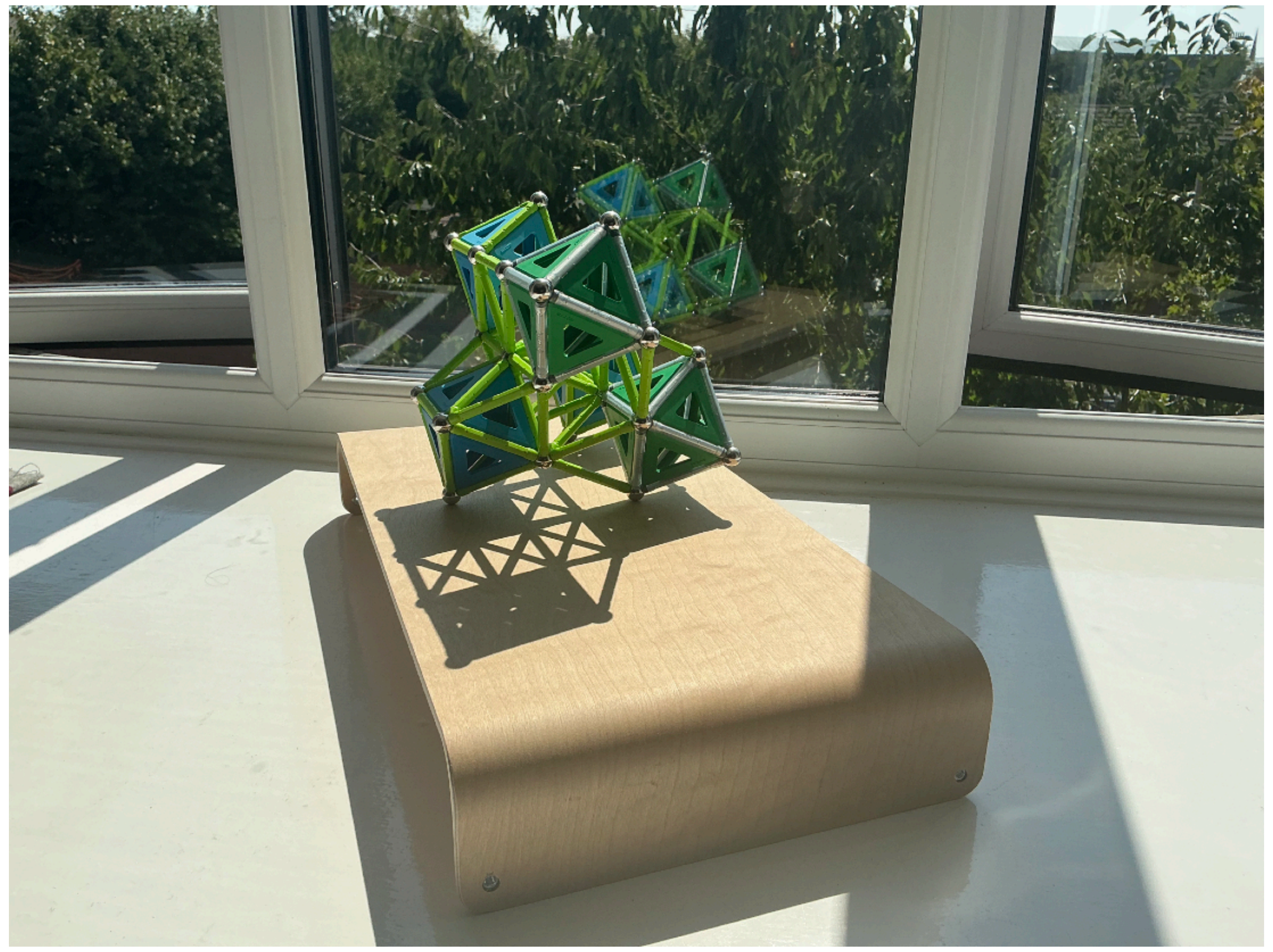
Symmetries of the tetrahedral and octahedral molecule packing models

1. *Inversions* – tetrahedra and octahedra of different colours are related by this isometry.









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Symmetries of the tetrahedral and octahedral molecule packing models

1. *Inversions* – tetrahedra and octahedra of different colours are related by this isometry.

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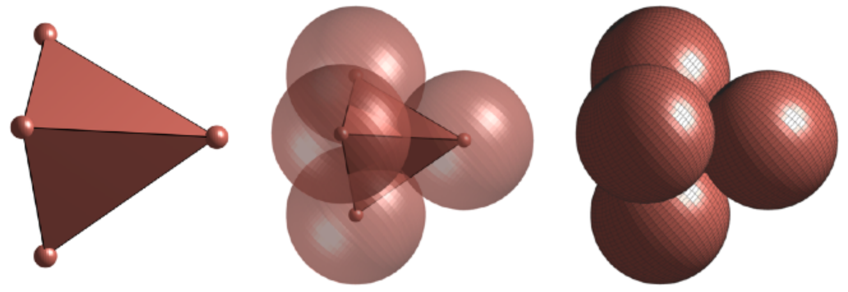
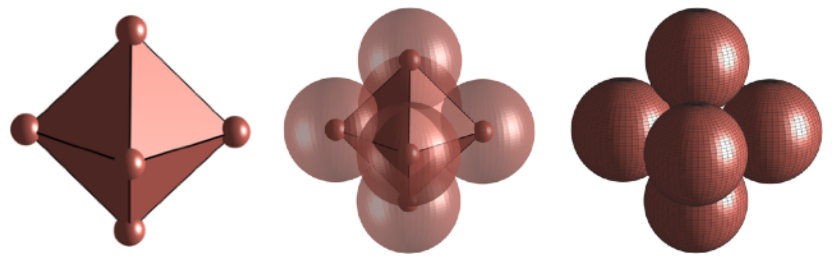
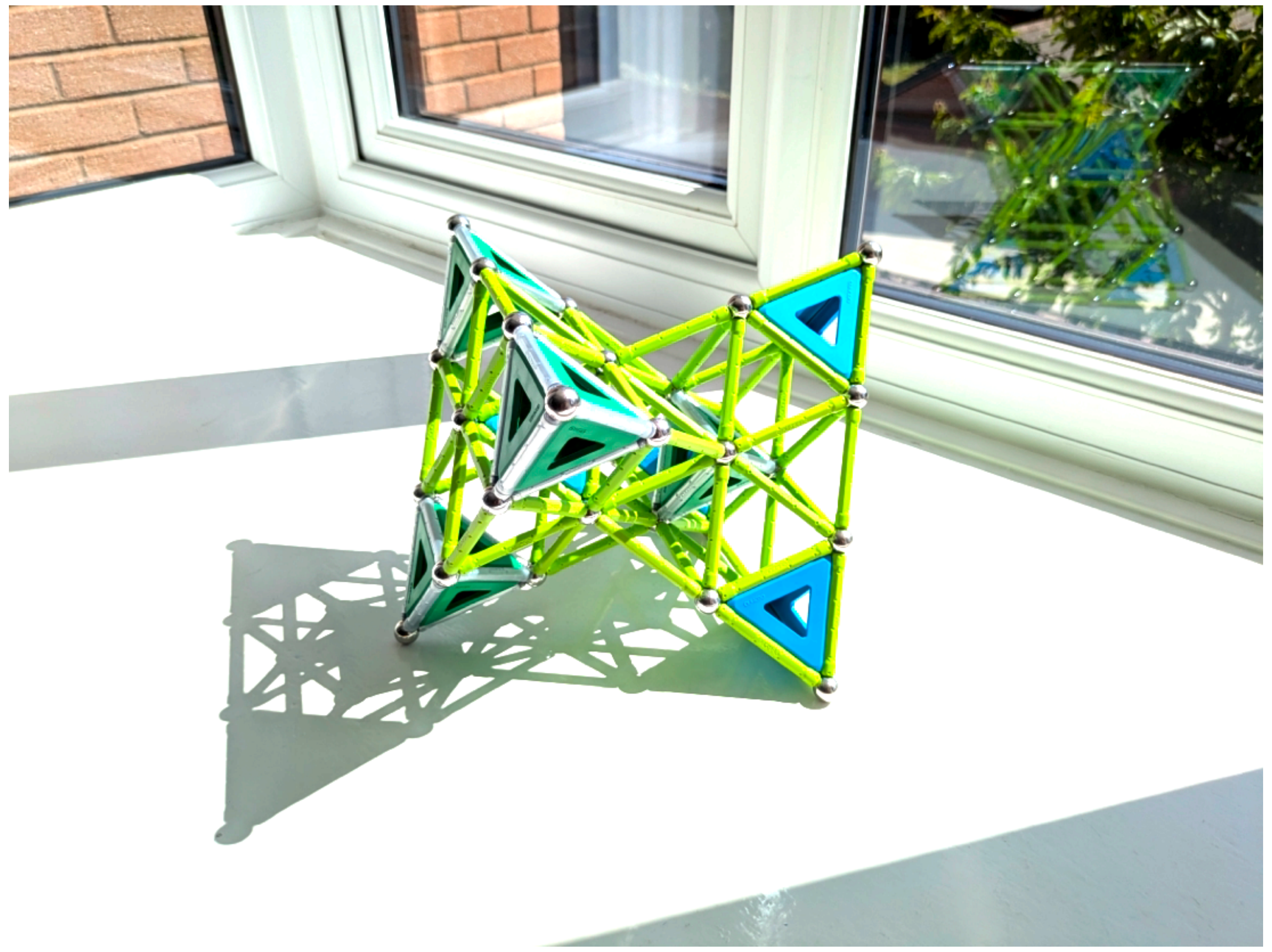
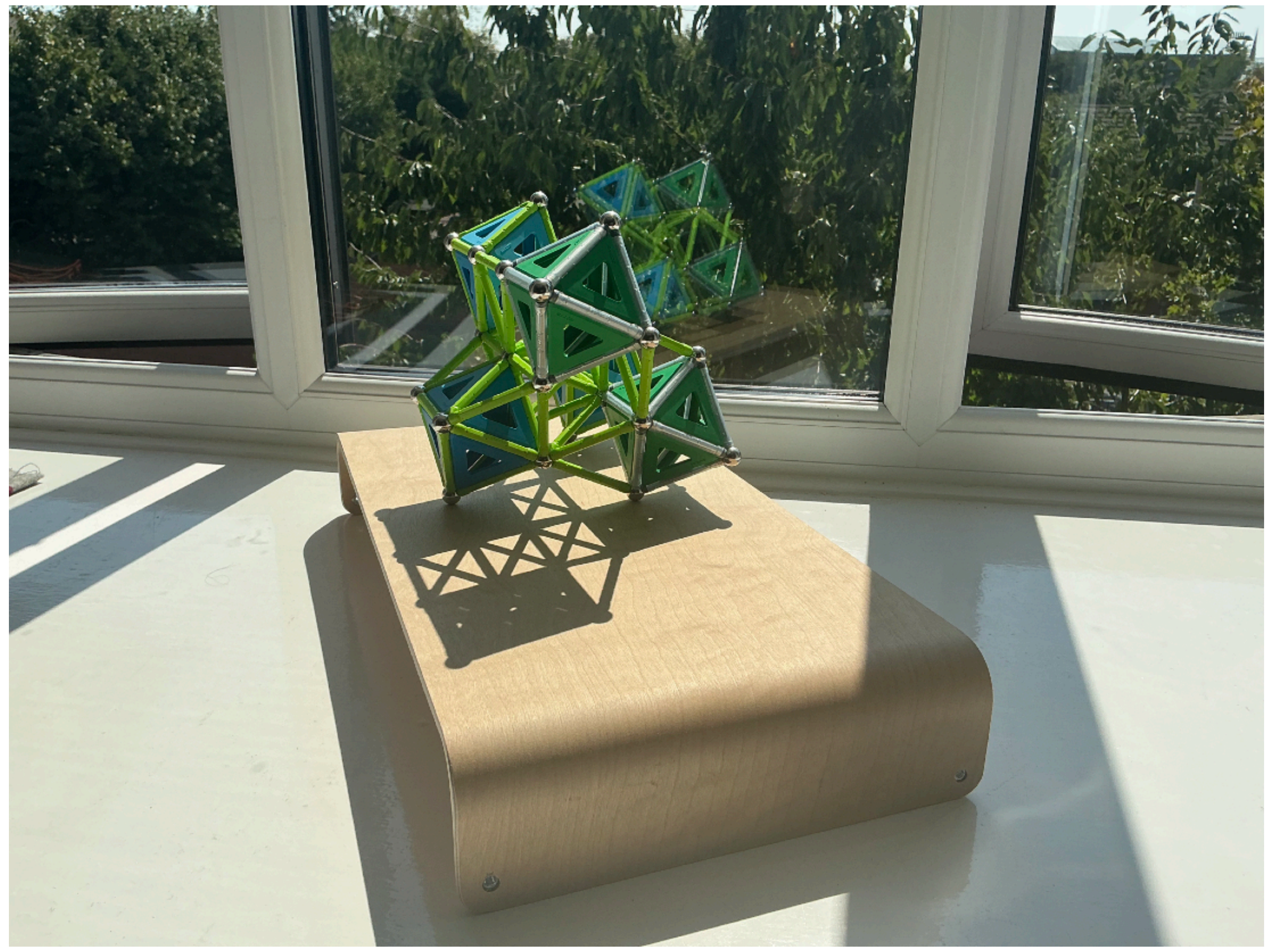








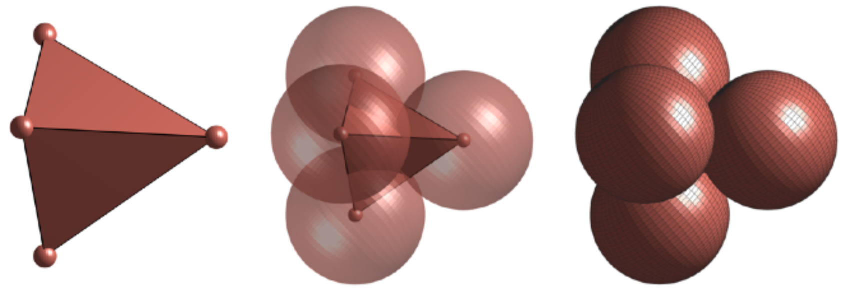
Which space group to search first?

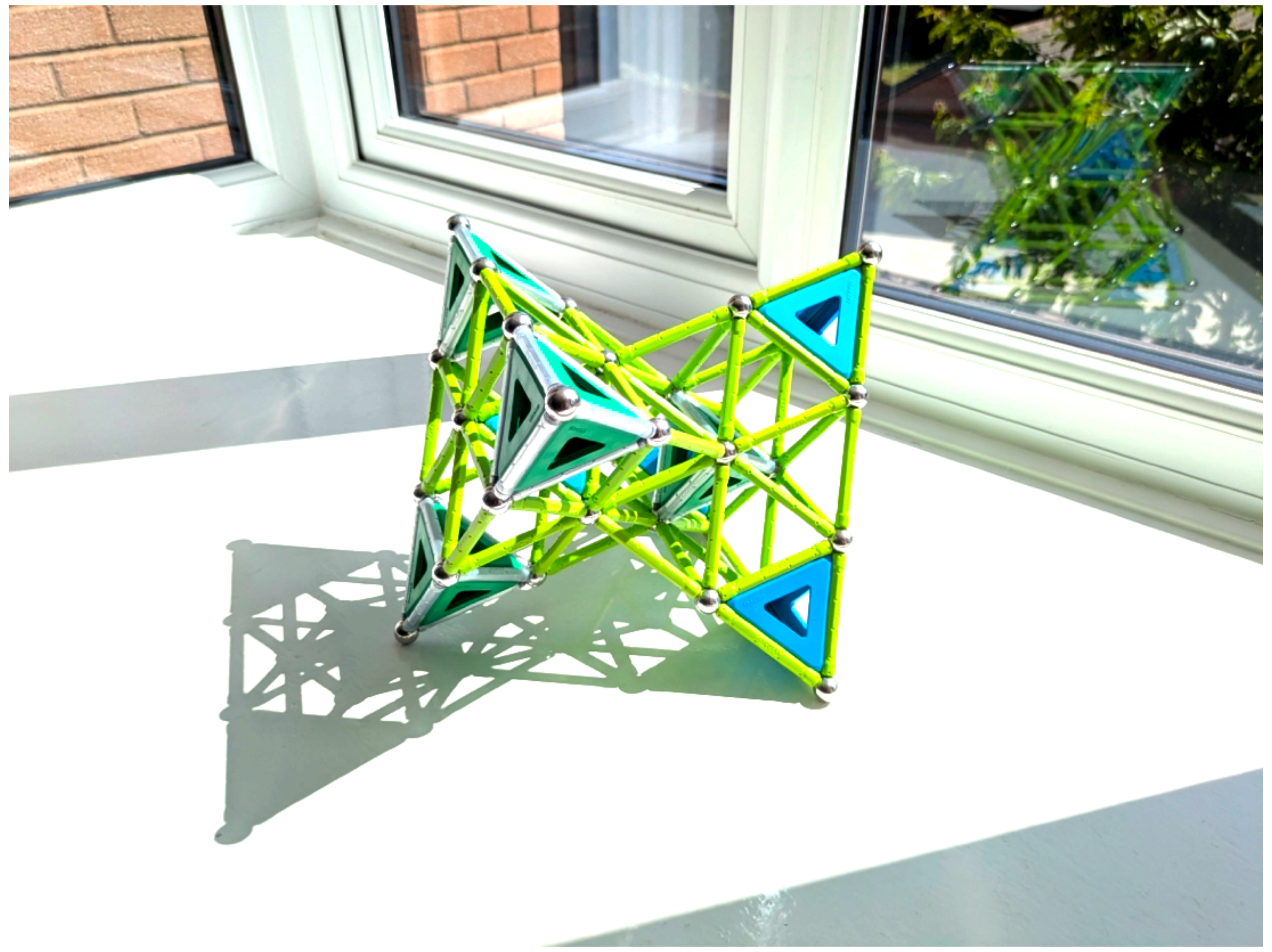
Symmetries of the tetrahedral and octahedral molecule packing models

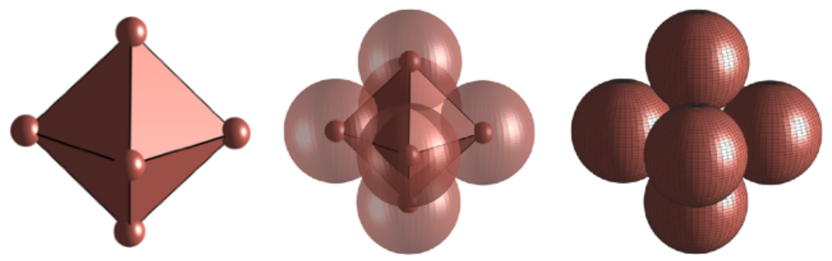
1. *Inversions* – tetrahedra and octahedra of different colours are related by this isometry.

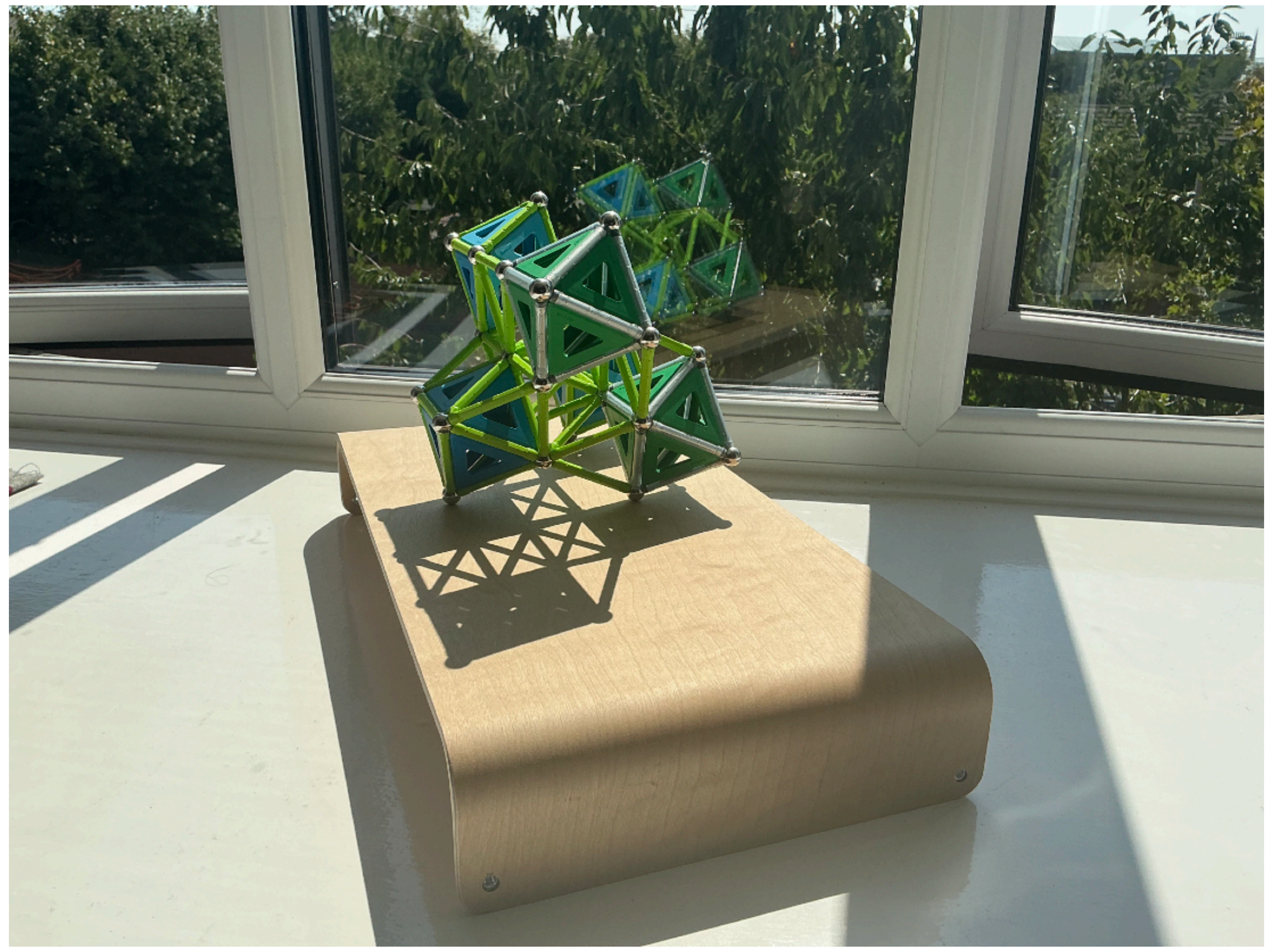
2. *Lattice translations* – tetrahedra with the same colour are related by this isometry.

   - The octahedral configuration is a lattice packing.









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Symmetries of the tetrahedral and octahedral molecule packing models

1. Inversions – tetrahedra and octahedra of different colours are related by this isometry.

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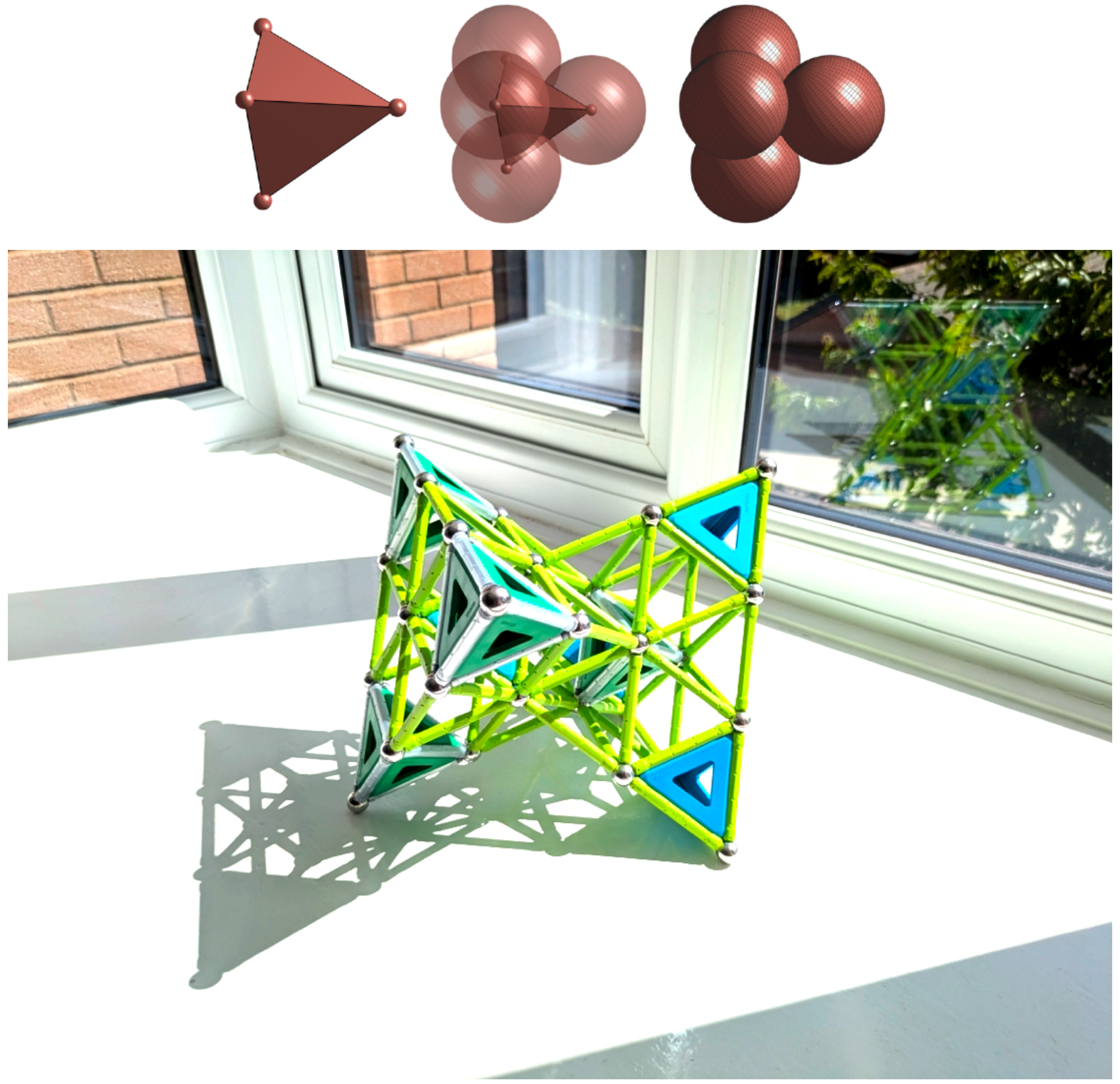
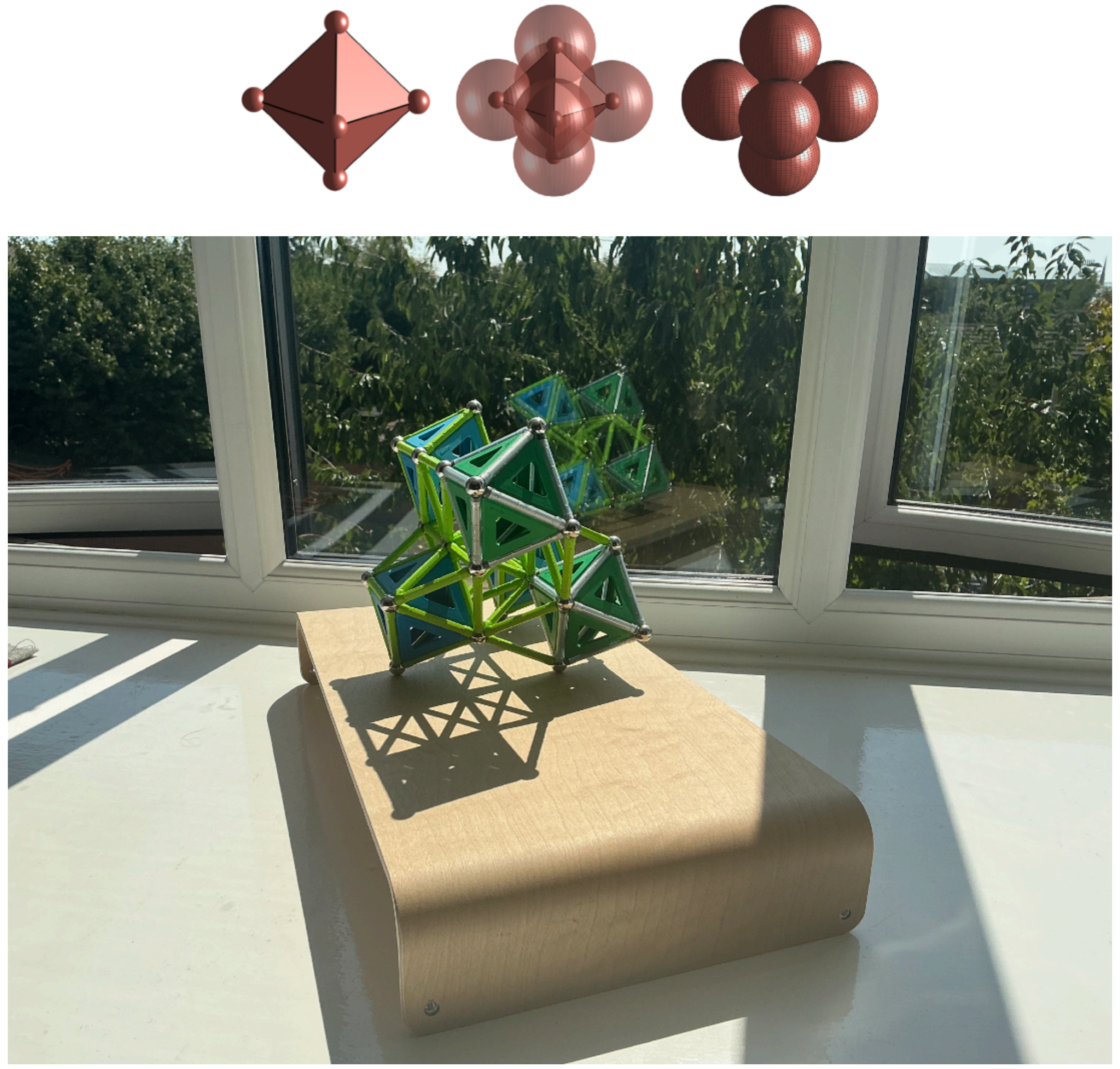
- The octahedral configuration is a lattice packing.

The obvious choice is to start with space group $P\bar{1}$

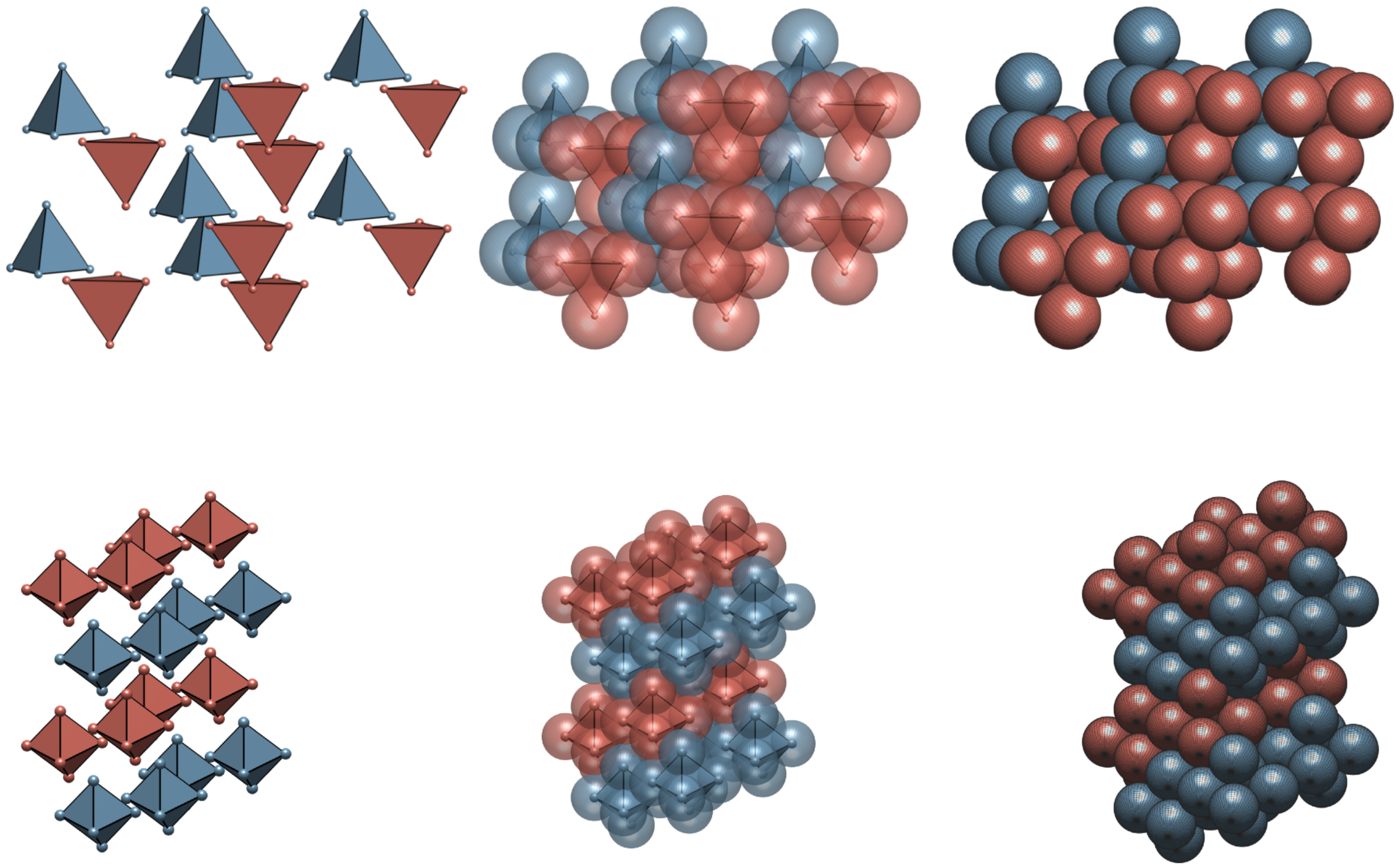




Densest $P\bar{1}$ Packing of Tetrahedral and Octahedral Molecules

- Packing density formula $\rho\left(\mathscr{K}_G\right) = \dfrac{N \text{ vol}(K)}{\text{vol}(U)}$

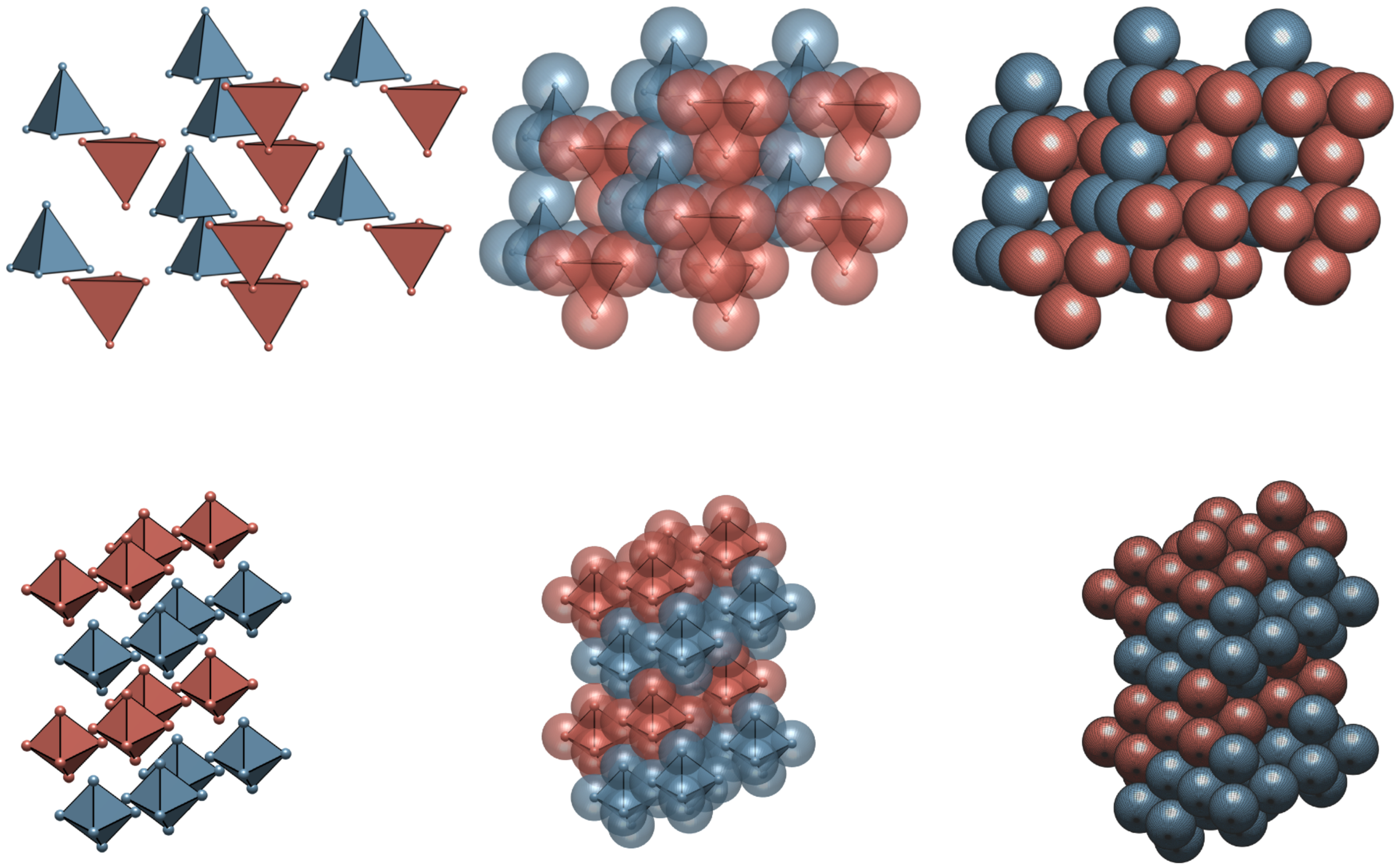
Densest packing configurations from the computational experiments



Densest $P\bar{1}$ Packing of Tetrahedral and Octahedral Molecules

- Packing density formula $\rho\left(\mathscr{K}_G\right) = \dfrac{N\ \text{vol}(K)}{\text{vol}(U)}$
- Volume of the unit cell $\text{vol}(U) = 2^7$

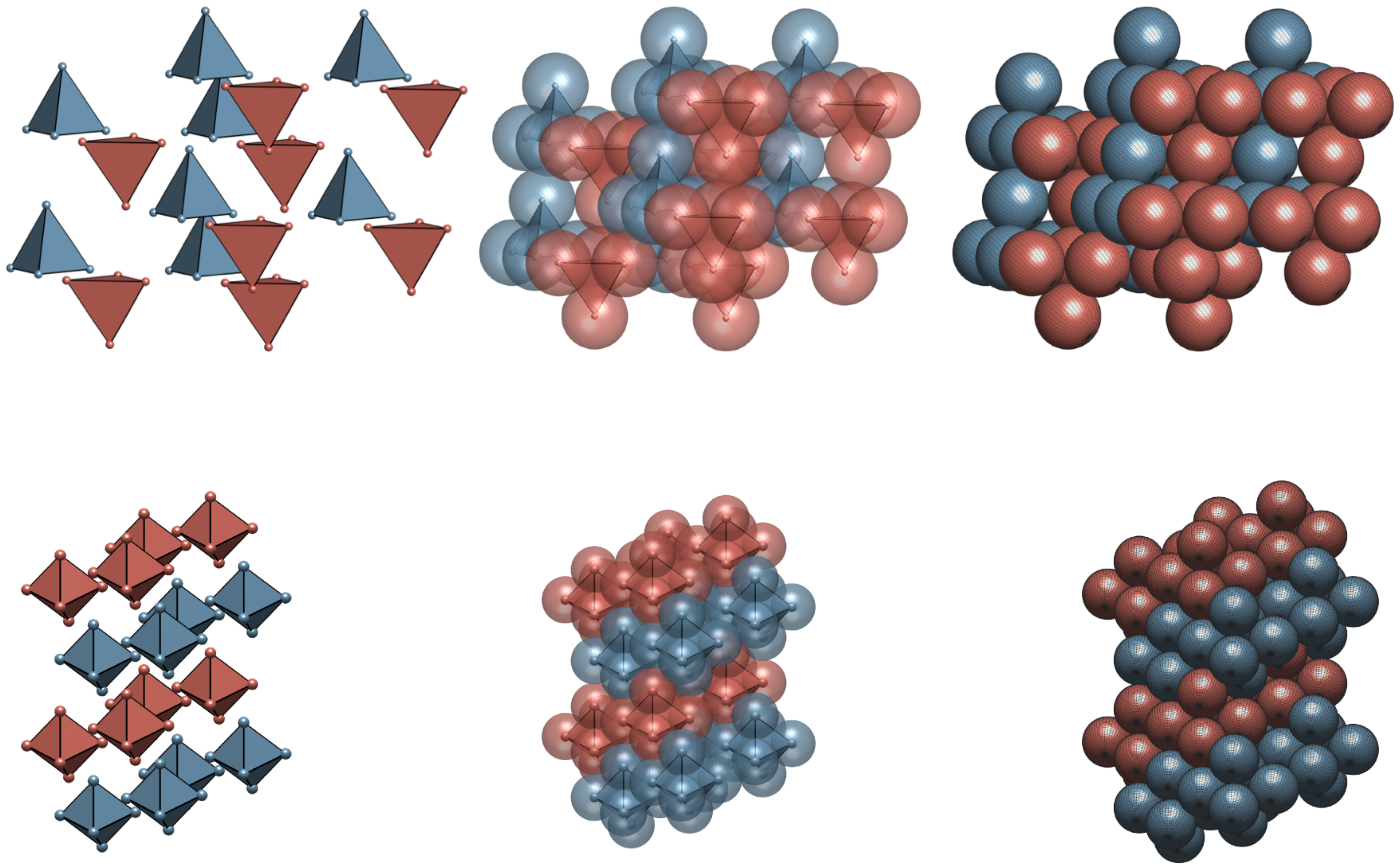
Densest packing configurations from the computational experiments



Densest $P\bar{1}$ Packing of Tetrahedral and Octahedral Molecules

- Packing density formula $\rho\left(\mathscr{K}_G\right) = \dfrac{N\,\text{vol}(K)}{\text{vol}(U)}$
- Volume of the unit cell vol$(U) = 2^7$
- Volume of the our tetrahedral molecule is vol$(K) = \dfrac{16}{3}\pi 2^{\frac{3}{2}}$

Densest packing configurations from the computational experiments



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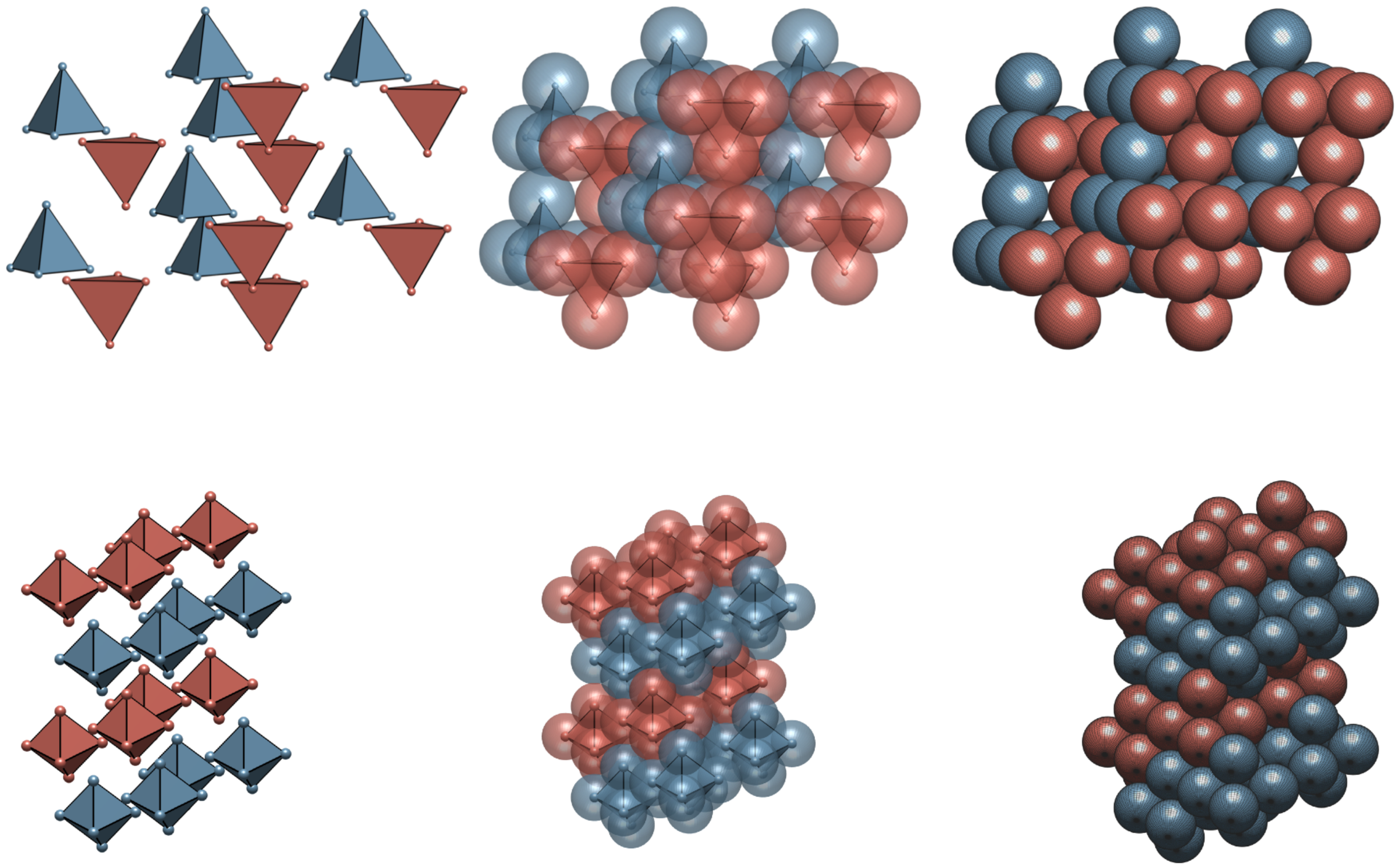
- Volume of the unit cell $\mathrm{vol}(U) = 2^7$
- Volume of the our tetrahedral molecule is $\mathrm{vol}(K) = \dfrac{16}{3}\pi 2^{\frac{3}{2}}$
- Number of elements of factor group G/L where L is the lattice subgroup of G is $N = 2$

Densest packing configurations from the computational experiments



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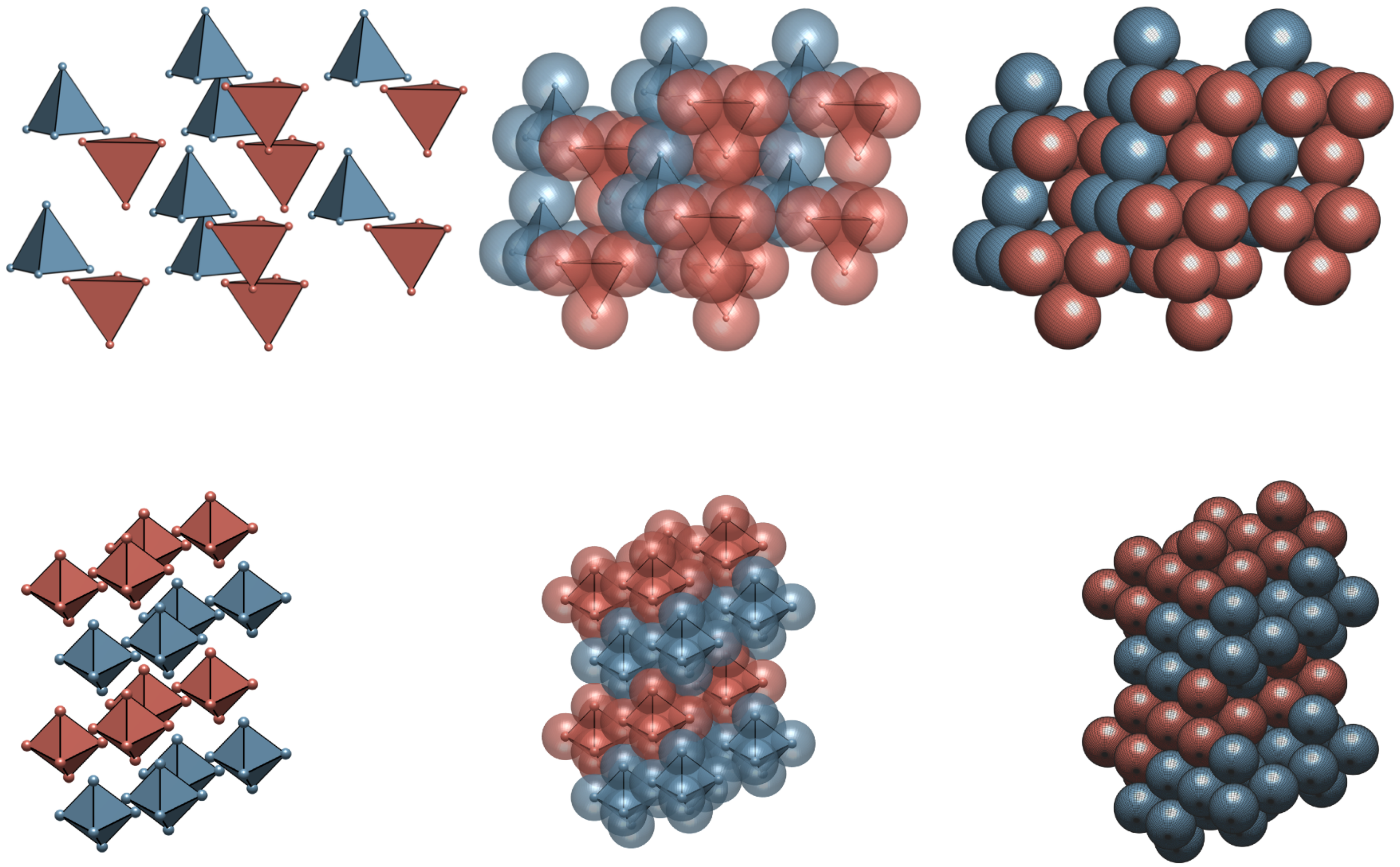
- Number of elements of factor group G/L where L is the lattice subgroup of G is $N = 2$
- Packing density of tetrahedral and octahedral molecule packings $\rho\left(\mathscr{K}_G\right) = \dfrac{\pi}{\sqrt{18}}$

Densest packing configurations from the computational experiments



Densest $P\bar{1}$ Packing of Tetrahedral and Octahedral Molecules

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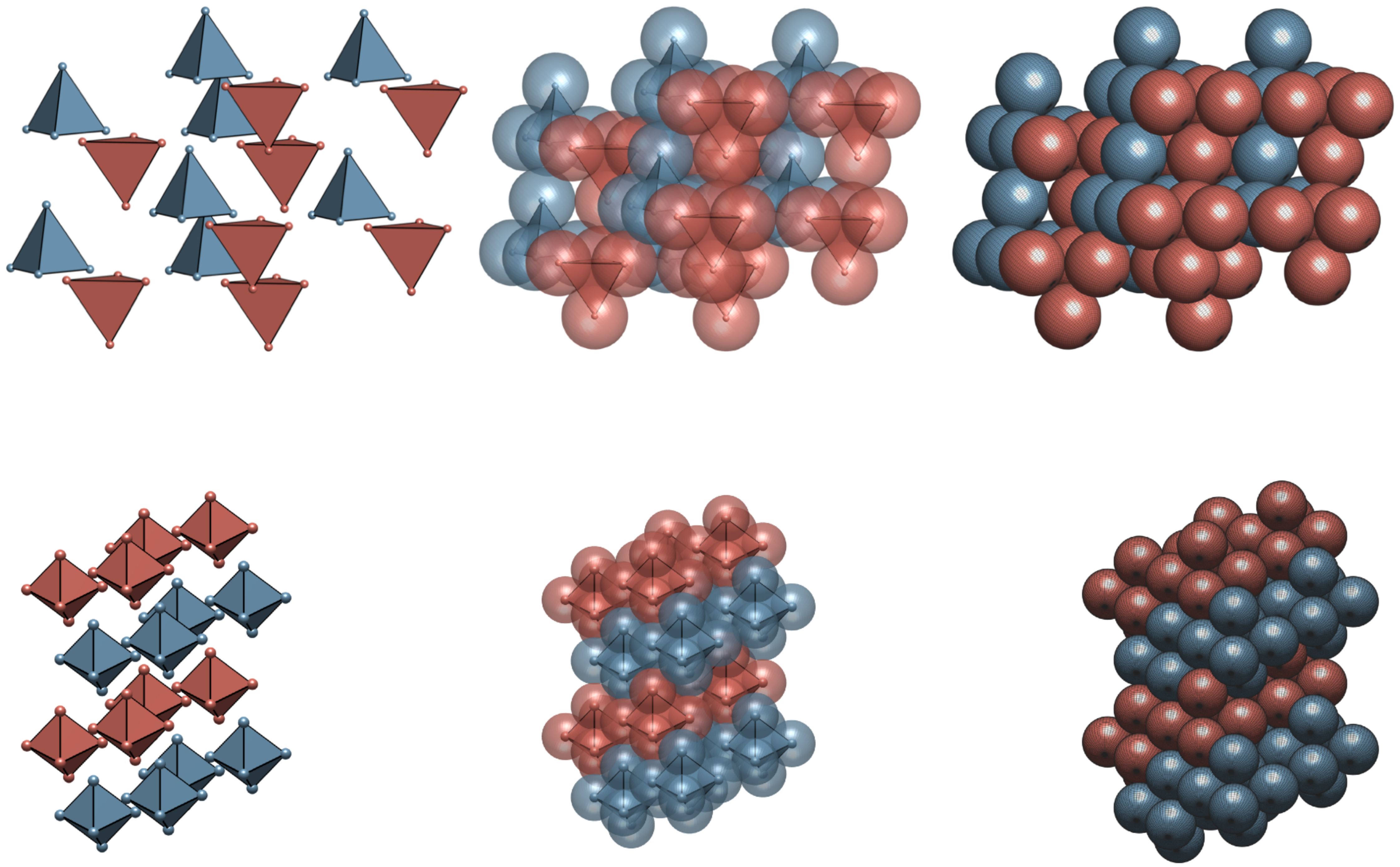
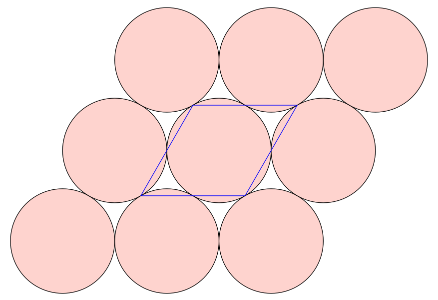
- Number of elements of factor group G/L where L is the lattice subgroup of G is $N = 2$
- Packing density of tetrahedral and octahedral molecule packings $\rho\left(\mathscr{K}_G\right) = \dfrac{\pi}{\sqrt{18}}$
- Which other space groups to search?

Densest packing configurations from the computational experiments

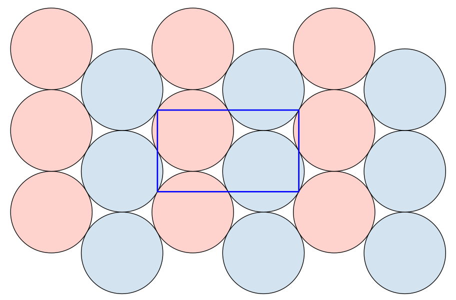


Fibrifold Space Group Notation

$p1$ packing



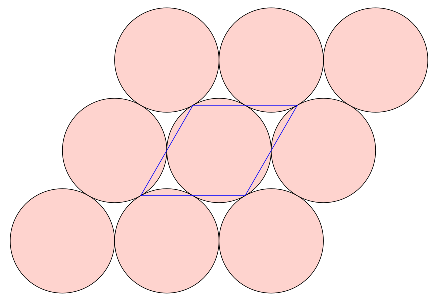
$p2$ packing



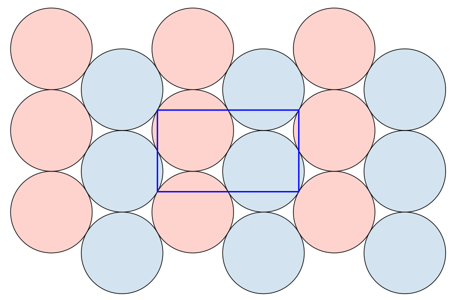
- Lattice points are centres of a 2-fold rotational symmetry.

Fibrifold Space Group Notation

$p1$ packing



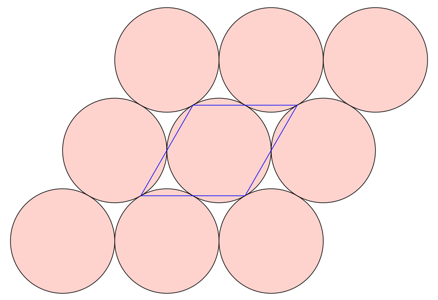
$p2$ packing



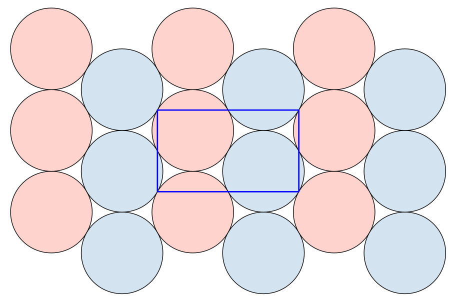
- Lattice points are centres of a 2-fold rotational symmetry.
- Centres of the discs of the lattice packing are centres of a 2-fold rotational symmetry.

Fibrifold Space Group Notation

$p1$ packing



$p2$ packing



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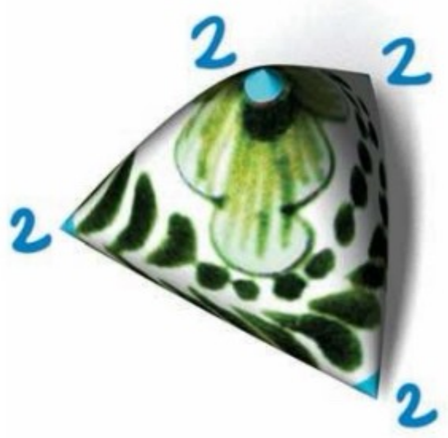
$p2$ orbifold signature: $2\ 2\ 2\ 2$



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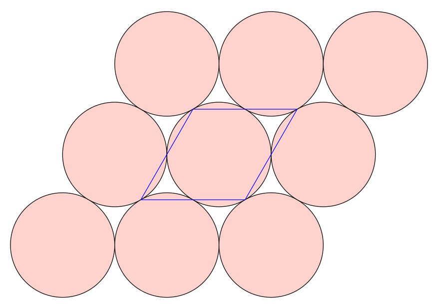
Fibrifold Space Group Notation

$p1$ packing



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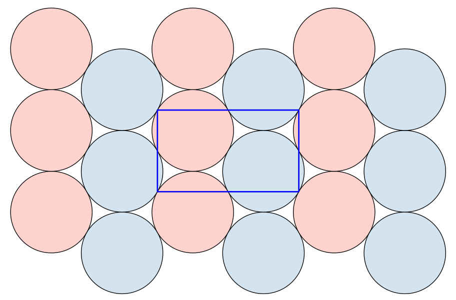

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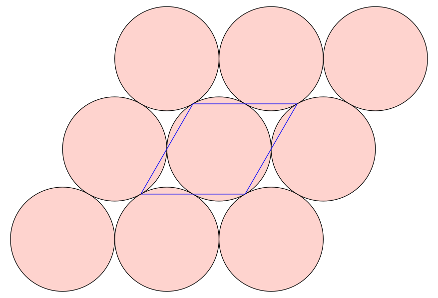

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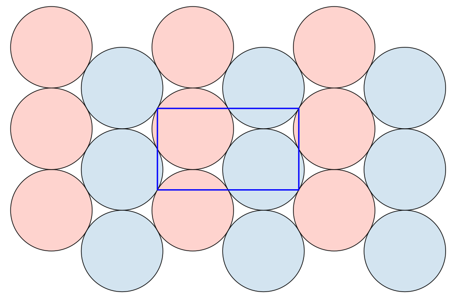

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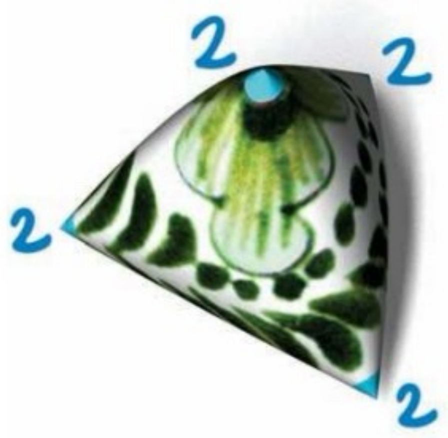

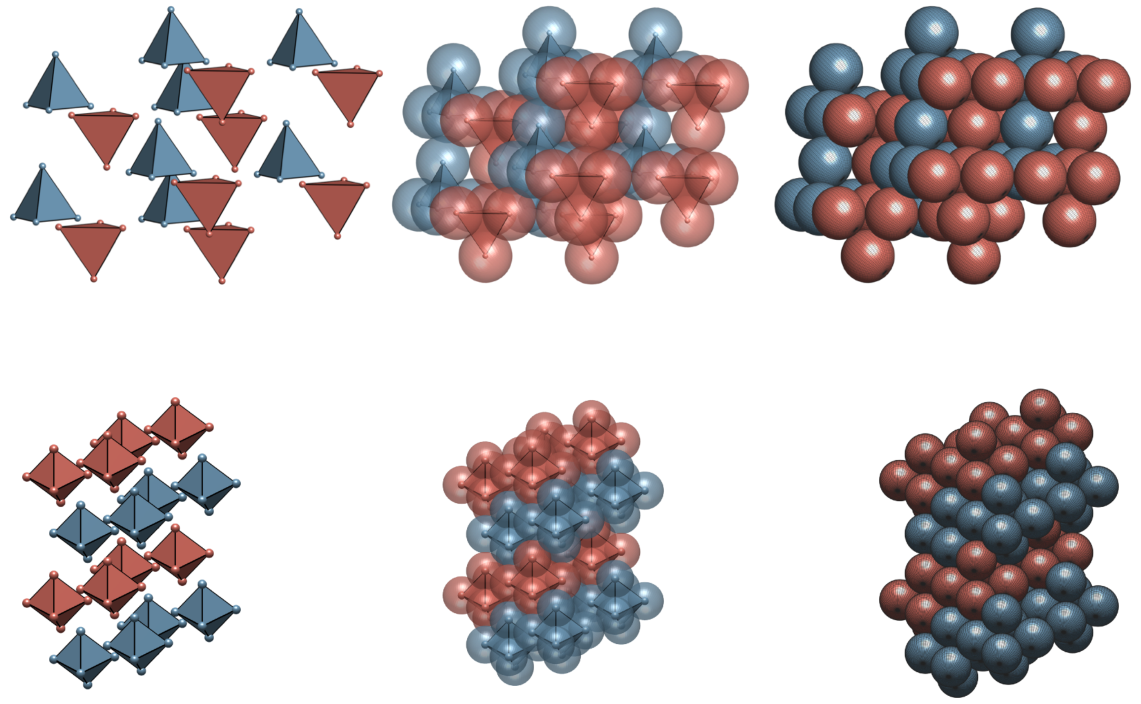

- Layers of $2\ 2\ 2\ 2$ orbifolds

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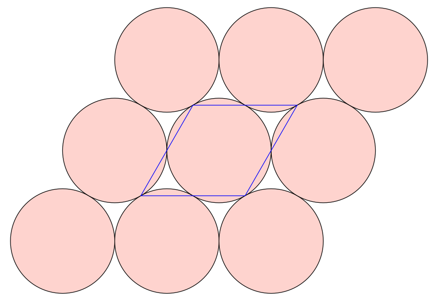

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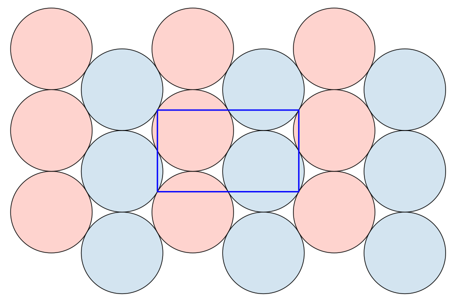

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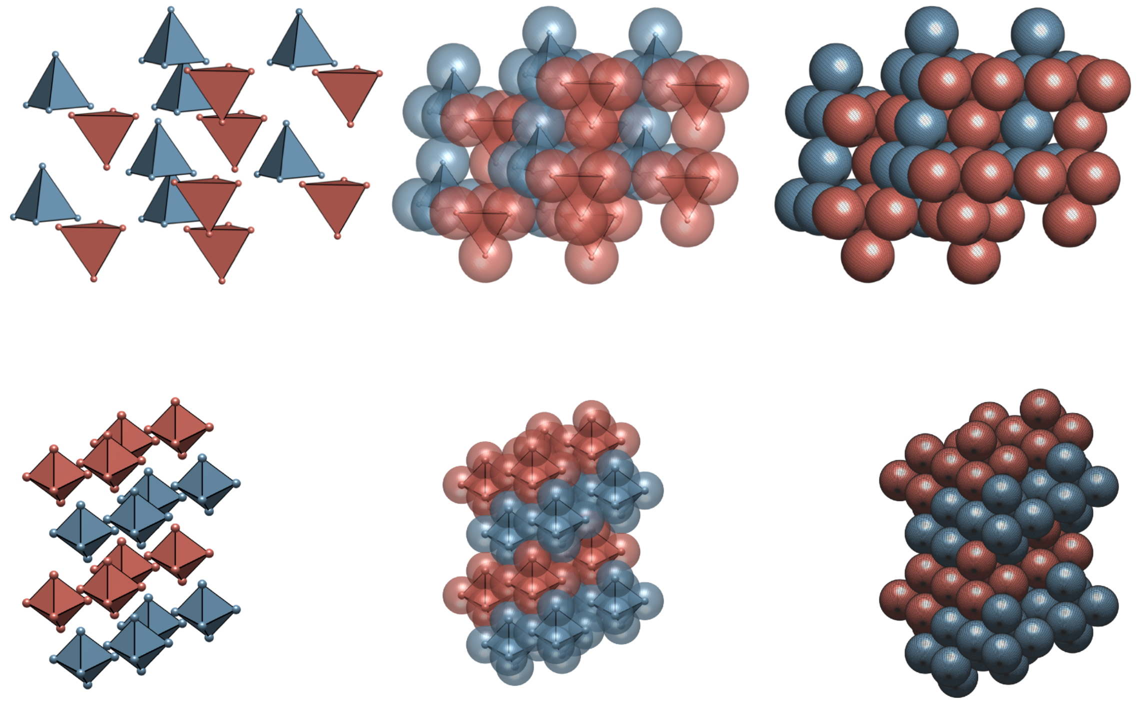

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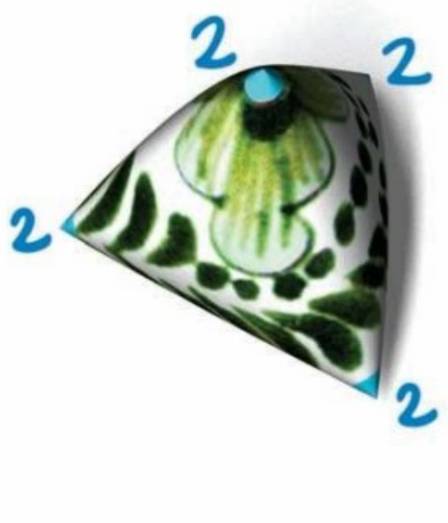

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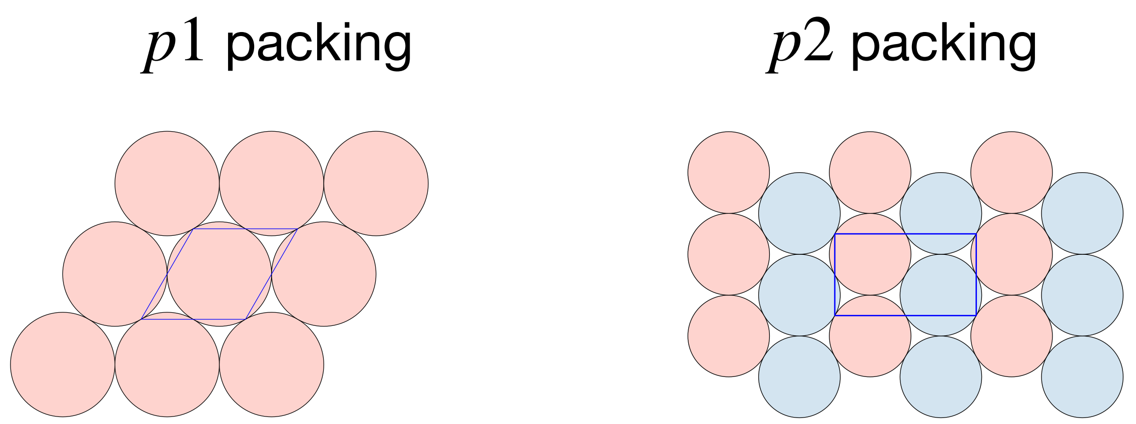

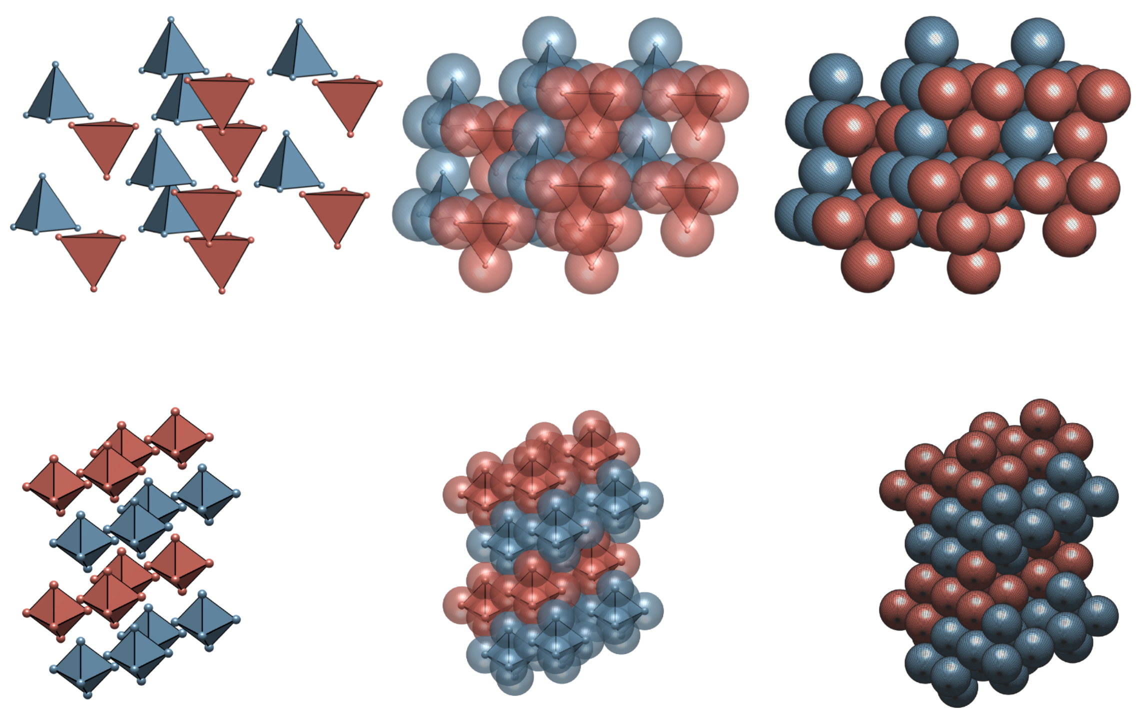

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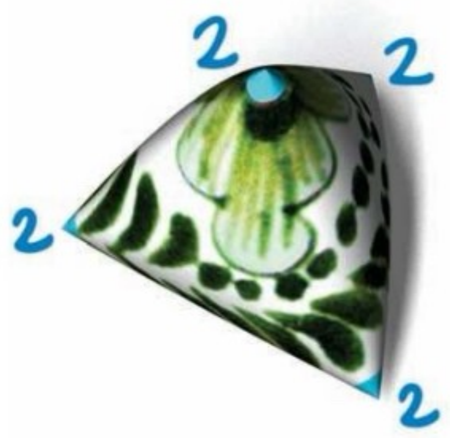
- Fibre-bundle whose base spaces and fibres are orbifolds:

$p2$ orbifold signature: $2\ 2\ 2\ 2$



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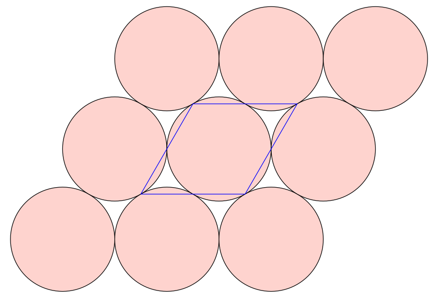

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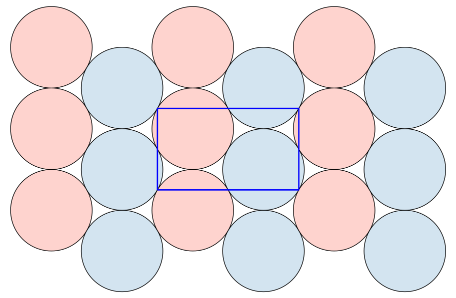

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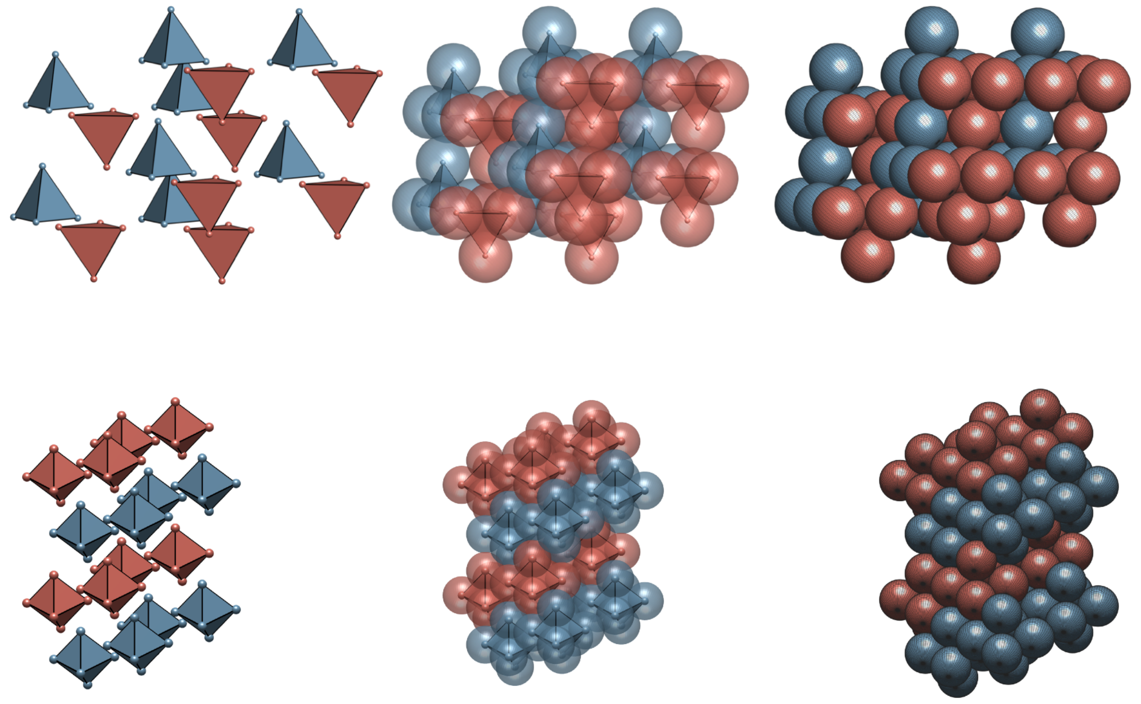

- Layers of $2\ 2\ 2\ 2$ orbifolds
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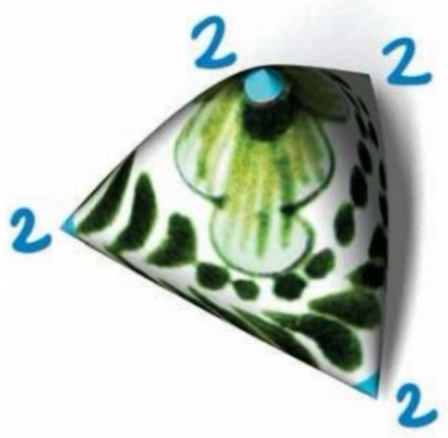

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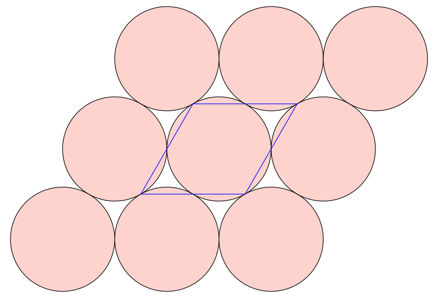

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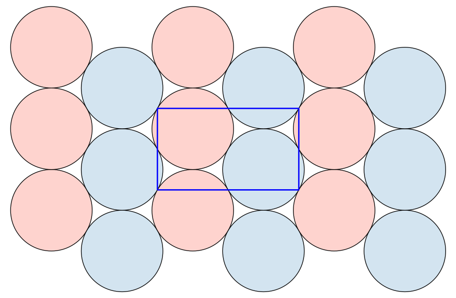

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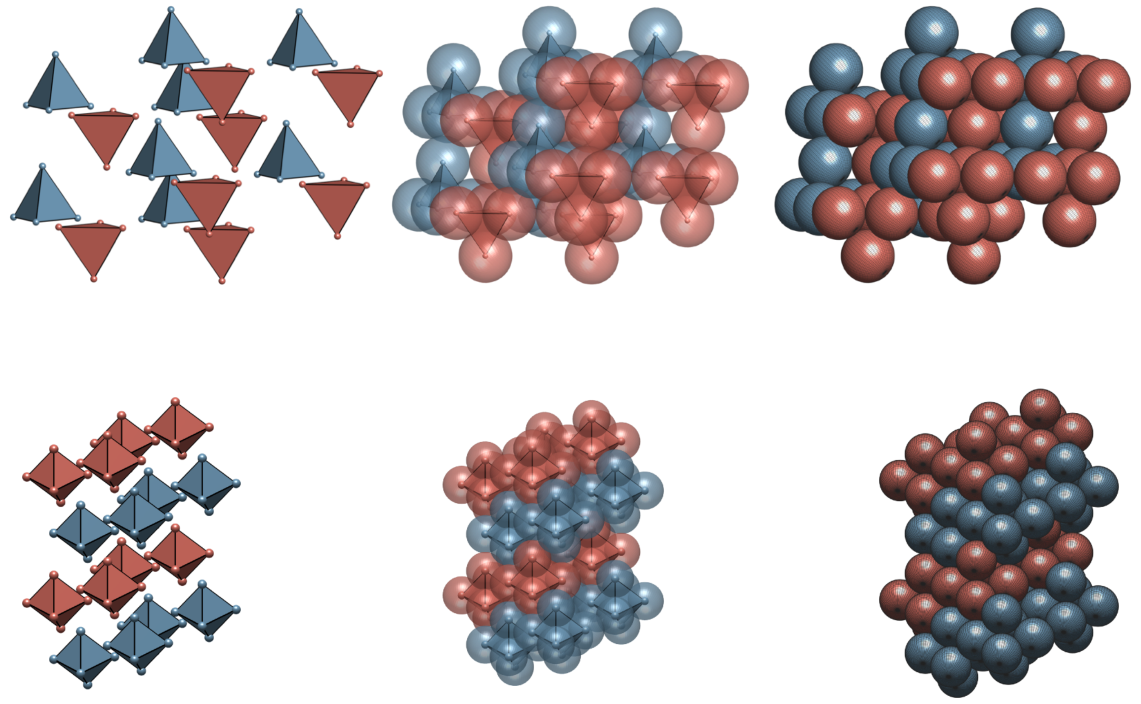

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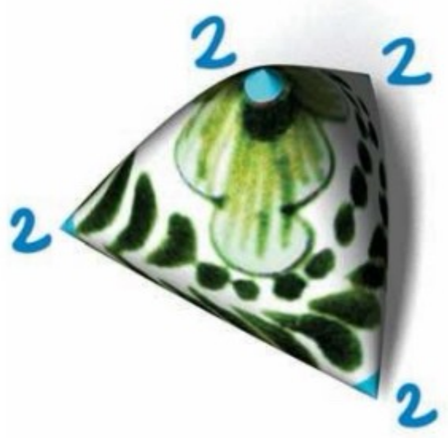

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Fibrifold Space Group Notation

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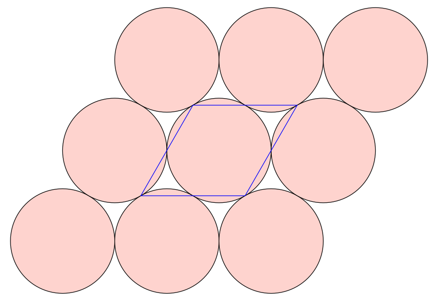

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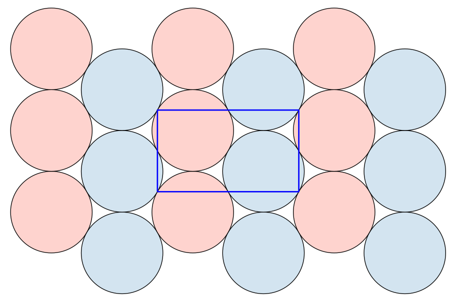

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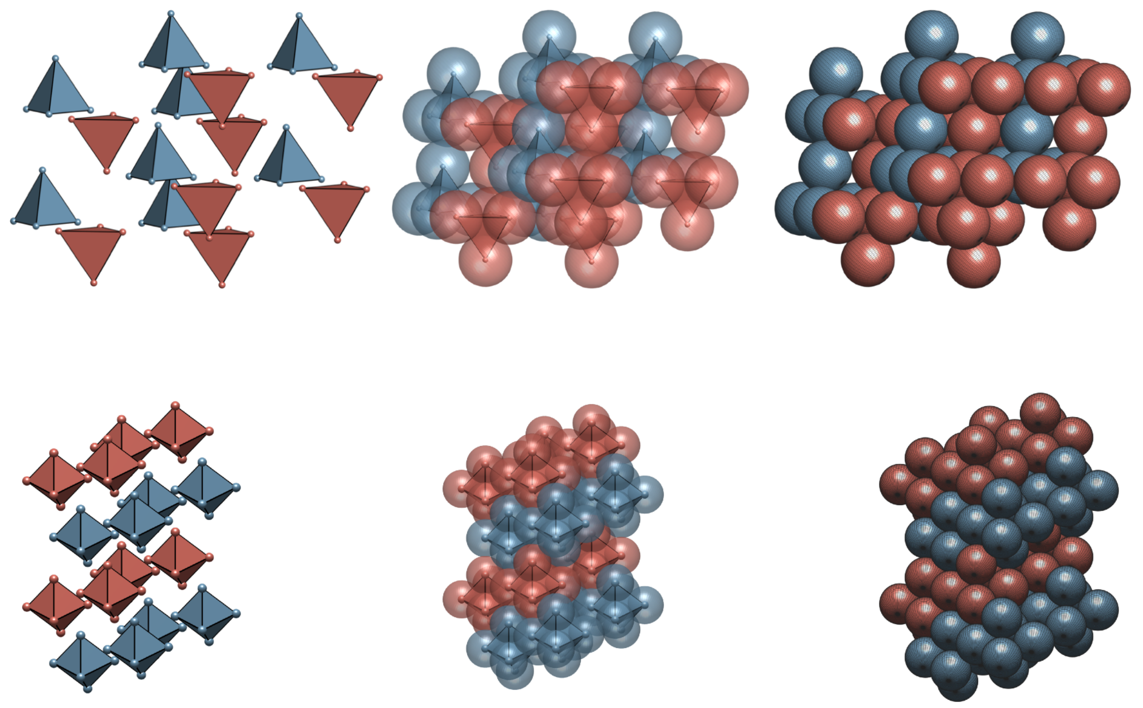

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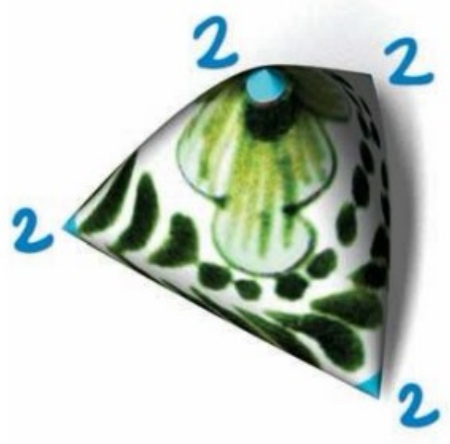

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Fibrifold Space Group Notation

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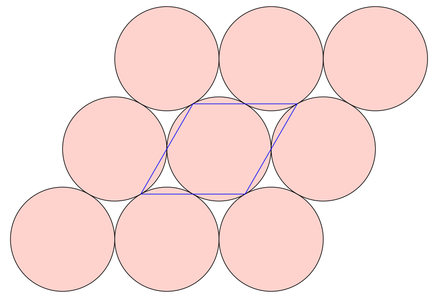

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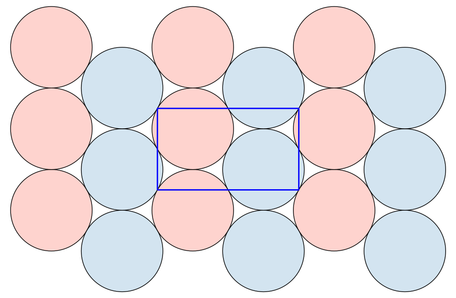

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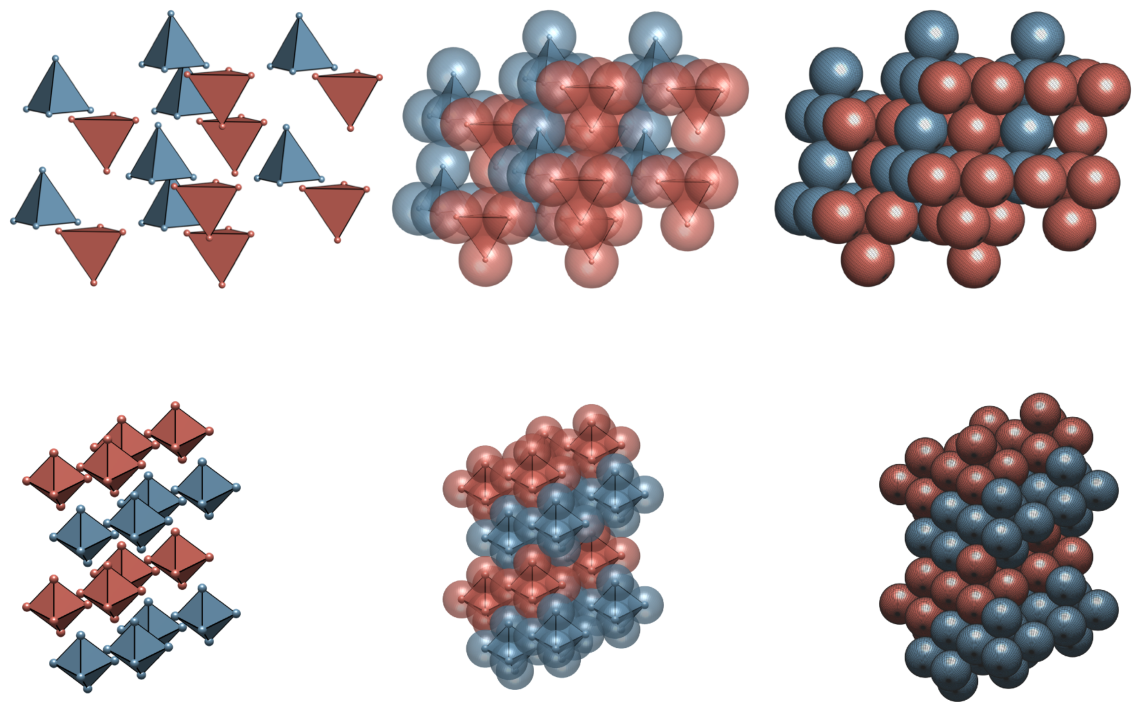

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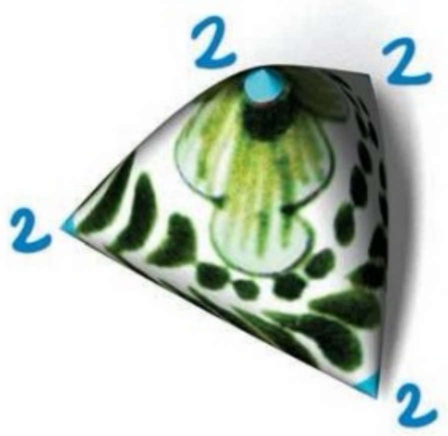

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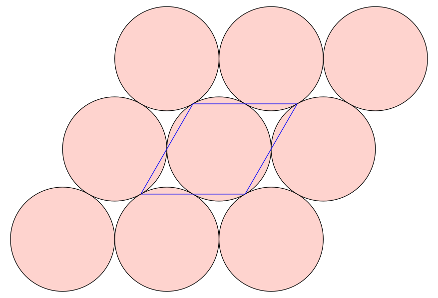

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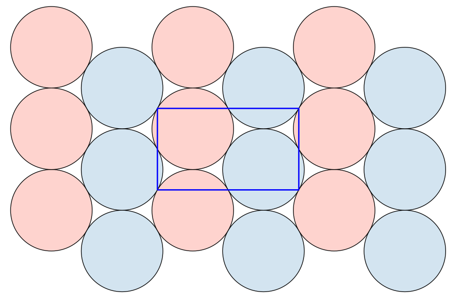

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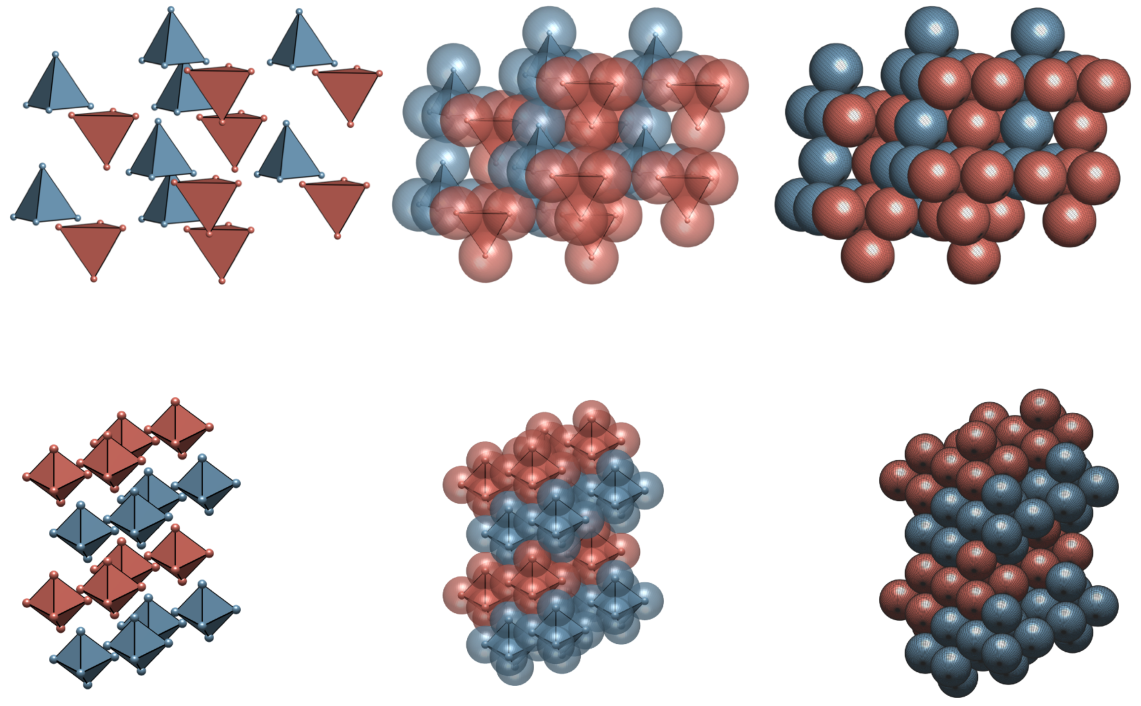

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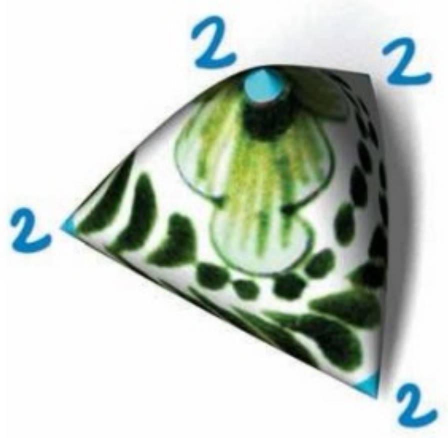

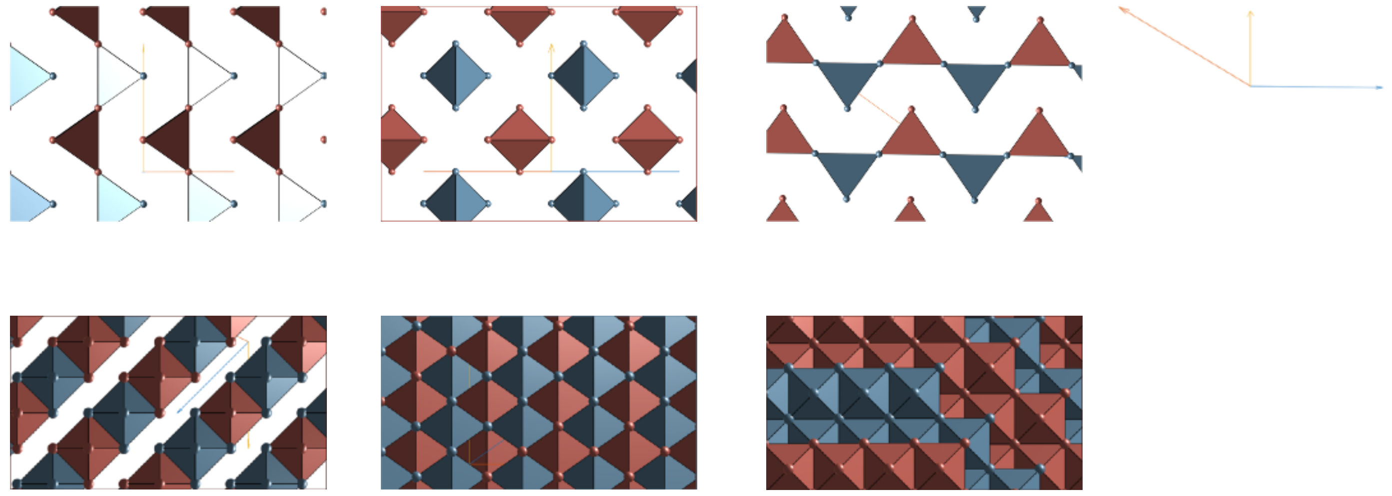

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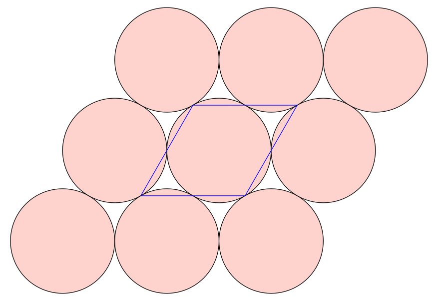

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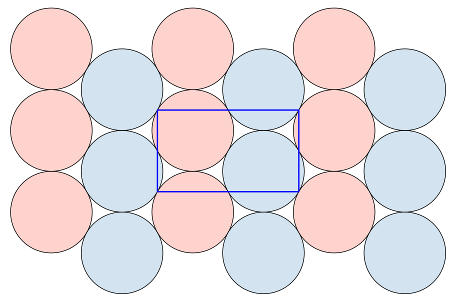

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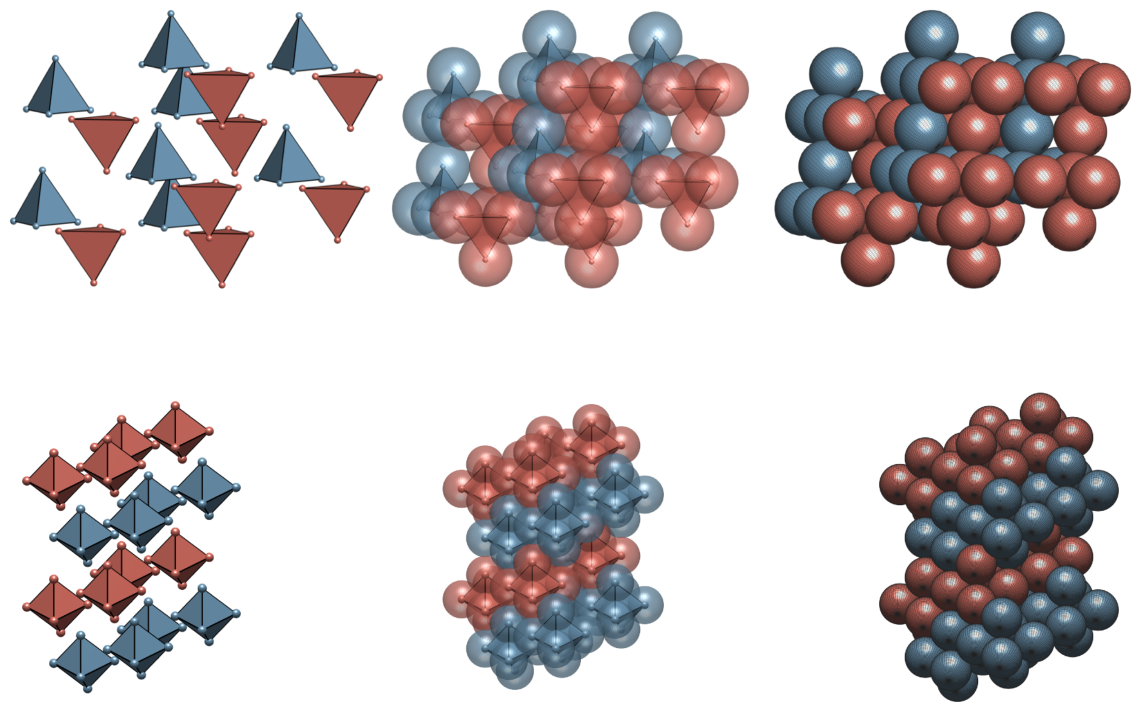

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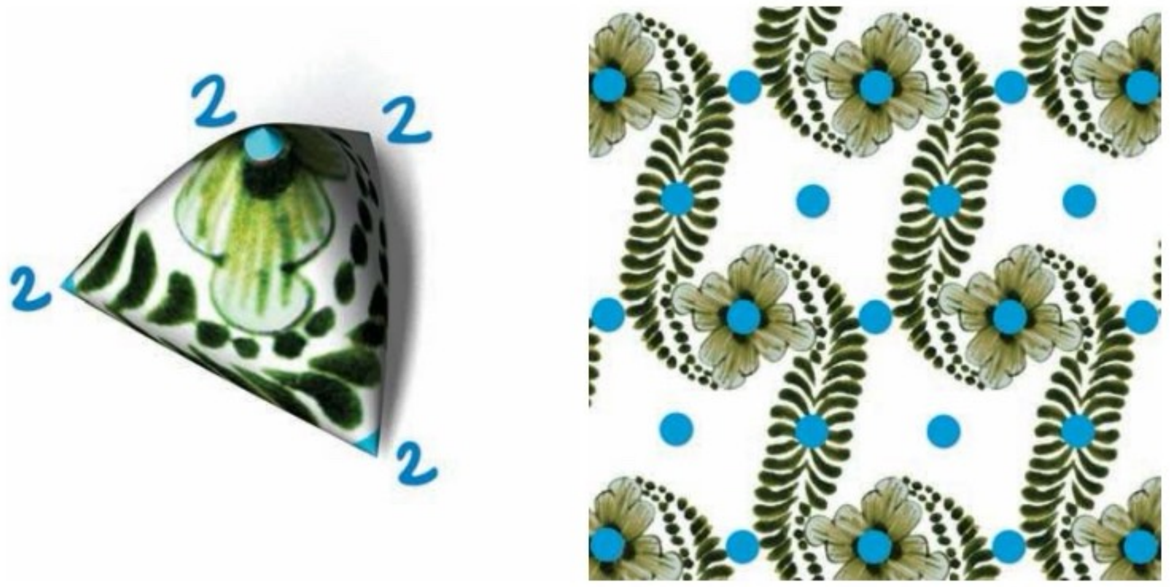

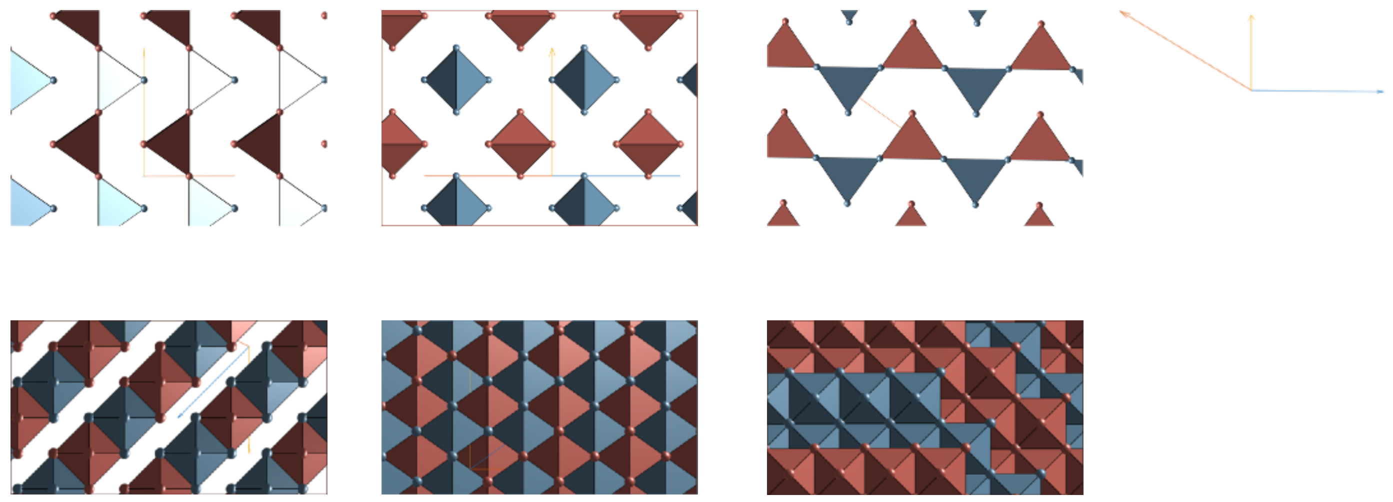

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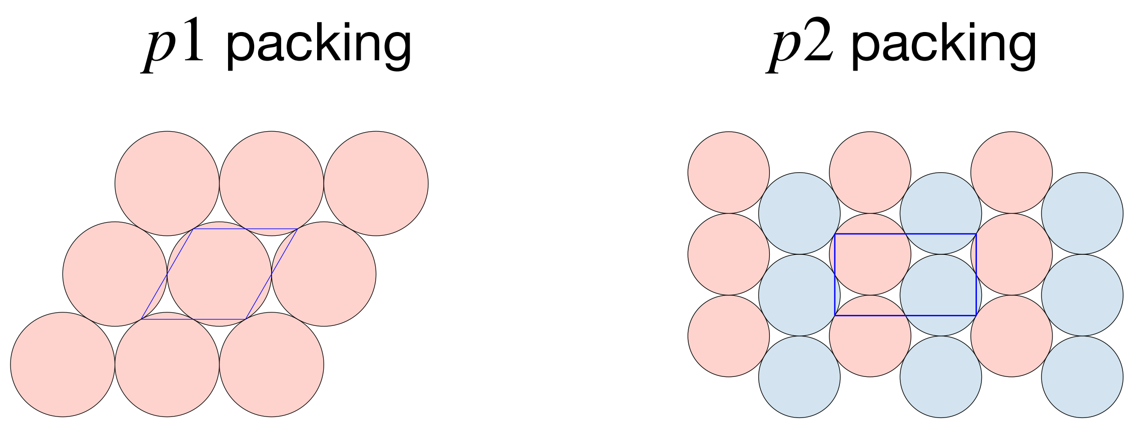

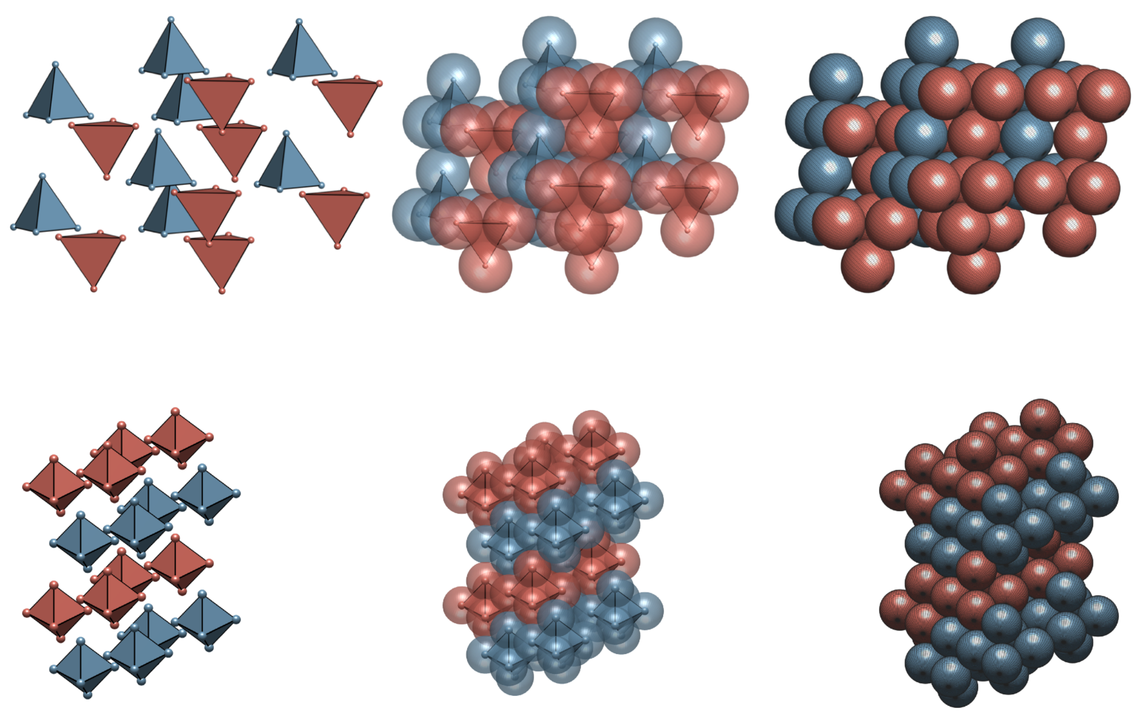

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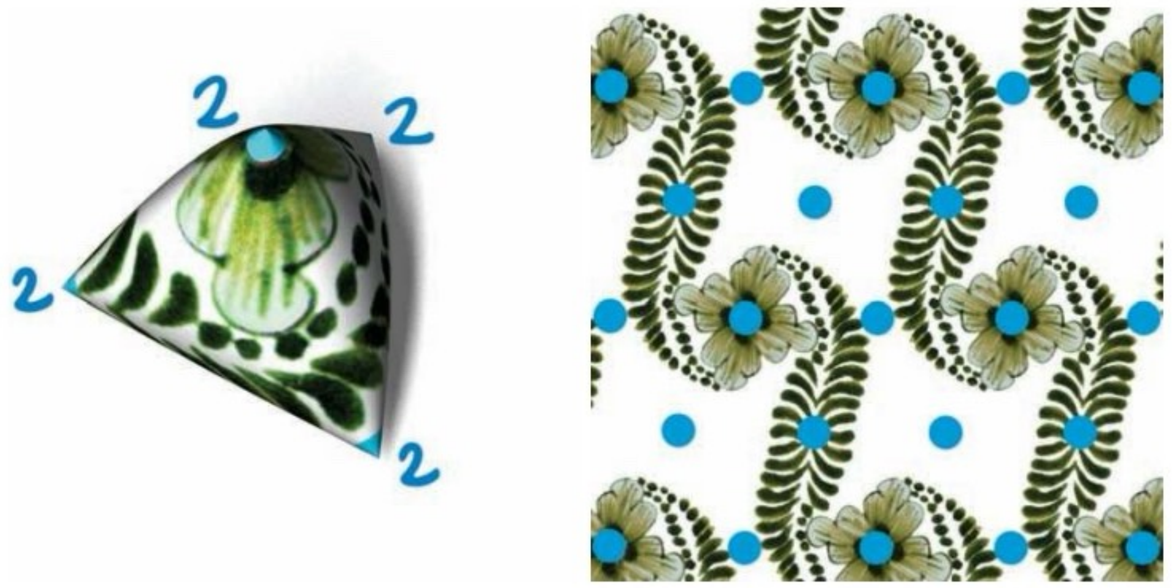

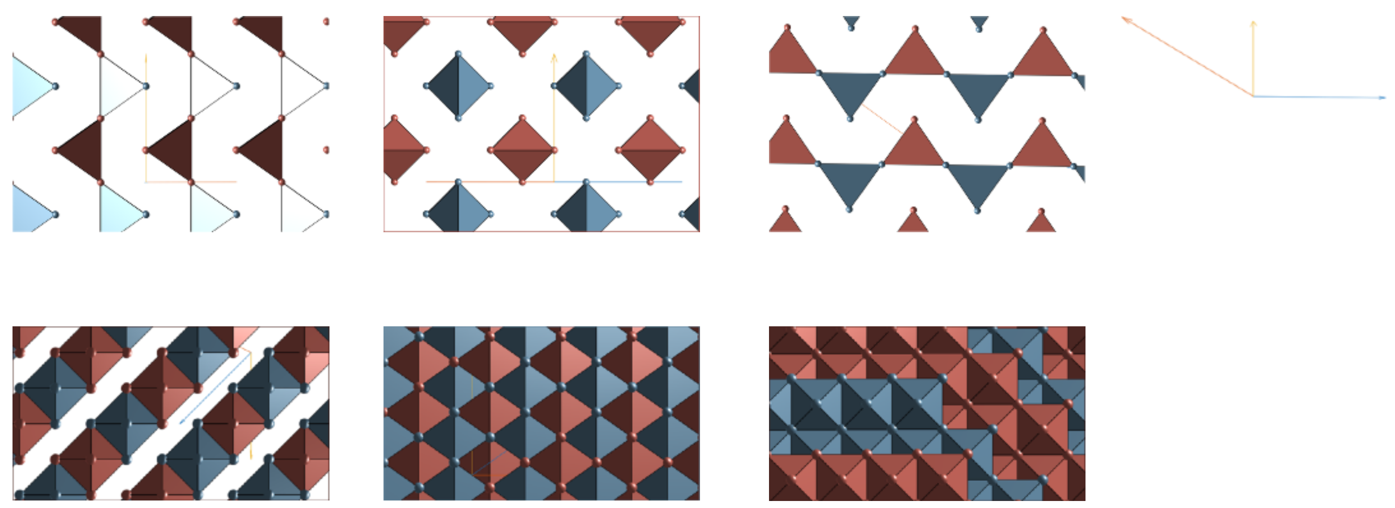

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Closest-Packed Space Groups

- Experimental analysis of symmetries of the densest packings of 34 regular polygons[1]: https://milotorda.net/packings/

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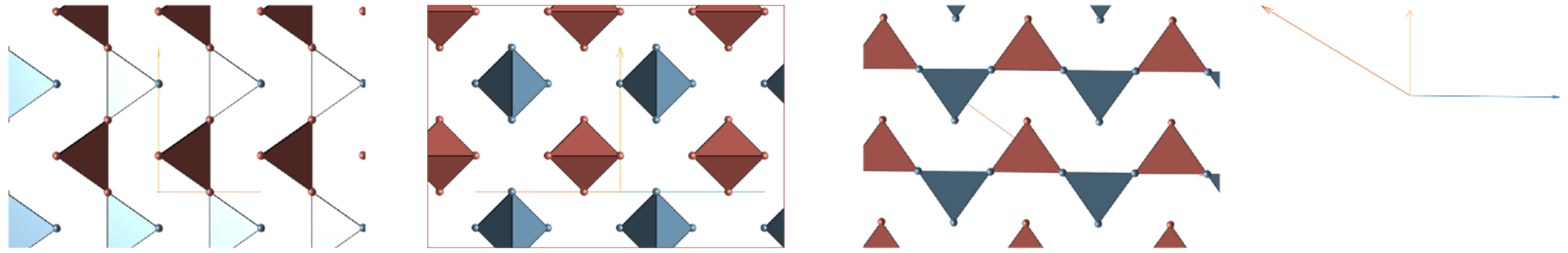
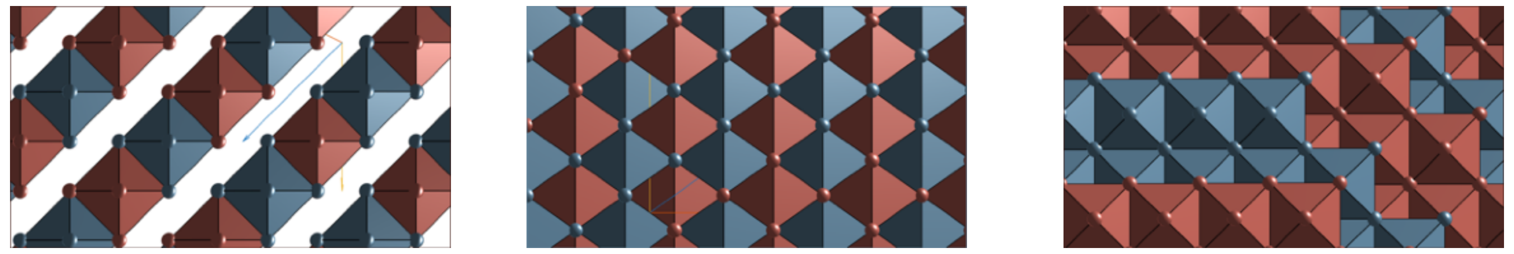
Densities of the densest plane group packings of regular convex n-gons obtained by the Entropic trust region packing algorithm. Each table entry contains a visualization of the packing configuration.

	3-gon	4-gon	5-gon	6-gon	7-gon	8-gon	9-gon	10-gon	11-gon	12-gon	13-gon	14-gon	15-gon	16-gon
p2	0.9999999	0.9999999	0.9213106	0.9999999	0.8926906	0.9061636	0.9010299	0.9137199	0.9076648	0.9282031	0.9043705	0.9074655	0.9047150	0.9090
p2gg	0.9999999	0.9999999	0.9213106	0.9999999	0.8926906	0.9061636	0.8998911	0.9137199	0.9076648	0.9282032	0.9043705	0.9074655	0.9040306	0.9090
pg	0.9999999	0.9999999	0.9213106	0.9999999	0.8926906	0.9061636	0.8986068	0.9137199	0.9076648	0.9282032	0.9043705	0.9074655	0.9023533	0.9090
p3	0.6666666	0.7737684	0.8704800	0.9999999	0.8808500	0.8766506	0.8877354	0.8877506	0.8989629	0.9282032	0.9000514	0.8972213	0.9001741	0.8995
p1	0.6666666	0.9999999	0.8172559	0.9999999	0.8501909	0.9061636	0.8877354	0.9137199	0.8891279	0.9282032	0.8938363	0.9074655	0.9001741	0.9090
p2mg	0.9999999	0.9999999	0.8541019	0.8571428	0.8422610	0.8655534	0.8341984	0.8372213	0.8311609	0.8615612	0.8330633	0.8382375	0.8399388	0.8485
cm	0.9999999	0.9999999	0.8541019	0.8571428	0.8422610	0.8655534	0.8341984	0.8372213	0.8279530	0.8615612	0.8321287	0.8382375	0.8399388	0.8485
p4	0.7128127	0.9999999	0.8421137	0.8177689	0.8421945	0.8503106	0.8303053	0.8300404	0.8378042	0.8615612	0.8369105	0.8352788	0.8376586	0.8461
p4gm	0.6961524	0.9999999	0.7111904	0.7461338	0.7647735	0.8284271	0.7659323	0.7720563	0.7762833	0.8038475	0.7766280	0.7786977	0.7802879	0.7956
c2mm	0.6666666	0.9999999	0.7171403	0.7499999	0.7625321	0.8284271	0.7669742	0.7725424	0.7757096	0.8038475	0.7769742	0.7788232	0.7800620	0.7956
pm	0.4999999	0.9999999	0.6909830	0.7499999	0.7382504	0.8284271	0.7571216	0.7725424	0.7665508	0.8038475	0.7719372	0.7788232	0.7753031	0.7956
p2mm	0.4999999	0.9999999	0.6909830	0.7499999	0.7382504	0.8284271	0.7571216	0.7725424	0.7665508	0.8038475	0.7719372	0.7788232	0.7753031	0.7956
p6	0.9999999	0.7219358	0.7593302	0.8571428	0.7574012	0.7643882	0.7853528	0.7693214	0.7729348	0.7956027	0.7725425	0.7732666	0.7799769	0.7742
p31m	0.7499999	0.6632301	0.7016619	0.7199999	0.7208406	0.7156544	0.7341084	0.7165394	0.7218280	0.7461339	0.7220589	0.7238032	0.7308747	0.7258
p3m1	0.9999999	0.4974226	0.5385407	0.6666666	0.5719655	0.5798083	0.6304149	0.5888775	0.5916426	0.6188021	0.5953579	0.5966415	0.6135979	0.5985
p4mm	0.5773502	0.4999999	0.5553763	0.5214872	0.5144618	0.5685424	0.5244326	0.5331442	0.5424065	0.5358983	0.5414412	0.5360762	0.5338570	0.5460
p6mm	0.4999999	0.4641016	0.4937279	0.4799999	0.4902521	0.4823532	0.4894056	0.4830540	0.4775021	0.4974226	0.4799512	0.4845448	0.4872498	0.4851

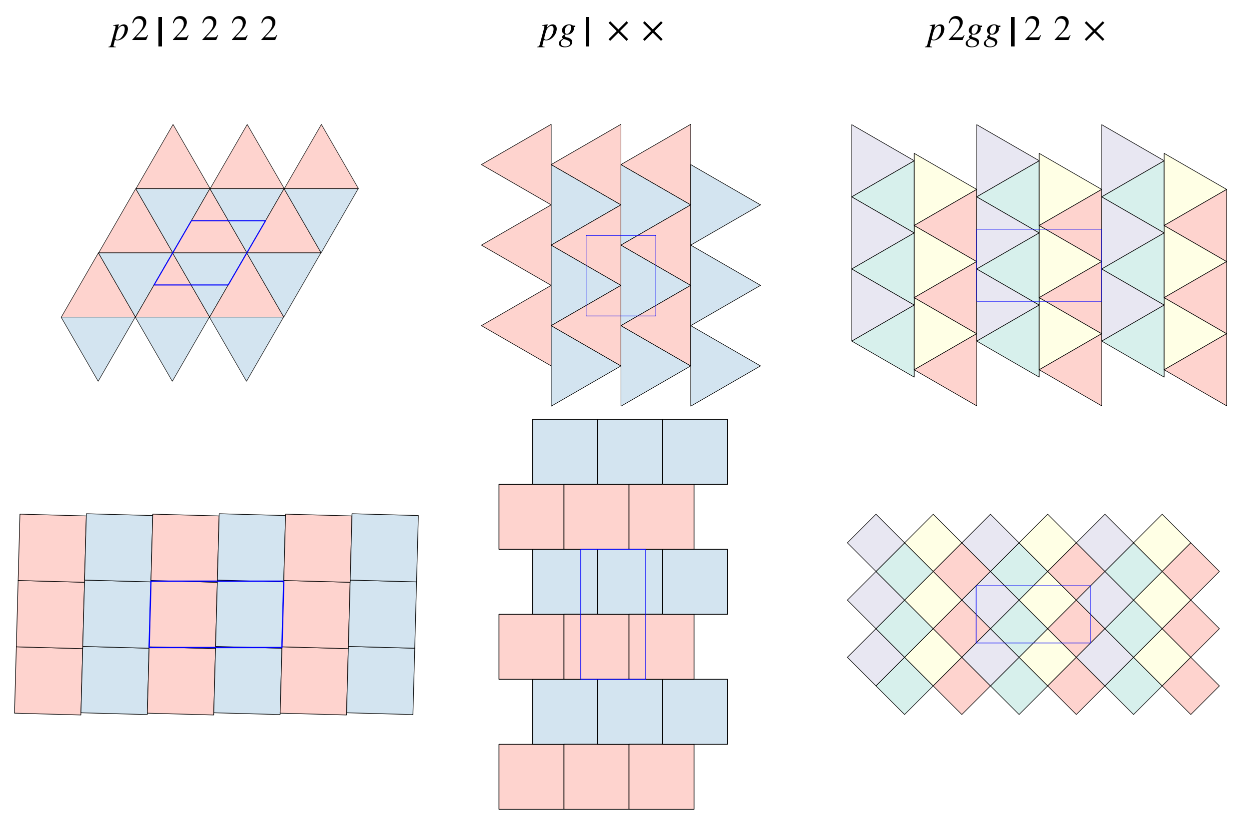


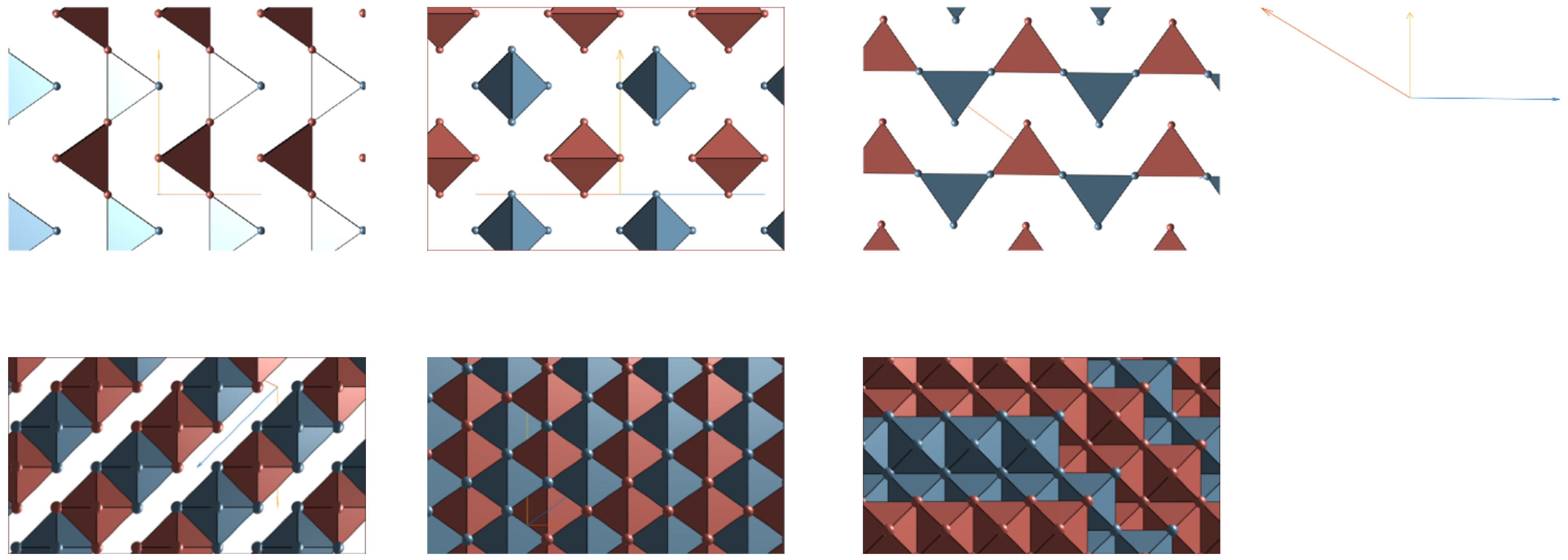


1. M. Torda, J. Y. Goulermas, V. Kurlin and G. M. Day. (2022). Densest plane group packings of regular polygons. *Physical Review E*, *106*(5), 054603.

Closest-Packed Space Groups

- Experimental analysis of symmetries of the densest packings of 34 regular polygons[1]: https://milotorda.net/packings/
  - Regular n-gons attain the maximum packing density in wallpaper groups $p2$, pg and $p2gg$ with orbifold names





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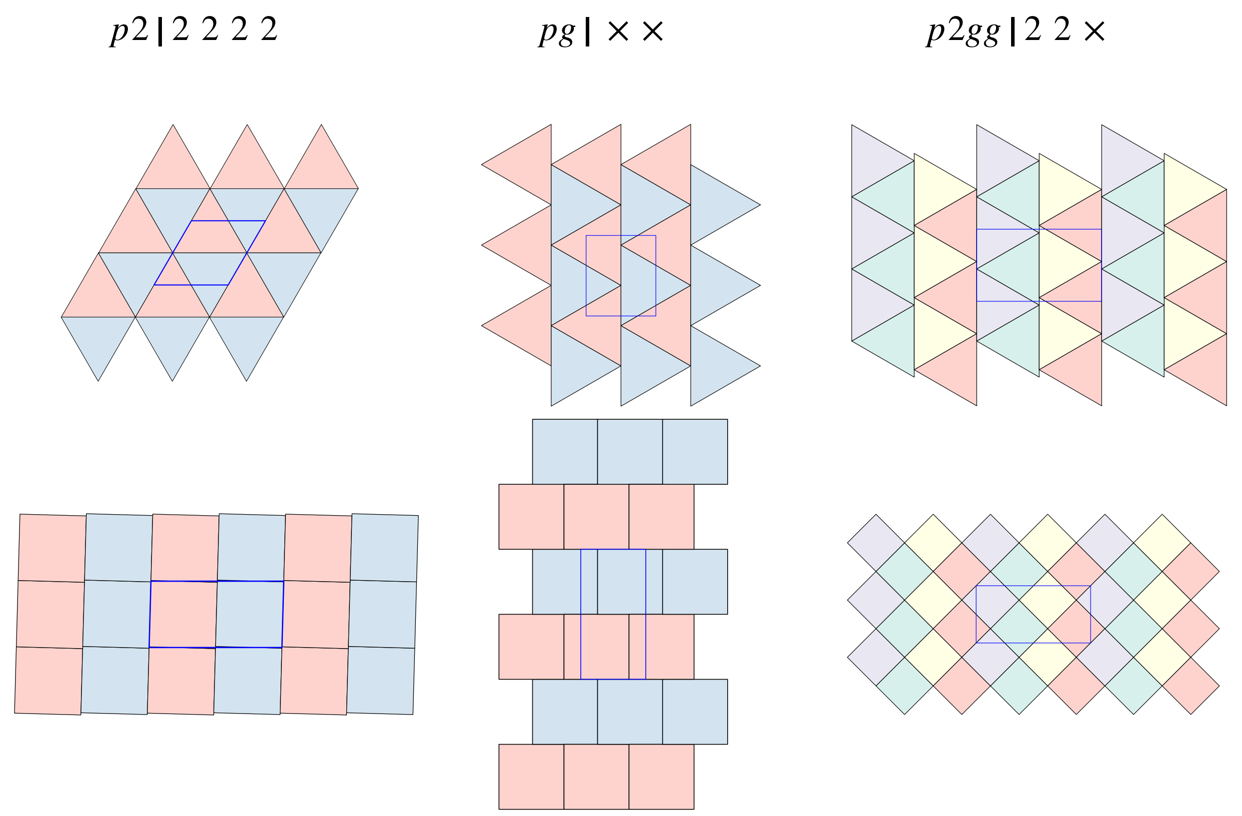

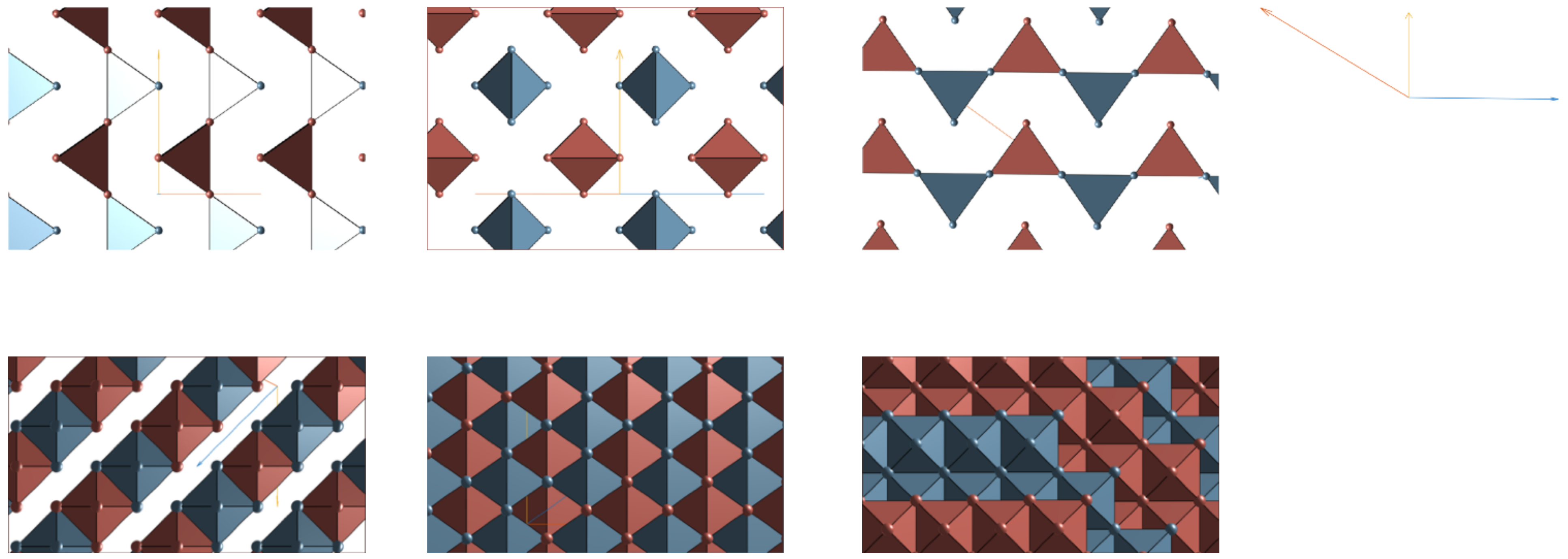

Symmetries of the $P\bar{1}$ | (2 2 2 2) Tetrahedral and Octahedral Molecule Packings							
Closest-Packed Space Groups		**Symmetries of Special Projections**					
H-M	*Fibrifold (primary)*	*H-M*	*Orbifold*	*H-M*	*Orbifold*	*H-M*	*Orbifold*
$P\bar{1}$	(2 2 2 2)	$p2$	2 2 2 2	$p2$	2 2 2 2	$p2$	2 2 2 2
$P2_1$	$(2_1\ 2_1\ 2_1\ 2_1)$	$p2$	2 2 2 2	pg	× ×	pg	× ×
$P2_12_12_1$	$(2_1\ 2_1\ \bar{\times})$	$p2gg$	2 2 ×	$p2gg$	2 2 ×	$p2gg$	2 2 ×

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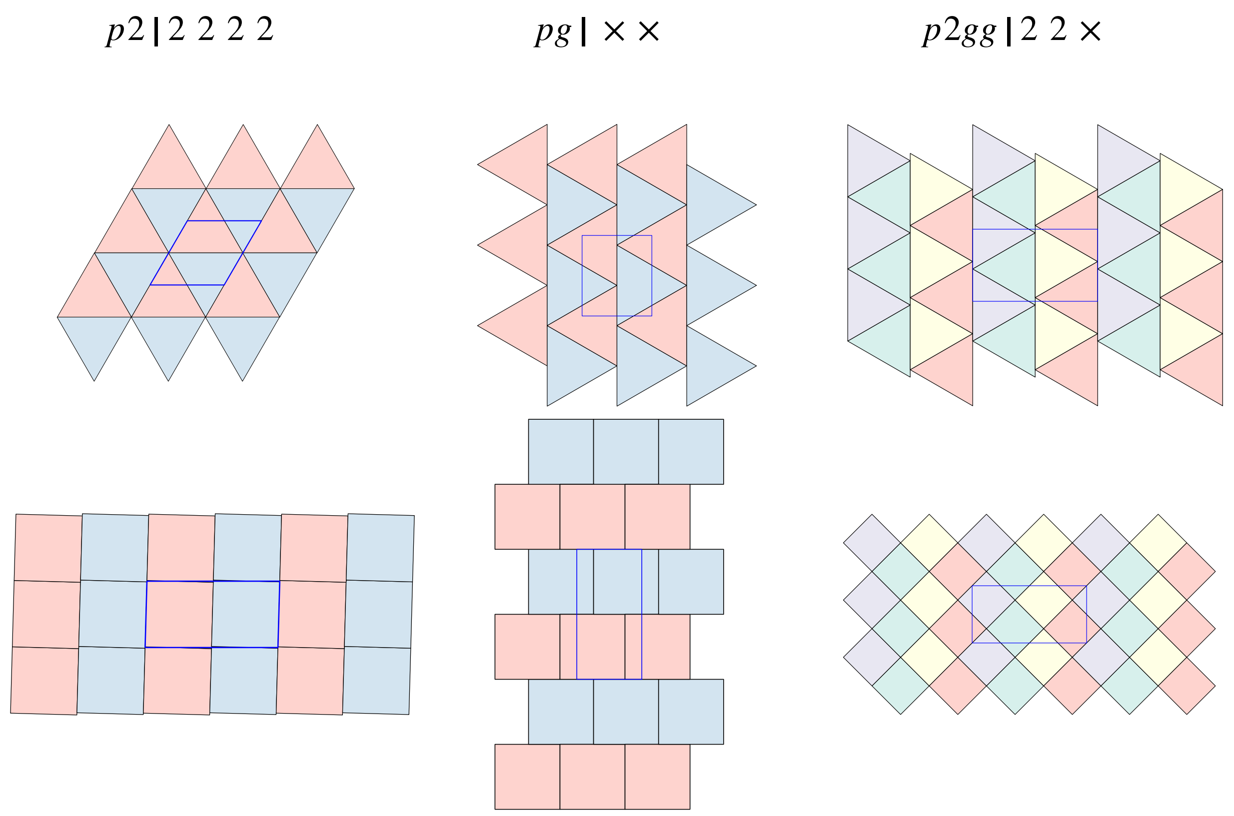
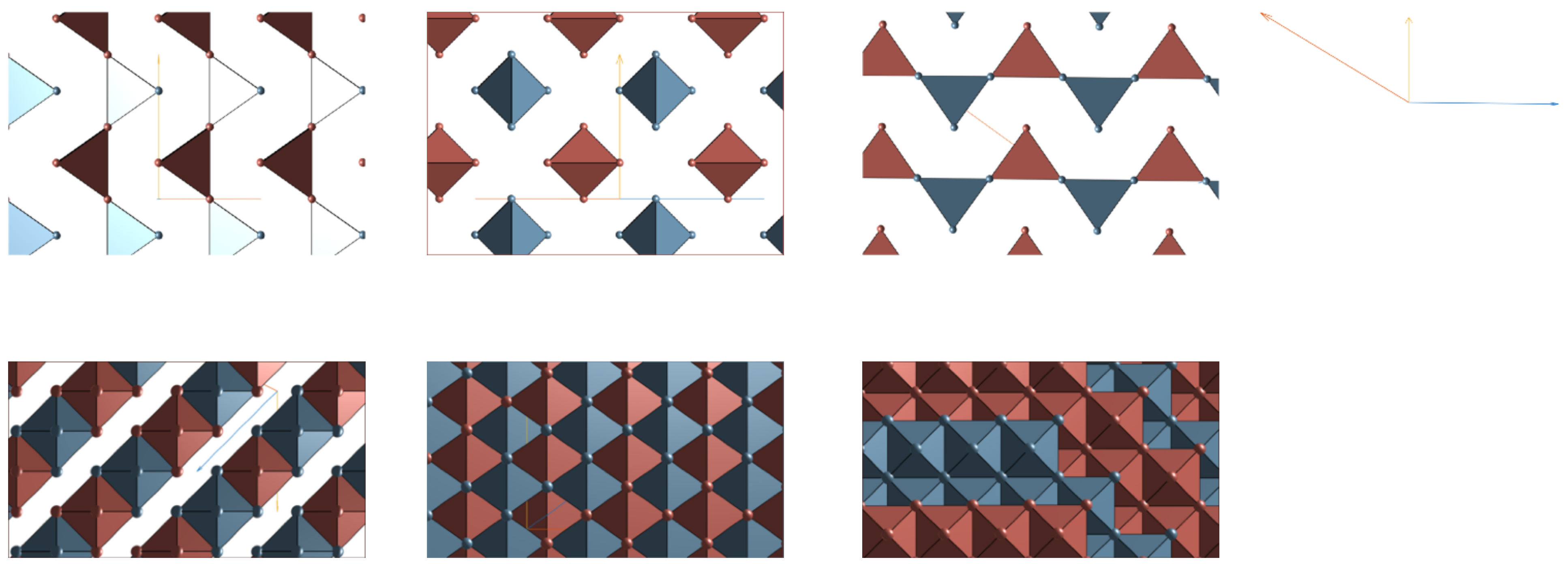
  - Only three space groups having special projections a combination of these three orbifolds
  - Are these the only symmetries of the tetrahedral molecular packing?





Symmetries of the $P\bar{1}$ | (2 2 2 2) Tetrahedral and Octahedral Molecule Packings							
Closest-Packed Space Groups		Symmetries of Special Projections					
H-M	*Fibrifold (primary)*	*H-M*	*Orbifold*	*H-M*	*Orbifold*	*H-M*	*Orbifold*
$P\bar{1}$	(2 2 2 2)	$p2$	2 2 2 2	$p2$	2 2 2 2	$p2$	2 2 2 2
$P2_1$	(2_1 2_1 2_1 2_1)	$p2$	2 2 2 2	pg	× ×	pg	× ×
$P2_12_12_1$	(2_1 2_1 $\bar{\times}$)	$p2gg$	2 2 ×	$p2gg$	2 2 ×	$p2gg$	2 2 ×

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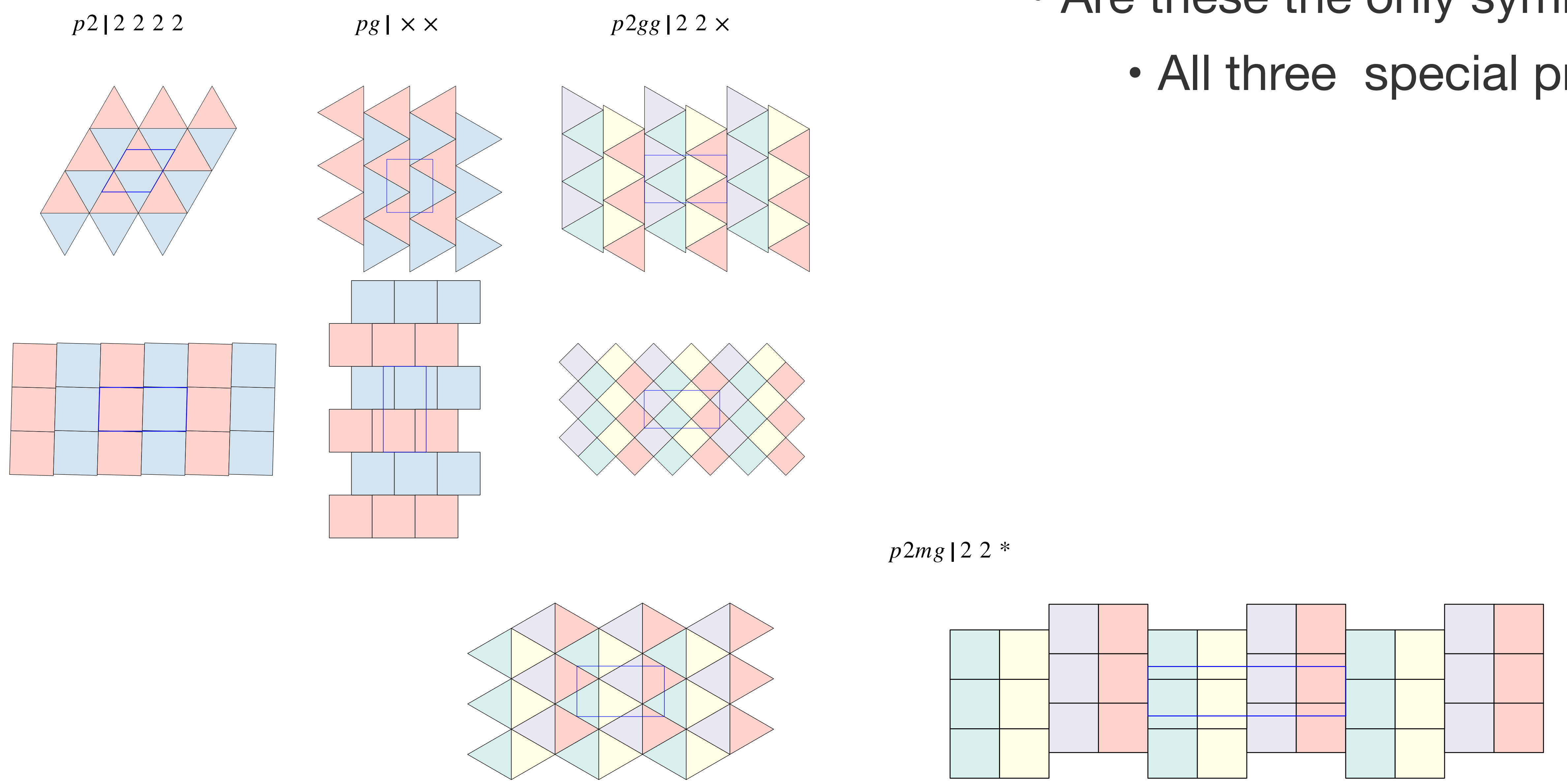
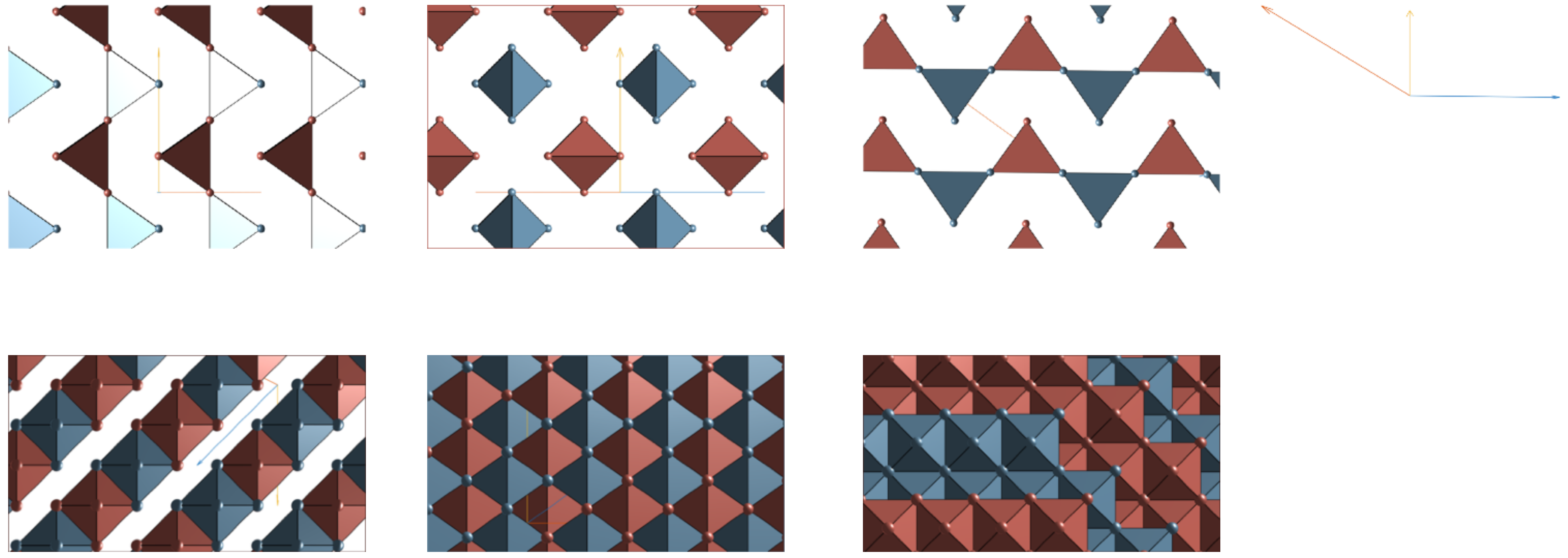
  - All three special projections contain a mirror reflection.





Symmetries of the $P\bar{1} \mid (2\ 2\ 2\ 2)$ Tetrahedral and Octahedral Molecule Packings							
Closest-Packed Space Groups		Symmetries of Special Projections					
H-M	Fibrifold (primary)	H-M	Orbifold	H-M	Orbifold	H-M	Orbifold
$P\bar{1}$	$(2\ 2\ 2\ 2)$	$p2$	$2\ 2\ 2\ 2$	$p2$	$2\ 2\ 2\ 2$	$p2$	$2\ 2\ 2\ 2$
$P2_1$	$(2_1\ 2_1\ 2_1\ 2_1)$	$p2$	$2\ 2\ 2\ 2$	pg	$\times\times$	pg	$\times\times$
$P2_12_12_1$	$(2_1\ 2_1\ \bar{\times})$	$p2gg$	$2\ 2\times$	$p2gg$	$2\ 2\times$	$p2gg$	$2\ 2\times$
$P2_1/c$	$(2_1\ 2_1\ 2\ 2)$	$p2$	$2\ 2\ 2\ 2$	$p2mg$	$2\ 2\ *$	$p2gg$	$2\ 2\times$
$Pbca$	$(2_1\ 2\ \bar{*}\ :)$	$p2mg$	$2\ 2\ *$	$p2mg$	$2\ 2\ *$	$p2mg$	$2\ 2\ *$

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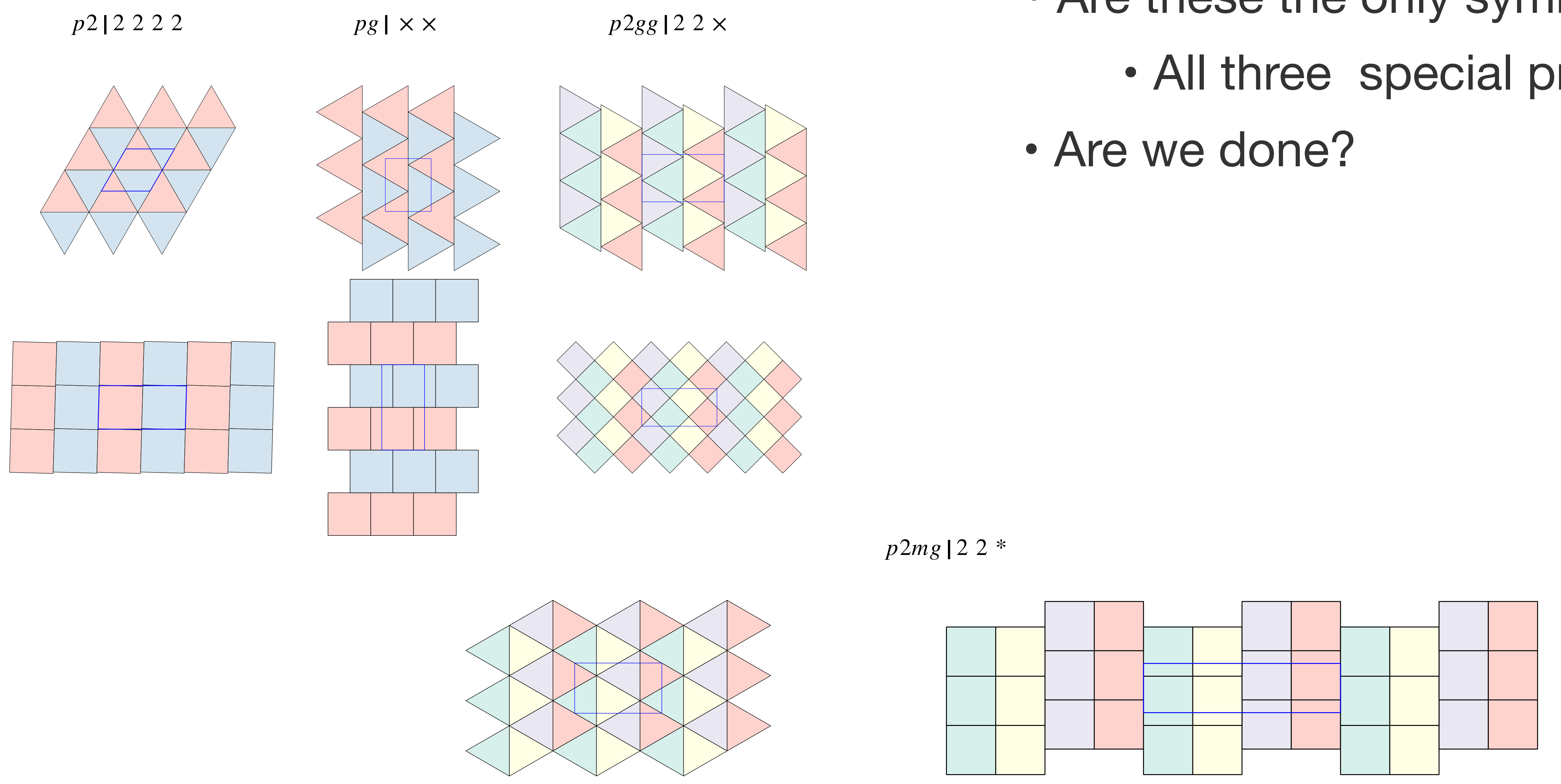
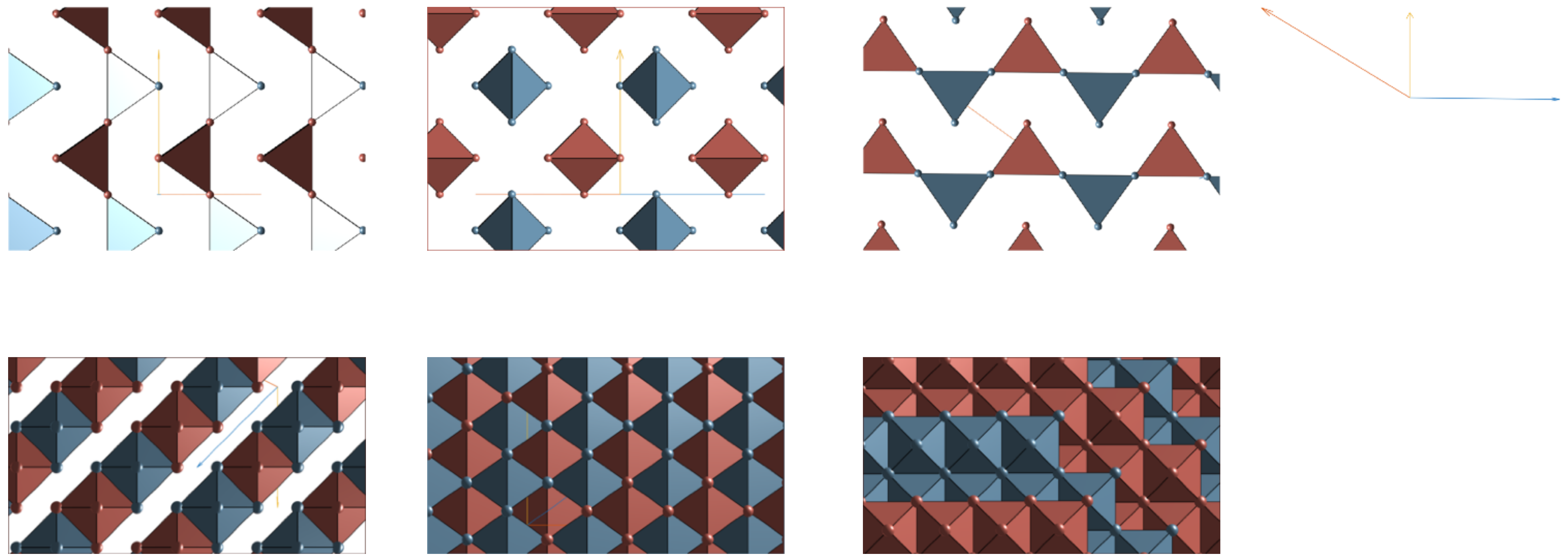


- Are these the only symmetries of the tetrahedral molecular packing?
    - All three special projections contain a mirror reflection.
- Are we done?



Symmetries of the $P\bar{1}\,|\,(2\ 2\ 2\ 2)$ Tetrahedral and Octahedral Molecule Packings							
Closest-Packed Space Groups		Symmetries of Special Projections					
H-M	Fibrifold (primary)	H-M	Orbifold	H-M	Orbifold	H-M	Orbifold
$P\bar{1}$	$(2\ 2\ 2\ 2)$	$p2$	$2\ 2\ 2\ 2$	$p2$	$2\ 2\ 2\ 2$	$p2$	$2\ 2\ 2\ 2$
$P2_1$	$(2_1\ 2_1\ 2_1\ 2_1)$	$p2$	$2\ 2\ 2\ 2$	pg	$\times\times$	pg	$\times\times$
$P2_12_12_1$	$(2_1\ 2_1\ \bar{\times})$	$p2gg$	$2\ 2\times$	$p2gg$	$2\ 2\times$	$p2gg$	$2\ 2\times$
$P2_1/c$	$(2_1\ 2_1\ 2\ 2)$	$p2$	$2\ 2\ 2\ 2$	$p2mg$	$2\ 2\ *$	$p2gg$	$2\ 2\times$
$Pbca$	$(2_1\ 2\ \bar{*}\ :)$	$p2mg$	$2\ 2\ *$	$p2mg$	$2\ 2\ *$	$p2mg$	$2\ 2\ *$

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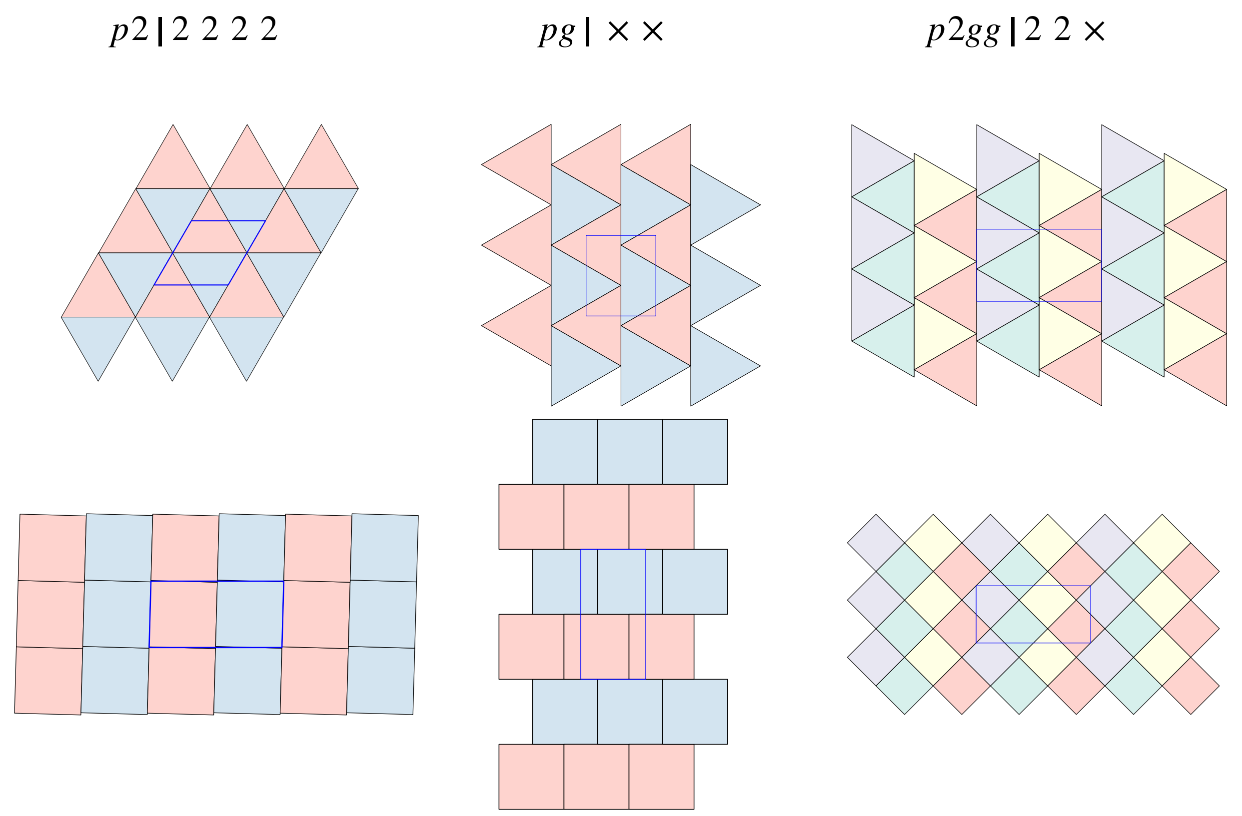

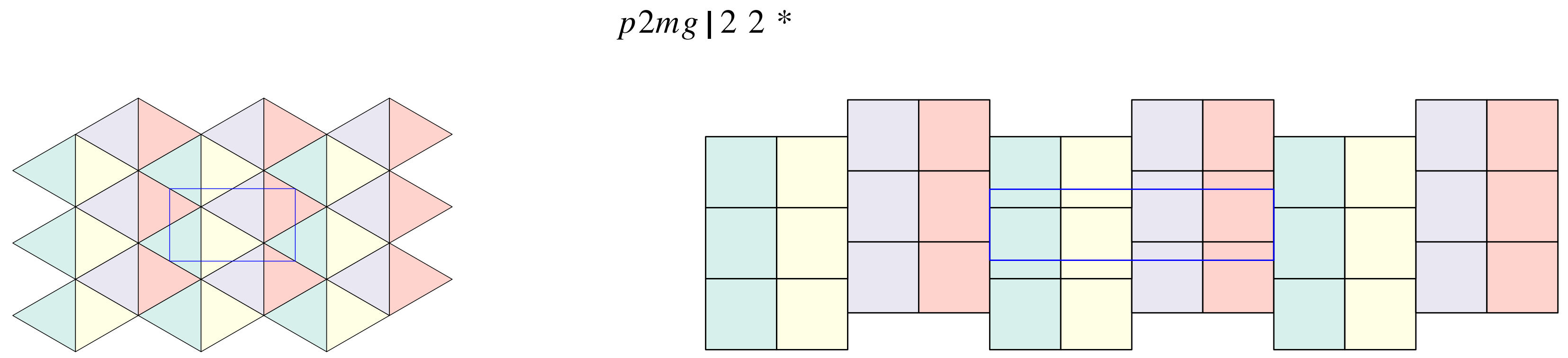

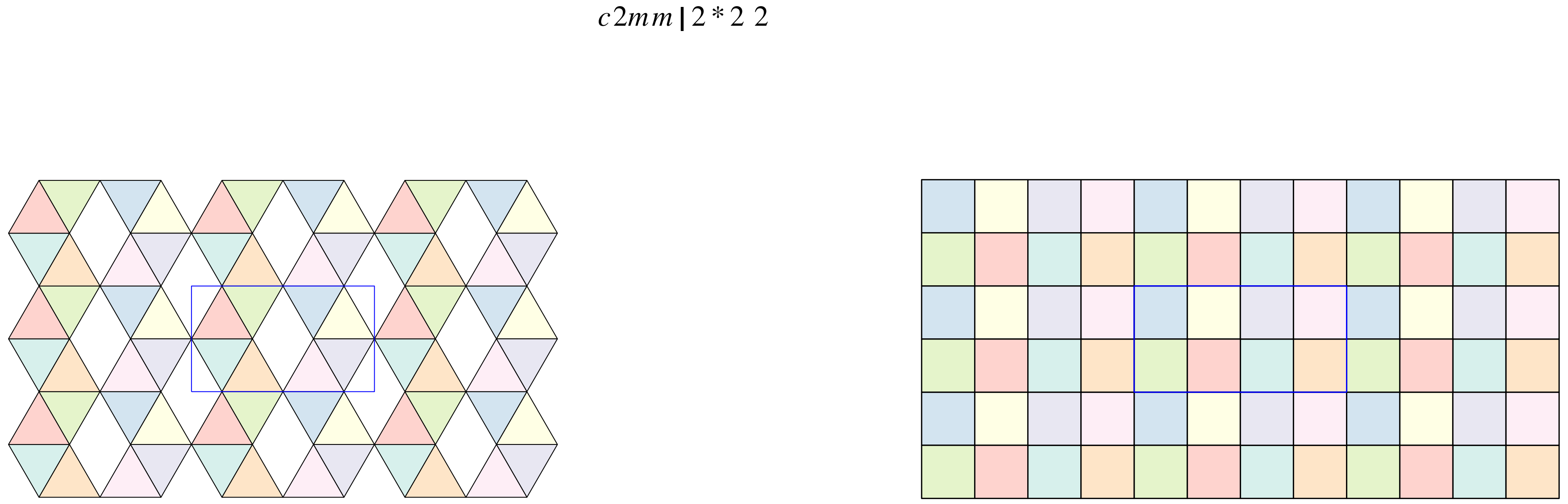

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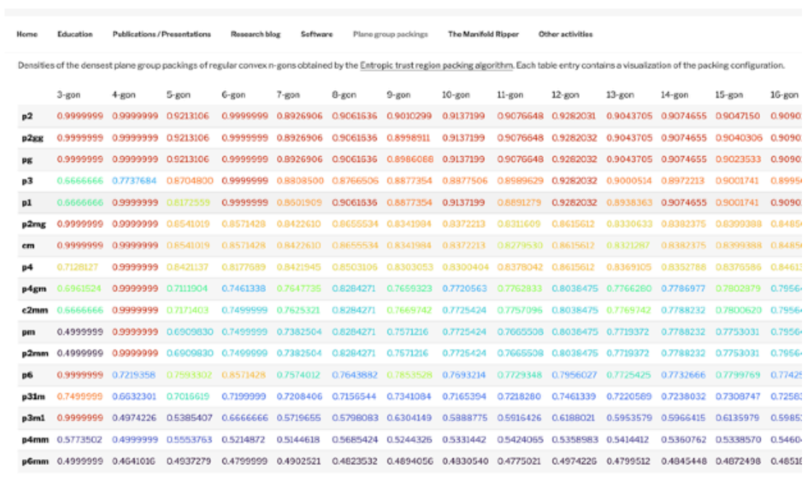

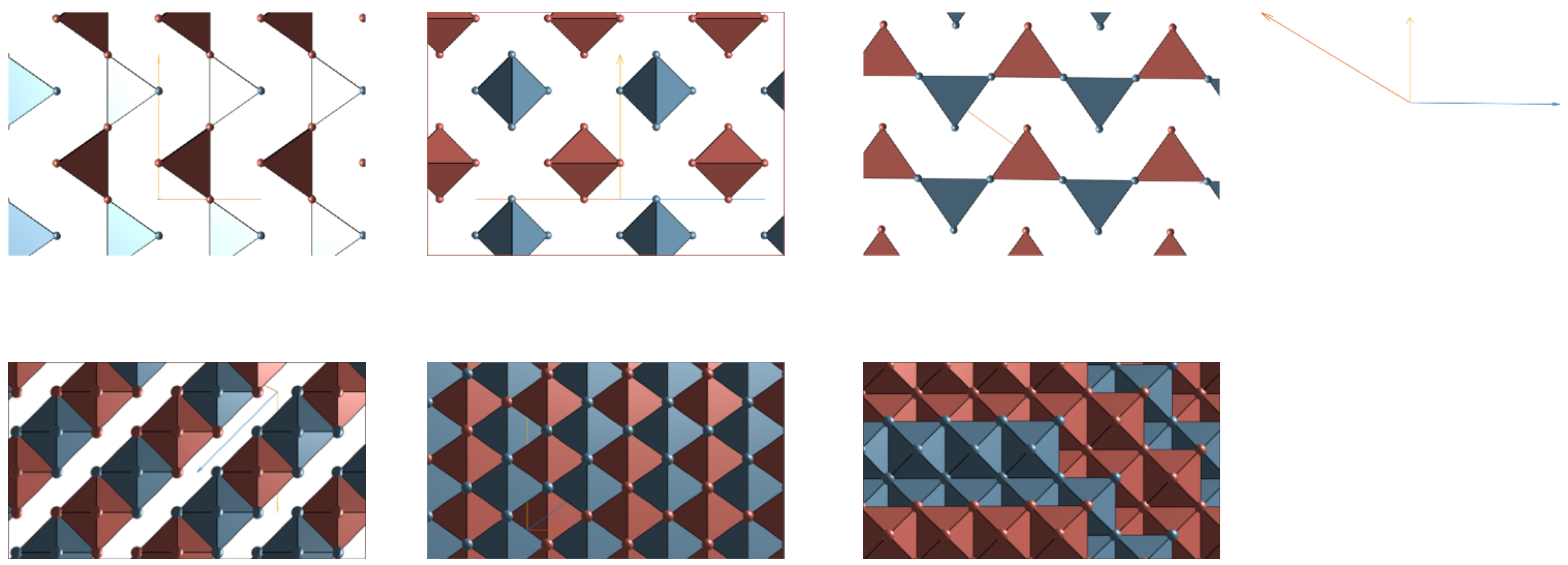

Symmetries of the $P\bar{1}$ | (2 2 2 2) Tetrahedral and Octahedral Molecule Packings							
Closest-Packed Space Groups		Symmetries of Special Projections					
H-M	Fibrifold (primary)	H-M	Orbifold	H-M	Orbifold	H-M	Orbifold
$P\bar{1}$	(2 2 2 2)	$p2$	2 2 2 2	$p2$	2 2 2 2	$p2$	2 2 2 2
$P2_1$	$(2_1\ 2_1\ 2_1\ 2_1)$	$p2$	2 2 2 2	pg	× ×	pg	× ×
$P2_12_12_1$	$(2_1\ 2_1\ \bar{\times})$	$p2gg$	2 2 ×	$p2gg$	2 2 ×	$p2gg$	2 2 ×
$P2_1/c$	$(2_1\ 2_1\ 2\ 2)$	$p2$	2 2 2 2	$p2mg$	2 2 *	$p2gg$	2 2 ×
$Pbca$	$(2_1\ 2\ \bar{*}\ :)$	$p2mg$	2 2 *	$p2mg$	2 2 *	$p2mg$	2 2 *
$C2/c$	$(2_0\ 2_1\ 2\ 2)$	$p2$	2 2 2 2	$c2mm$	2 * 2 2	$p2mg$	2 2 *

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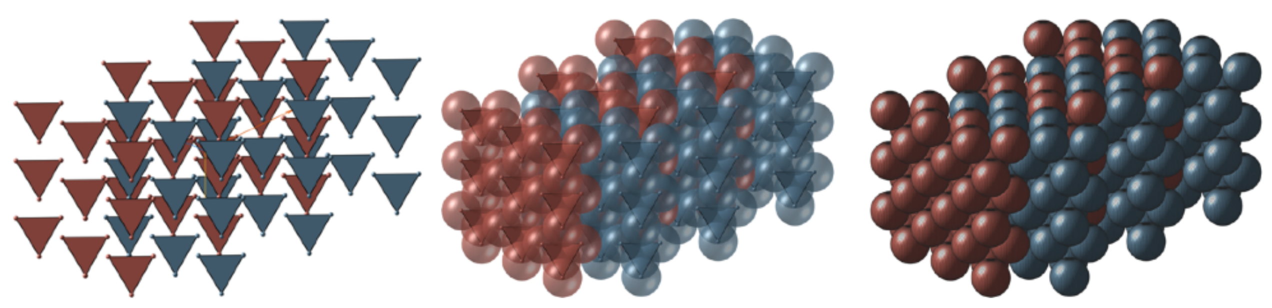
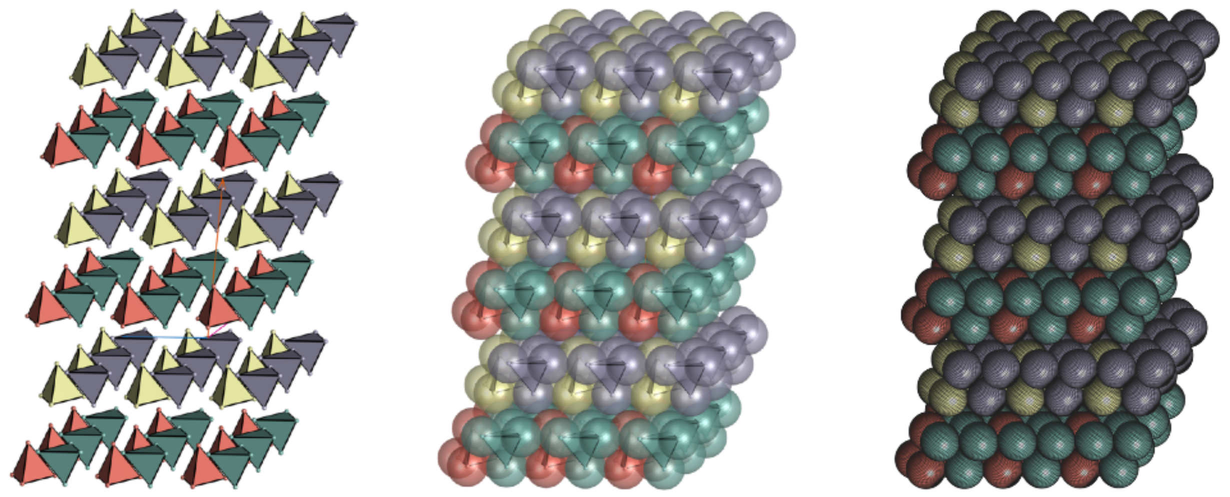
Densest $P2_1$, $P2_1/c$, $C2/c$, $P2_12_12_1$ and $Pbca$ Tetrahedral Molecule Packings

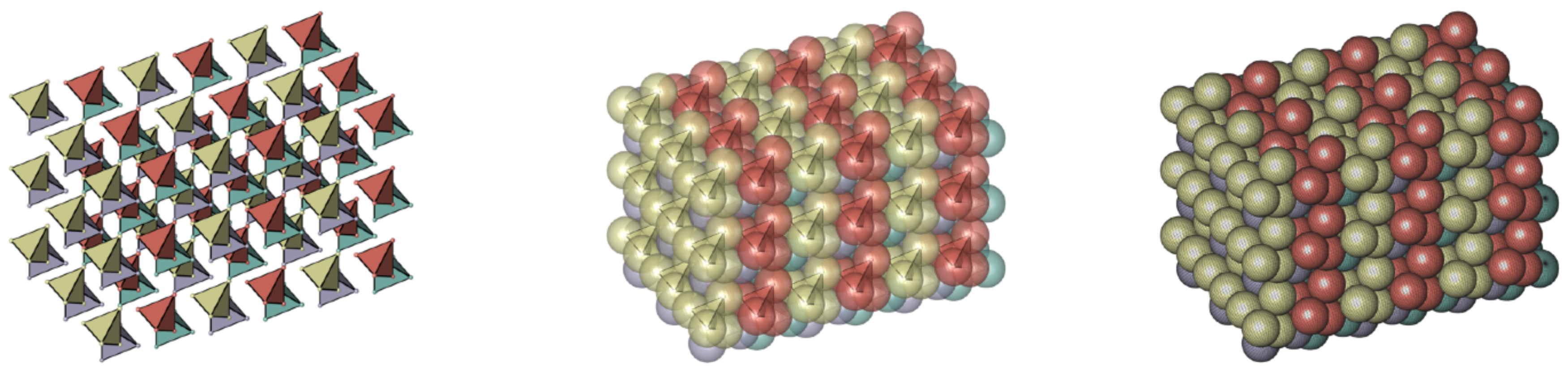
$P2_1 \,|\, (2_1\ 2_1\ 2_1\ 2_1) \,|\, 0.74048... \approx \frac{\pi}{\sqrt{18}}$



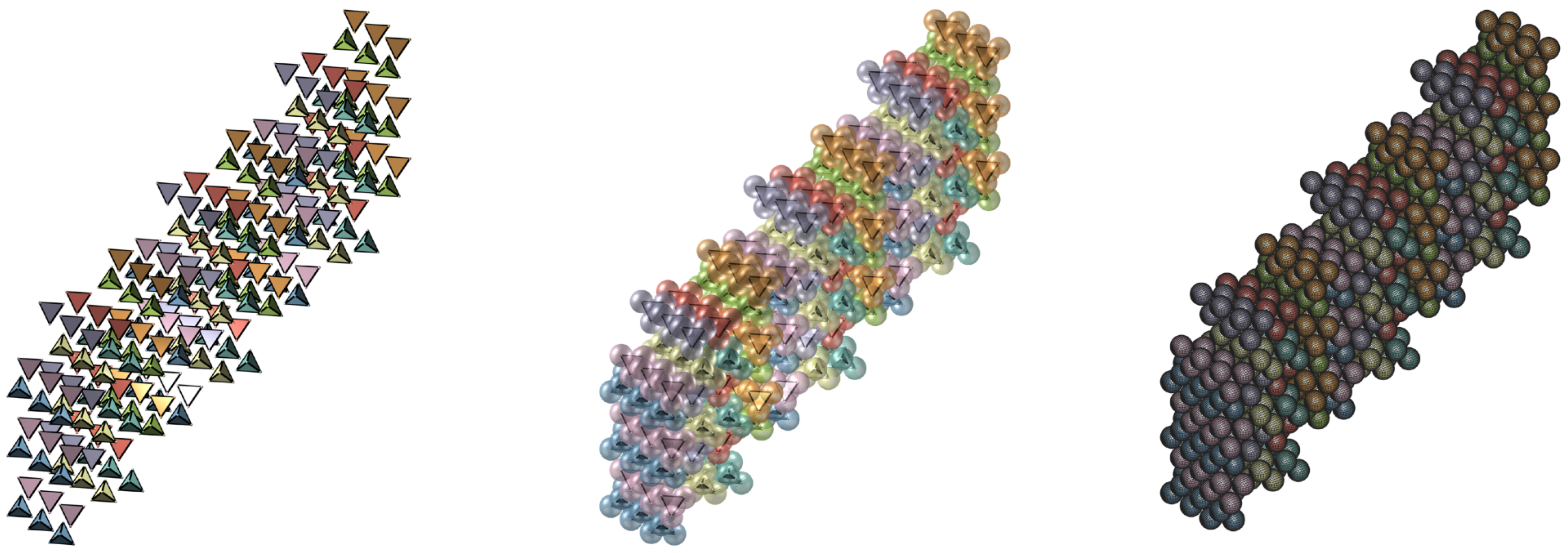
$P2_1/c \,|\, (2_1\ 2_1\ 2\ 2) \,|\, 0.74048... \approx \frac{\pi}{\sqrt{18}}$



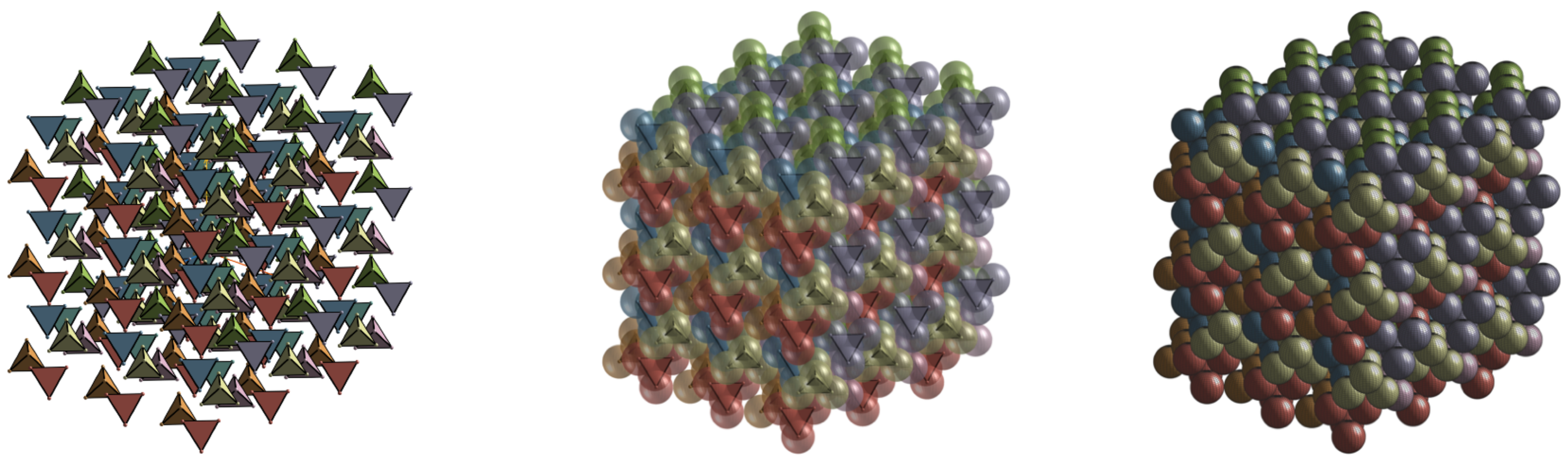
$P2_12_12_1 \,|\, (2_1\ 2_1\ \bar{\times}) \,|\, 0.74048... \approx \frac{\pi}{\sqrt{18}}$



$C2/c \,|\, (2_0\ 2_1\ 2\ 2) \,|\, 0.74048... \approx \frac{\pi}{\sqrt{18}}$

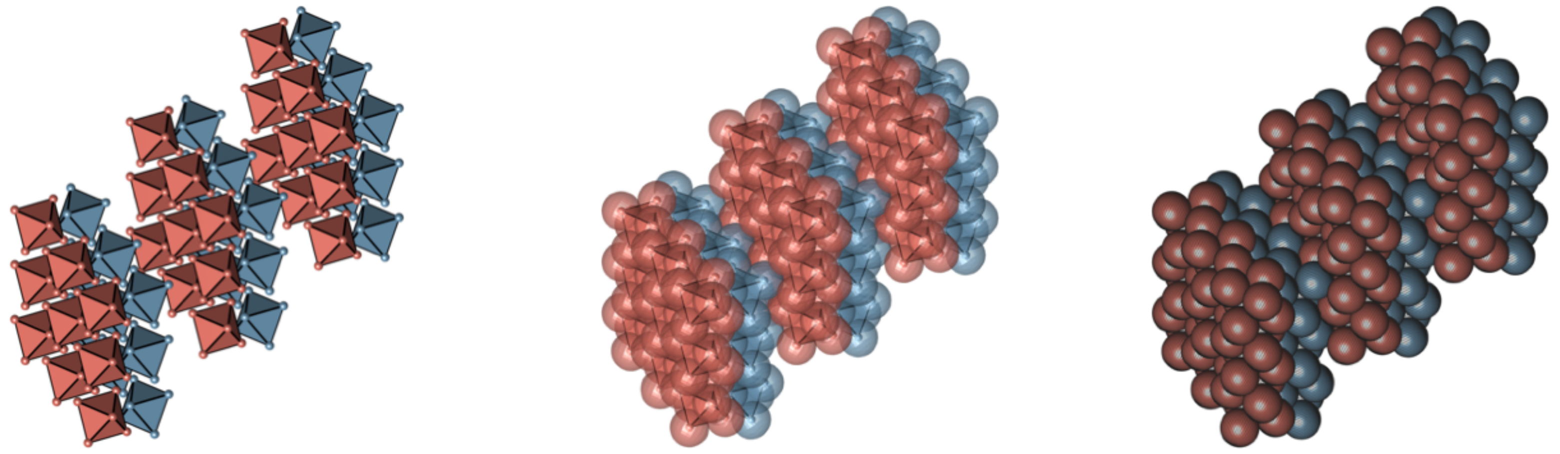


$Pbca \,|\, (2_1\ 2\ \bar{*}\ :) \,|\, 0.74048... \approx \frac{\pi}{\sqrt{18}}$

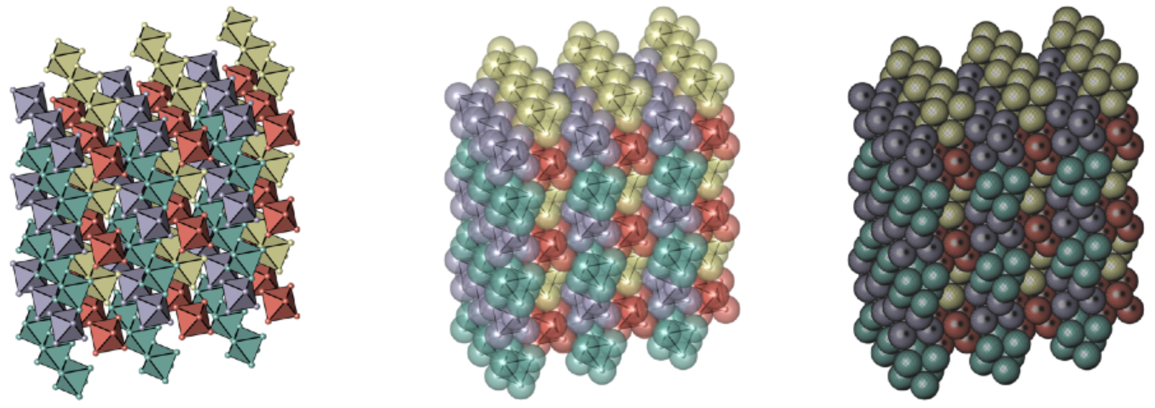


Densest $P2_1$, $P2_1/c$, $C2/c$, $P2_12_12_1$ and $Pbca$ Octahedral Molecule Packings

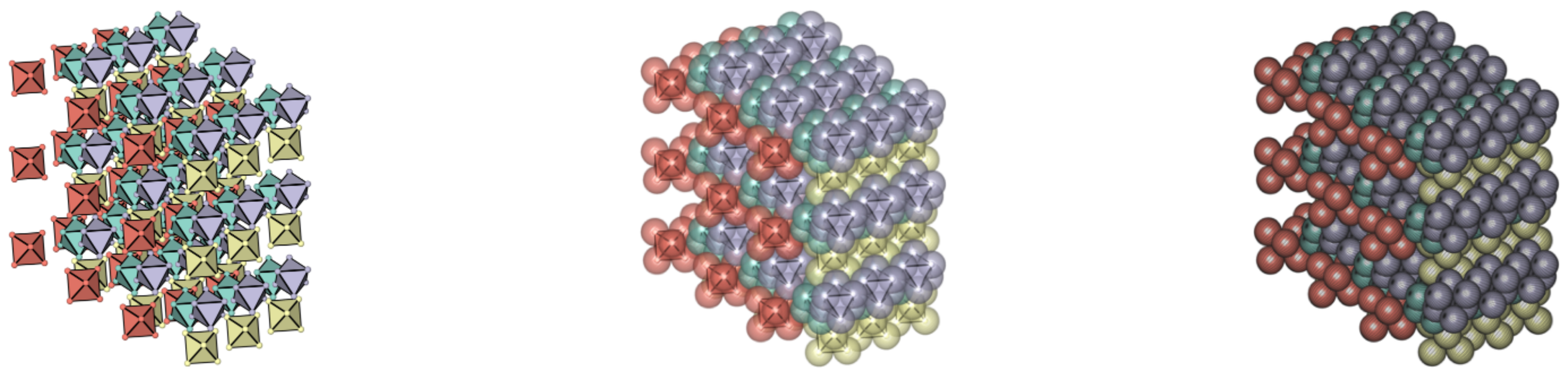
$P2_1 \,|\, (2_1\ 2_1\ 2_1\ 2_1) \,|\, 0.74048\ldots \approx \frac{\pi}{\sqrt{18}}$



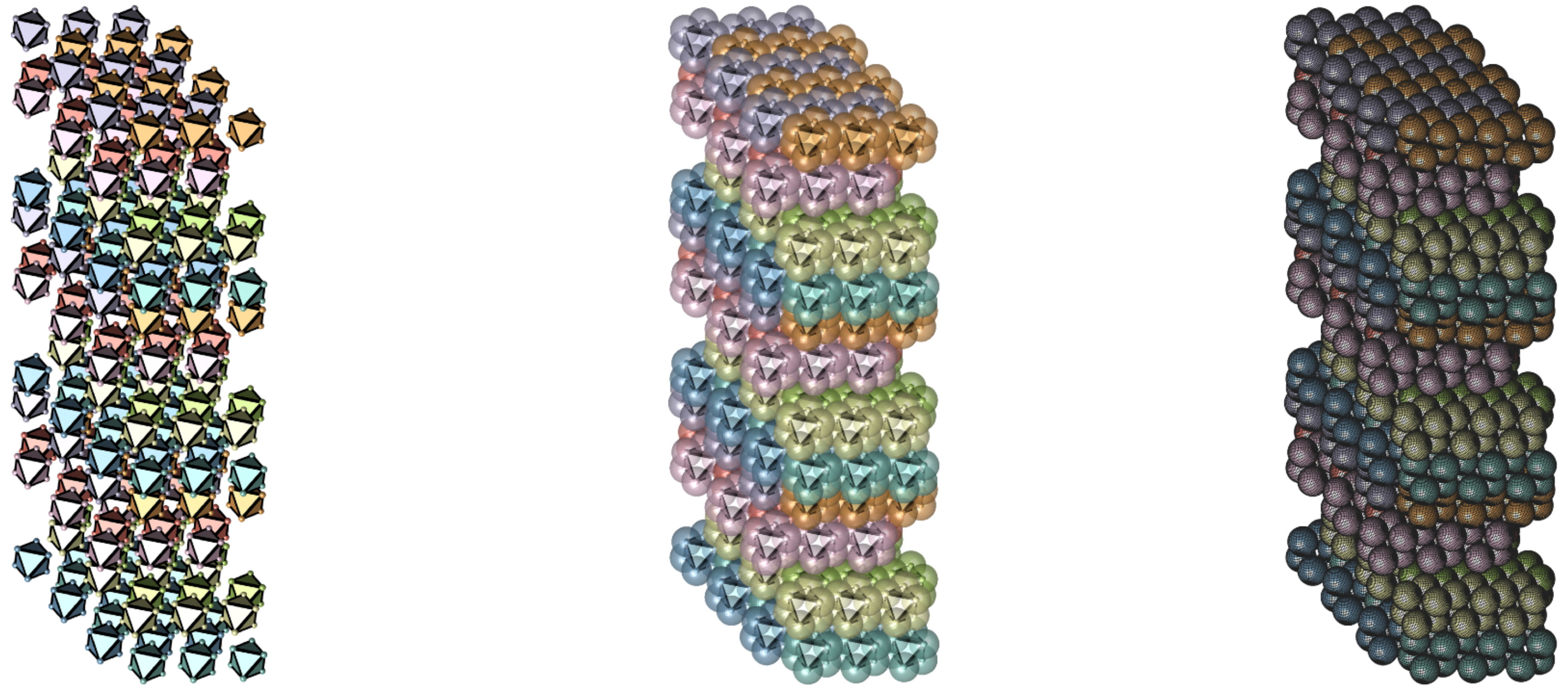
$P2_1/c \,|\, (2_1\ 2_1\ 2\ 2) \,|\, 0.74048\ldots \approx \frac{\pi}{\sqrt{18}}$



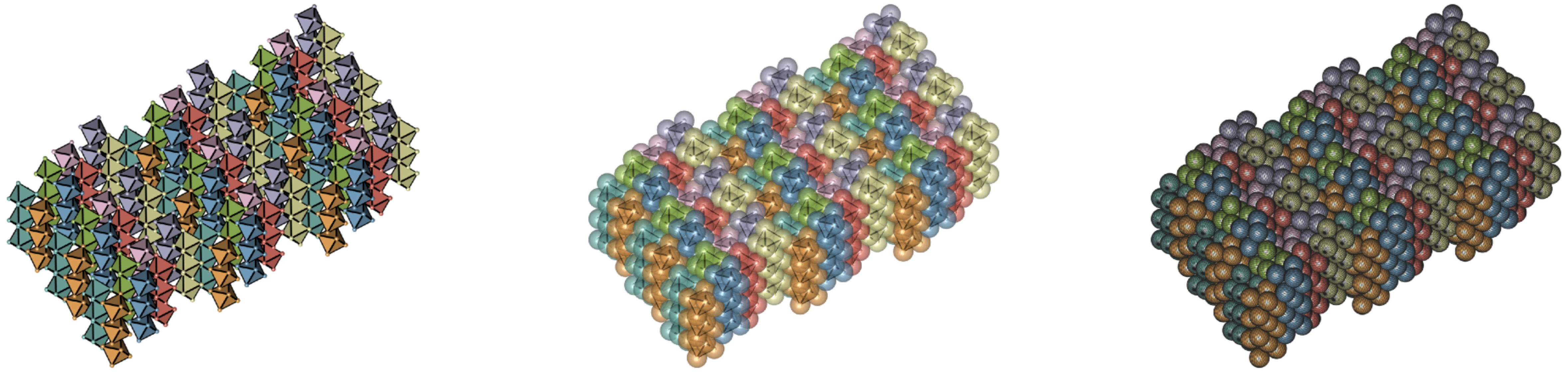
$P2_12_12_1 \,|\, (2_1\ 2_1\ \bar{\times}) \,|\, 0.74048\ldots \approx \frac{\pi}{\sqrt{18}}$



$C2/c \,|\, (2_0\ 2_1\ 2\ 2) \,|\, 0.74048\ldots \approx \frac{\pi}{\sqrt{18}}$

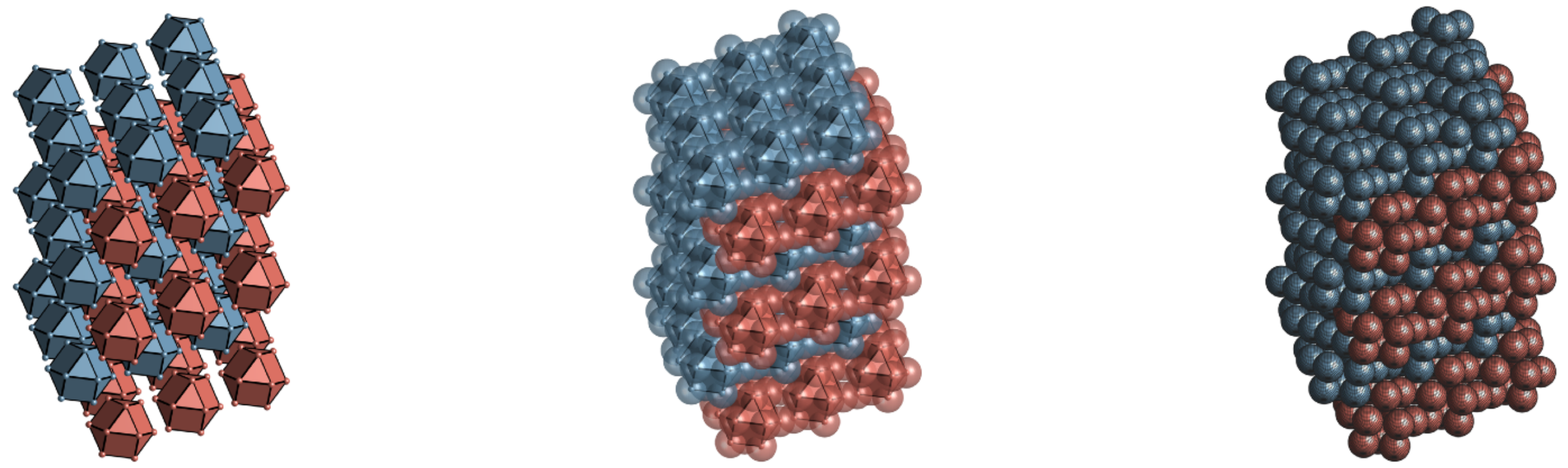


$Pbca \,|\, (2_1\ 2\ \bar{*}\ :) \,|\, 0.74048\ldots \approx \frac{\pi}{\sqrt{18}}$

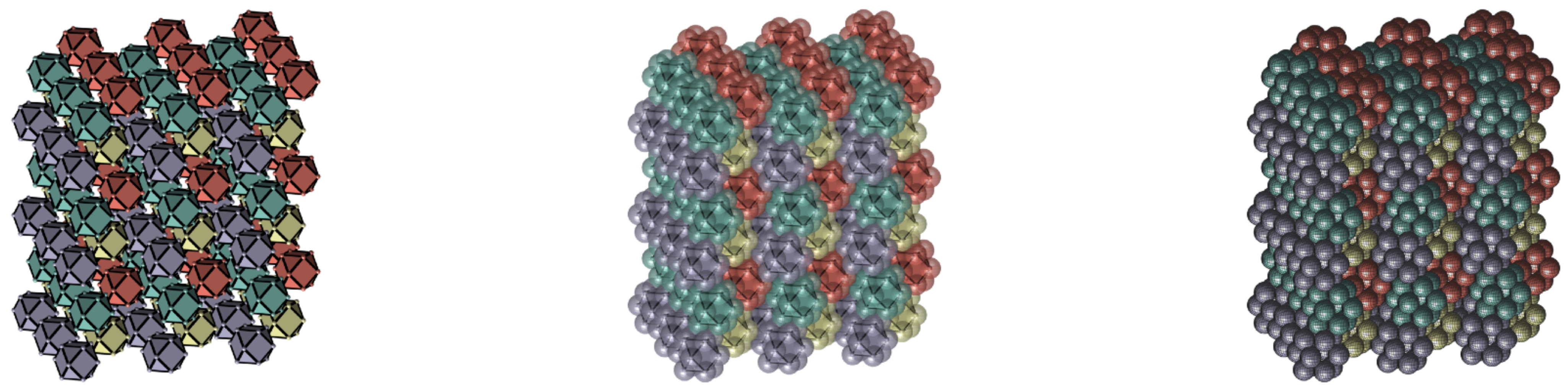


Densest $P\bar{1}$, $P2_1$, $P2_1/c$,$C2/c$,$P2_12_12_1$ and $Pbca$ Cuboctahedral Molecule Packings

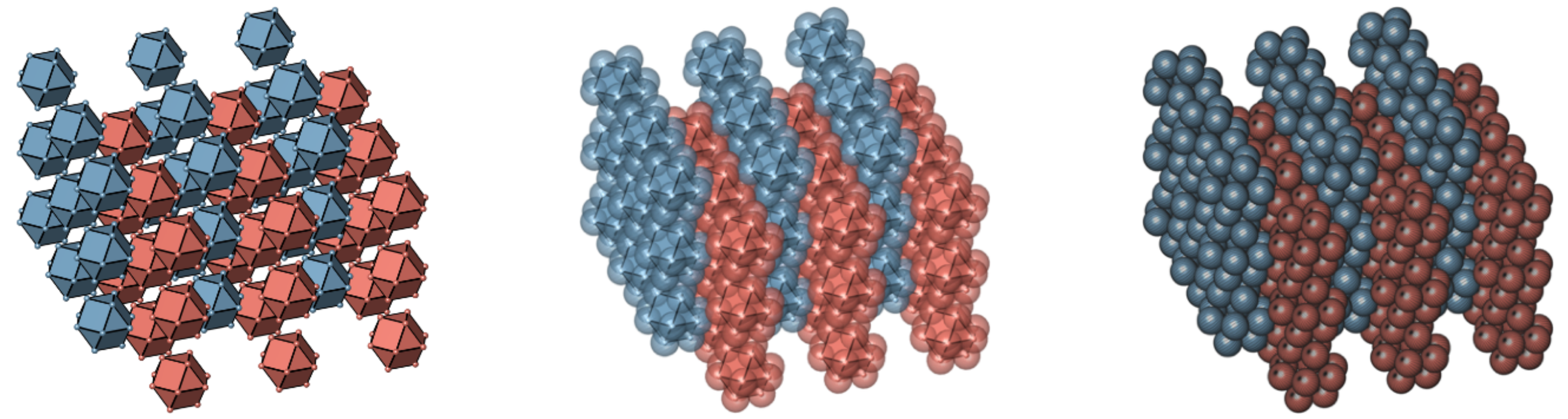
$P\bar{1}\,|\,(2\ 2\ 2\ 2)\,|\,0.68352... \approx \frac{12}{13}\frac{\pi}{\sqrt{18}}$



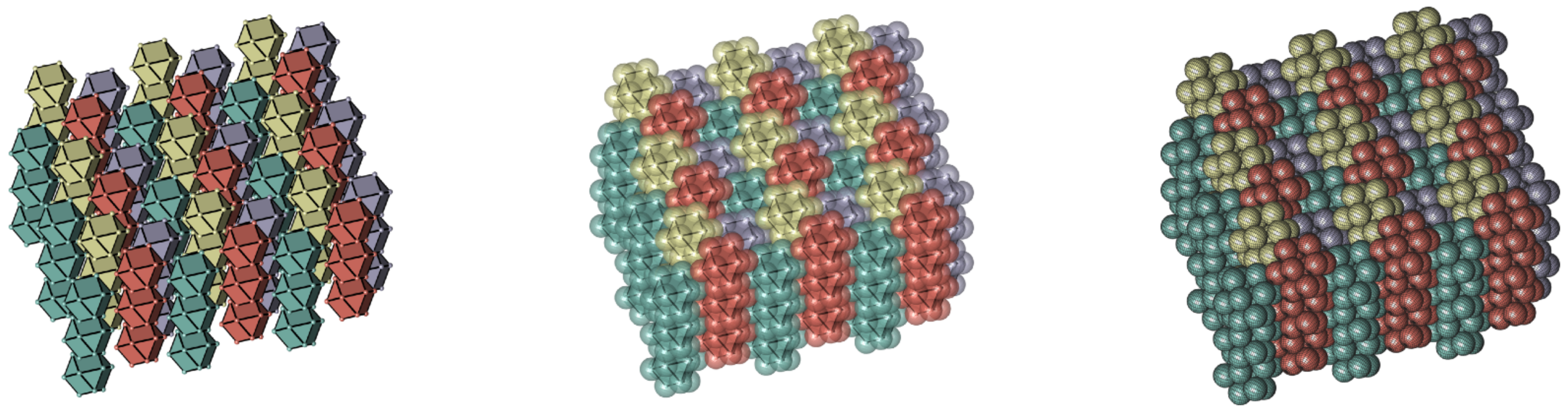
$P2_1/c\,|\,(2_1\ 2_1\ 2\ 2)\,|\,0.65820... \approx \frac{8}{9}\frac{\pi}{\sqrt{18}}$



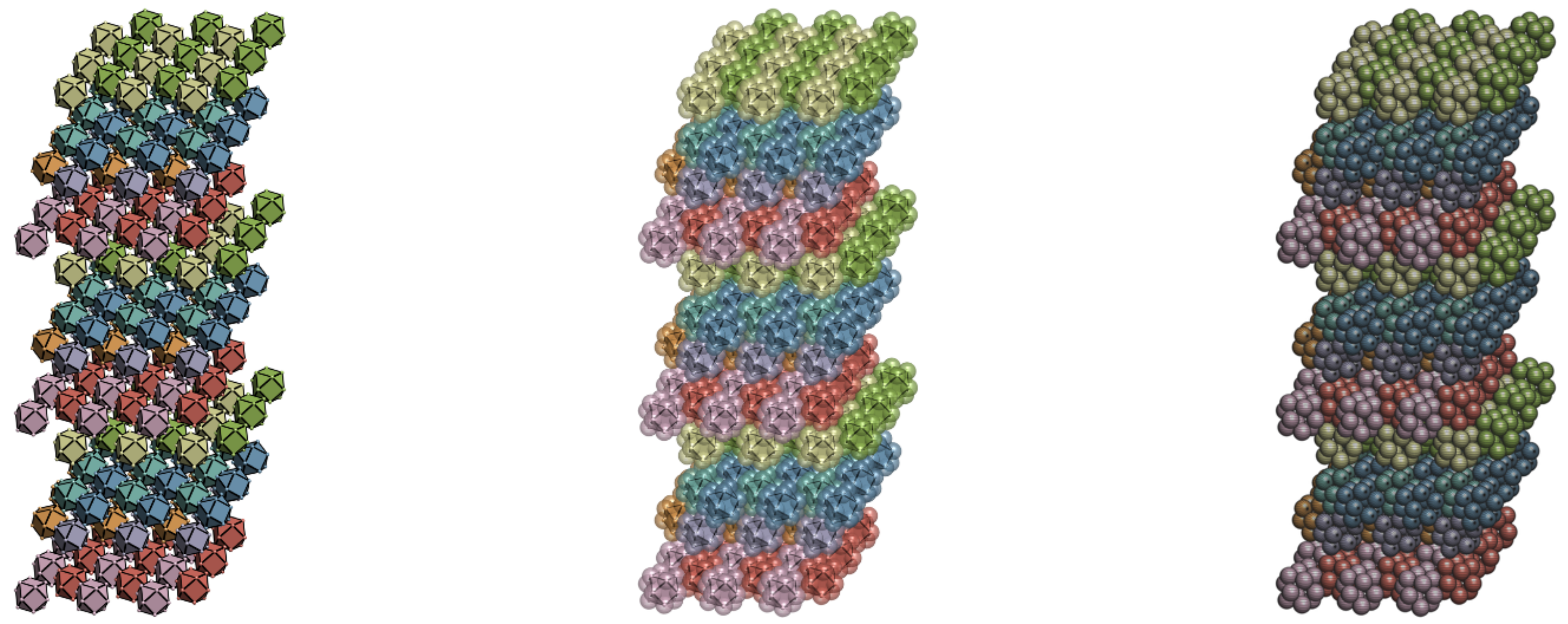
$P2_1\,|\,(2_1\ 2_1\ 2_1\ 2_1)\,|\,0.60584... \approx \frac{9}{11}\frac{\pi}{\sqrt{18}}$



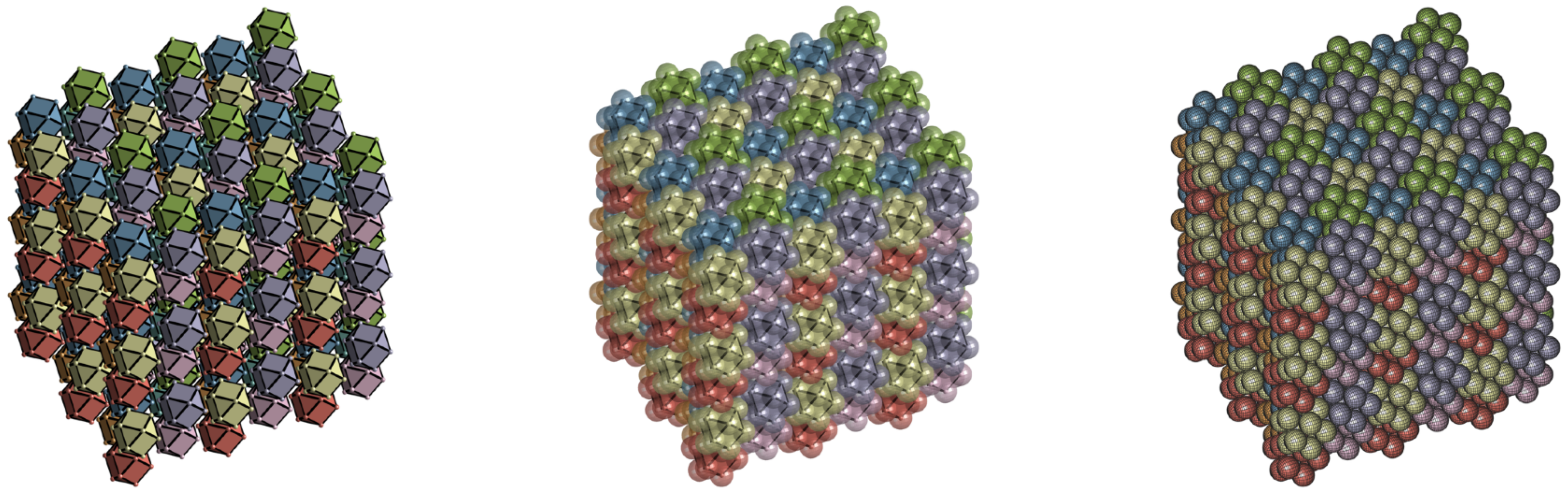
$P2_12_12_1\,|\,(2_1\ 2_1\ \bar{\times})\,|\,0.58959...$



$C2/c\,|\,(2_0\ 2_1\ 2\ 2)\,|\,0.63435...$

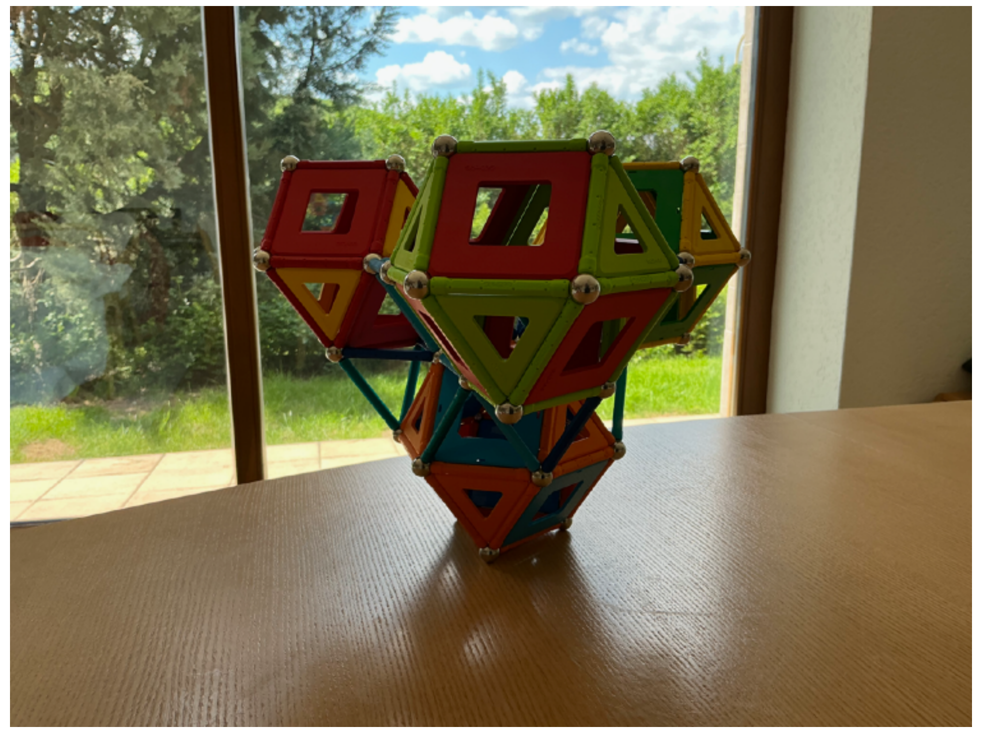


$Pbca\,|\,(2_1\ 2\ \bar{*}\ :)\,|\,0.65820... \approx \frac{8}{9}\frac{\pi}{\sqrt{18}}$



Global Cuboctahedral Molecule Packing Maximiser

- *Is the* GEOMAG cuboctahedral molecule packing model *the global packing density maximum?*



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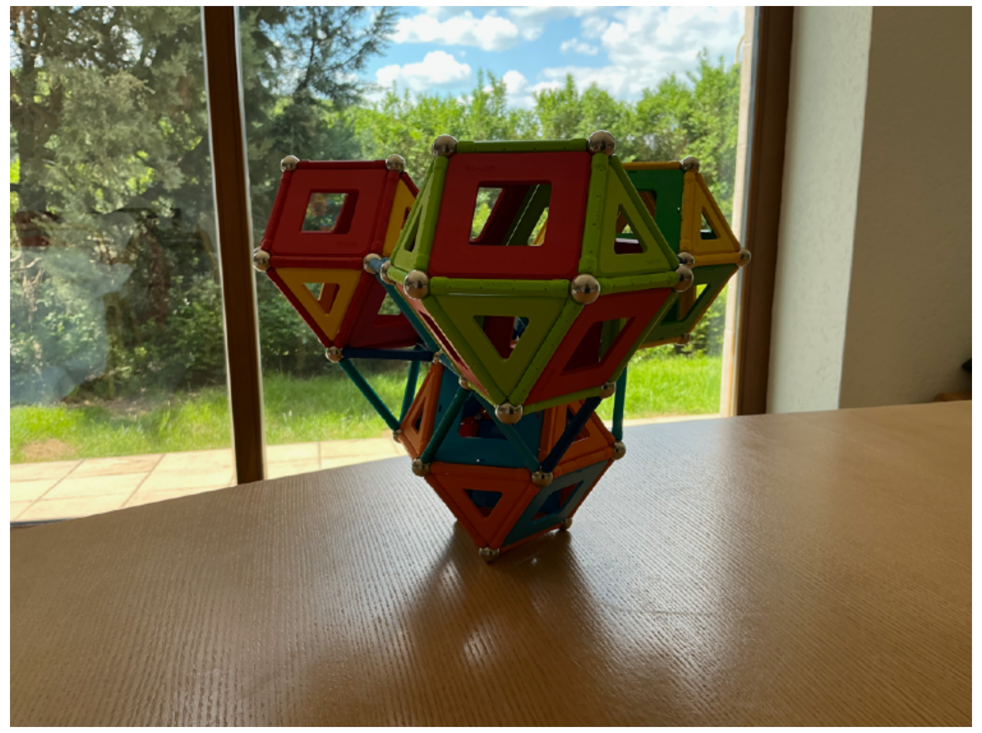
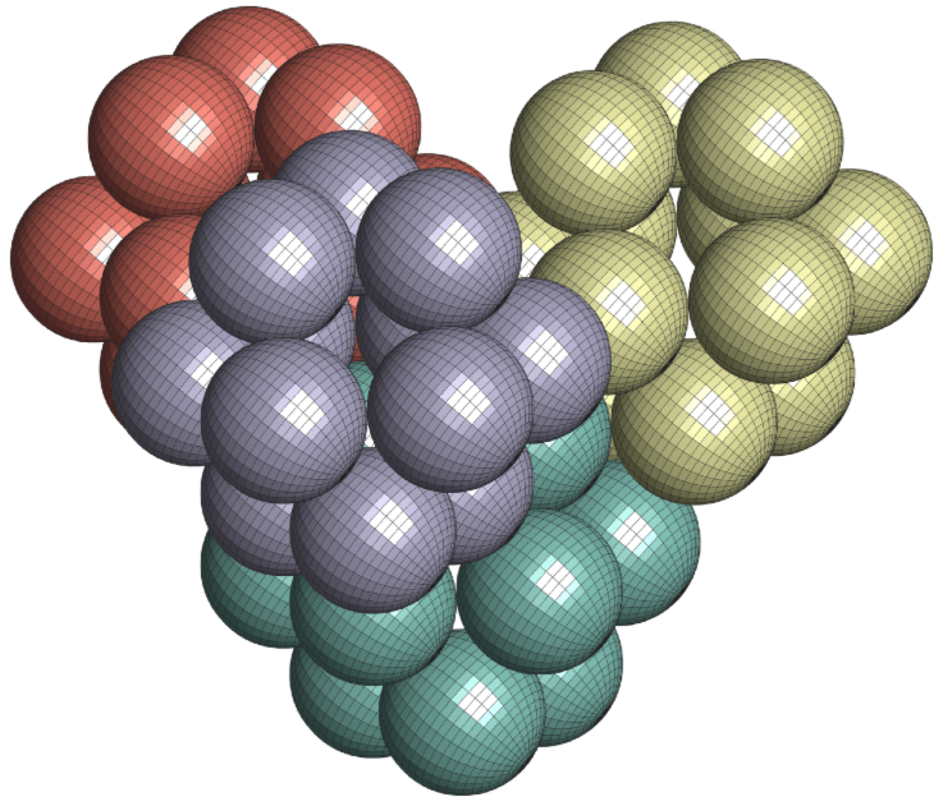
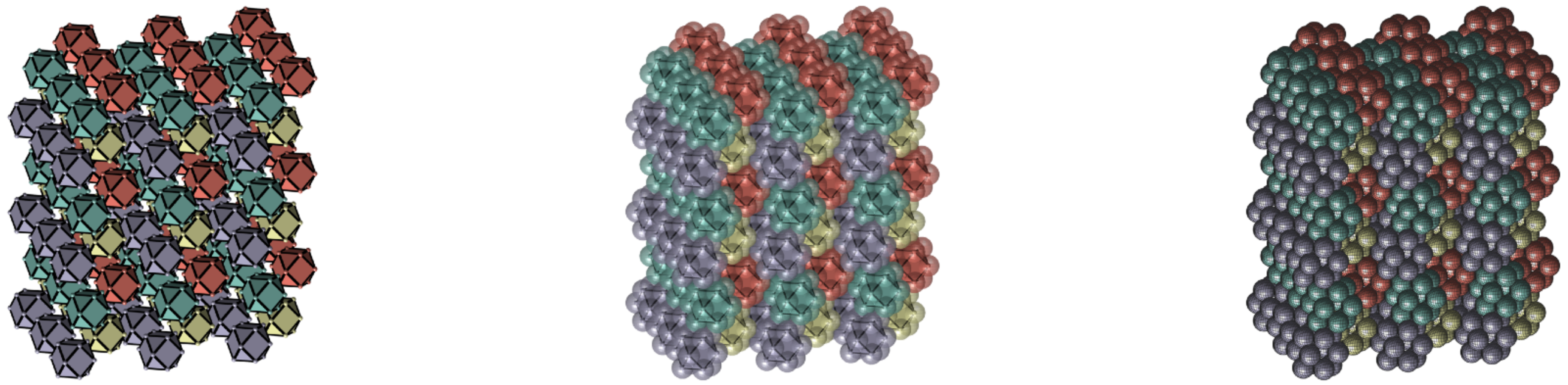
- *Is the* GEOMAG cuboctahedral molecule packing model *the global packing density maximum?*
- No. It is the second densest configuration.

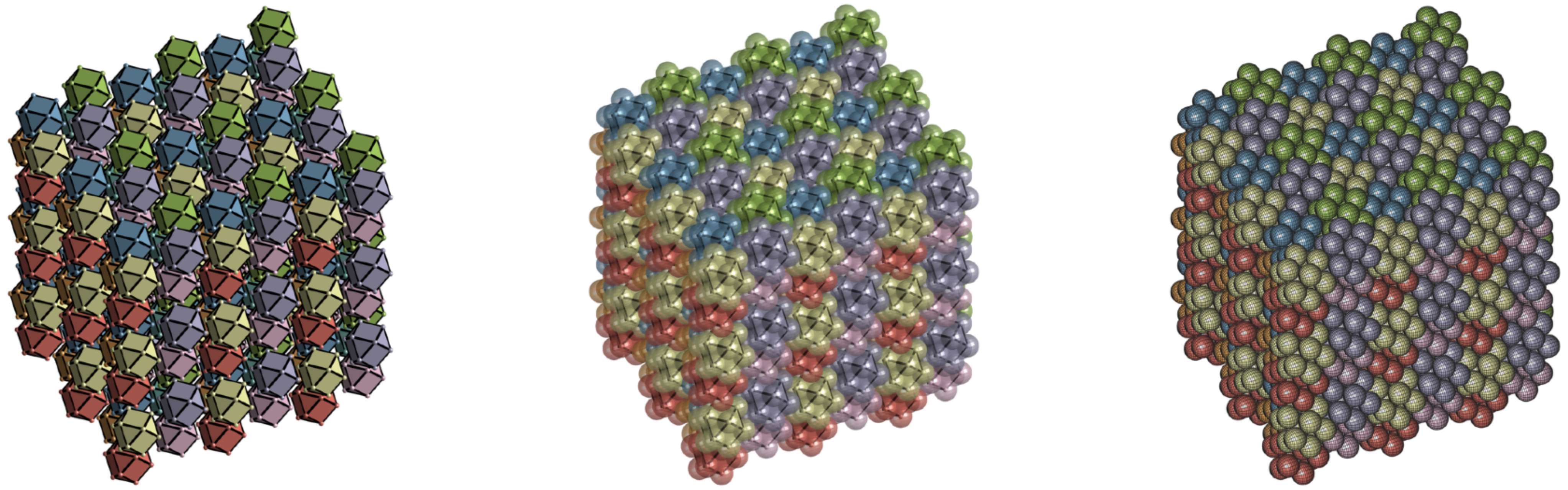




$P2_1/c \mid (2_1\ 2_1\ 2\ 2) \mid 0.65820... \approx \frac{8}{9}\frac{\pi}{\sqrt{18}}$



$Pbca \mid (2_1\ 2\ \bar{*}\ :) \mid 0.65820... \approx \frac{8}{9}\frac{\pi}{\sqrt{18}}$



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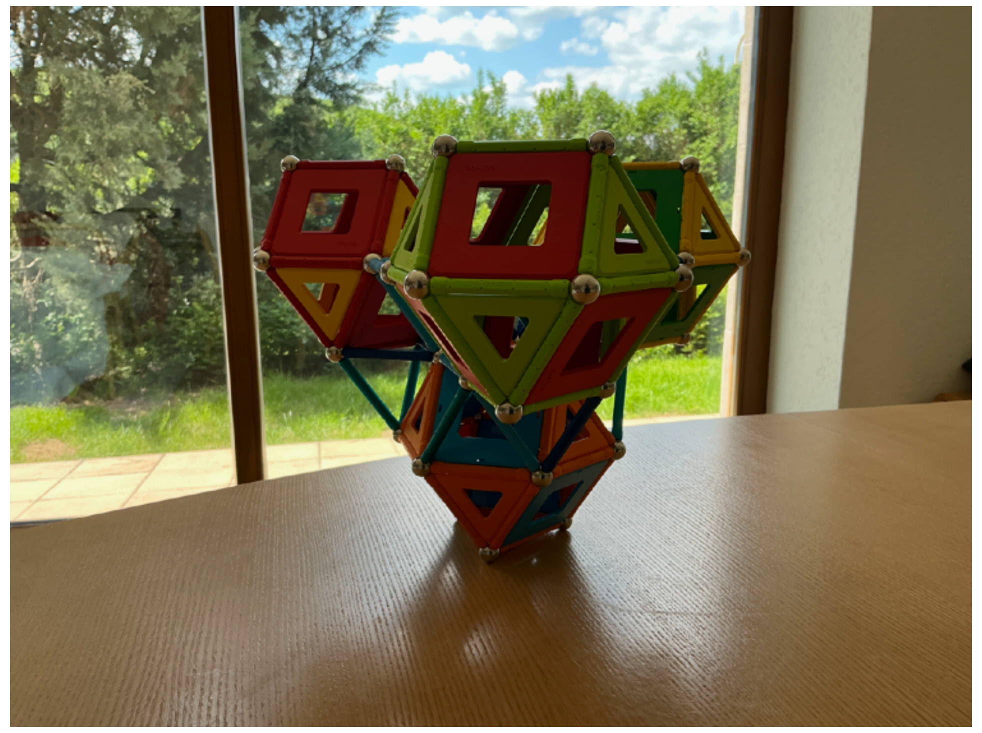

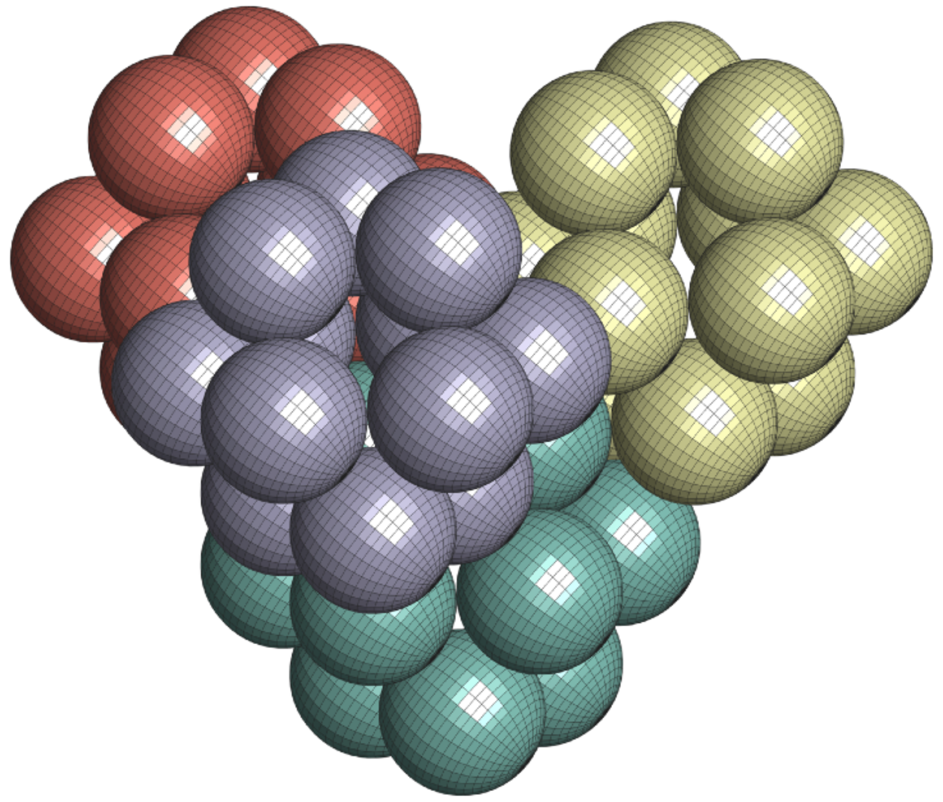

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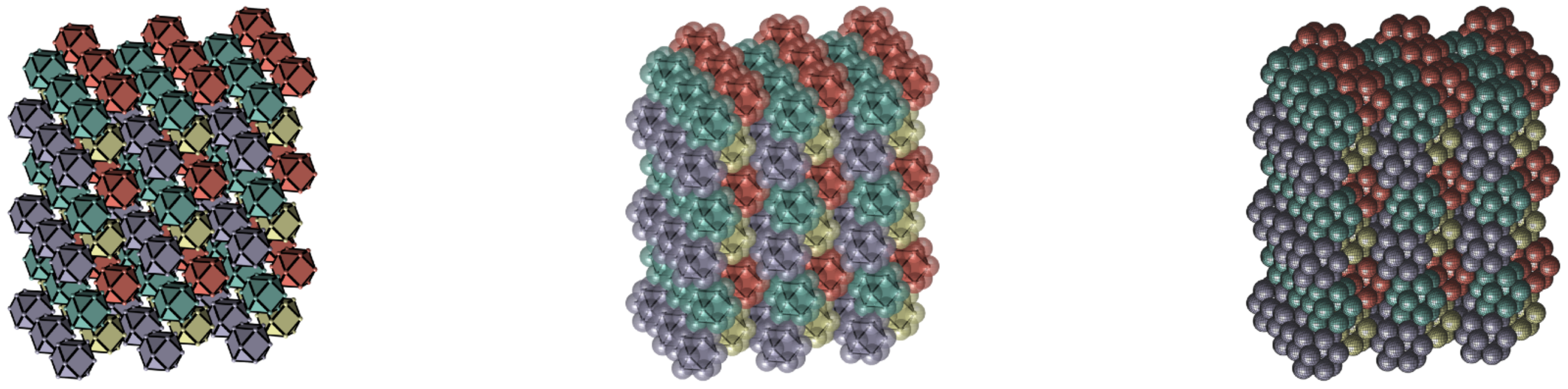

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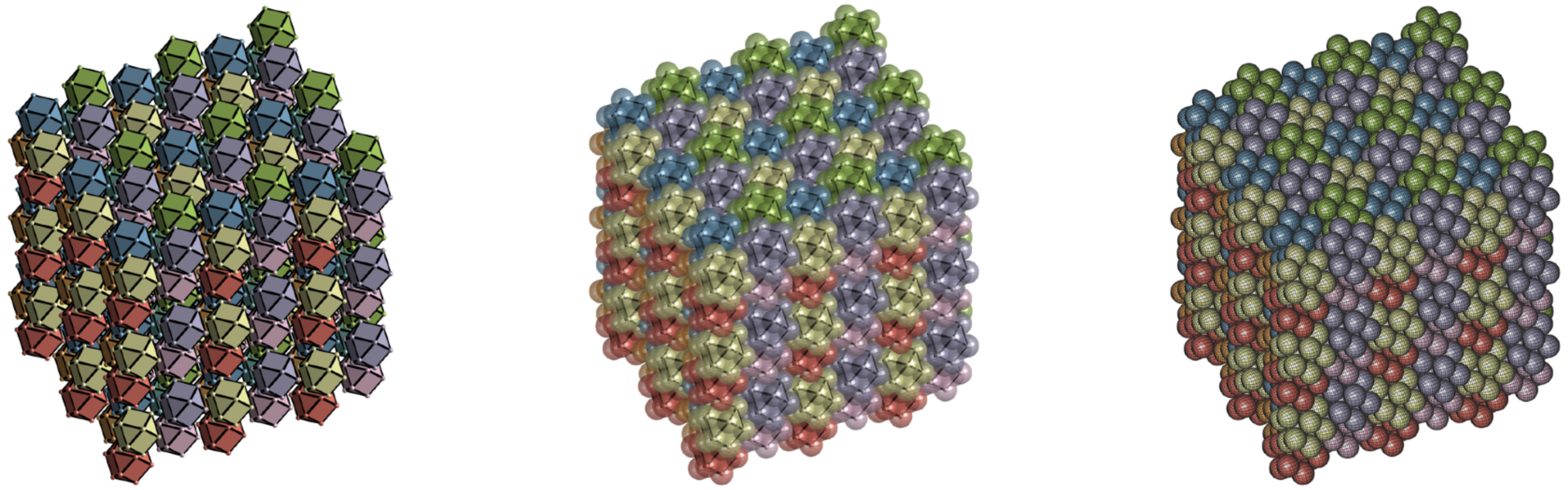
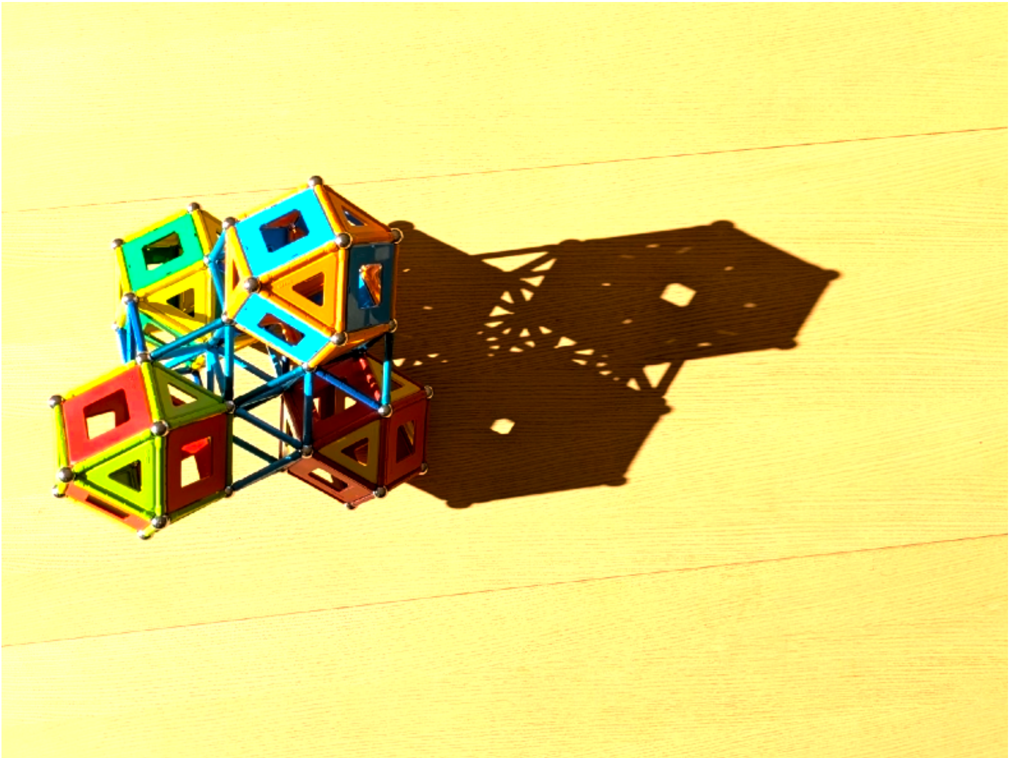
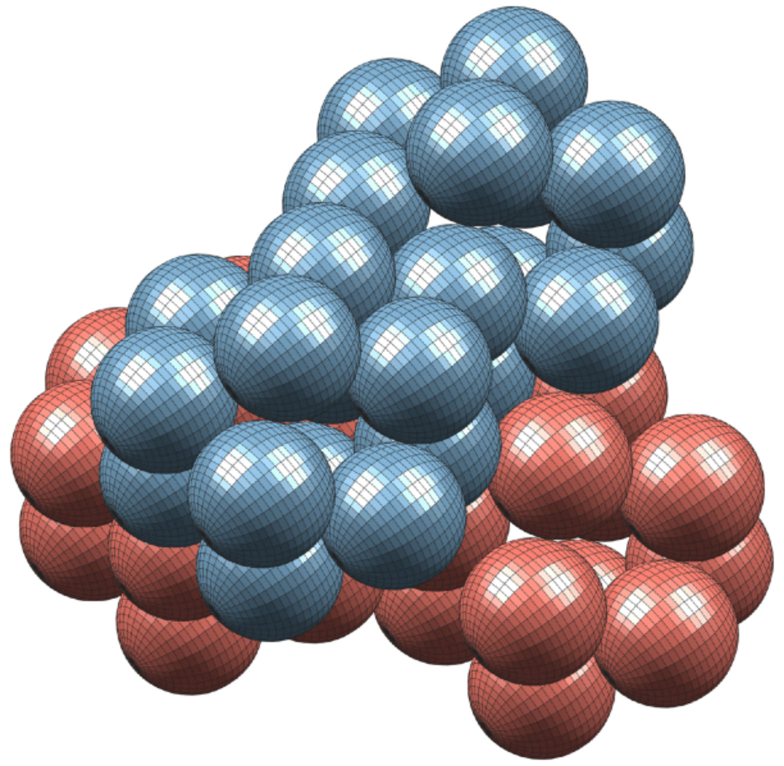
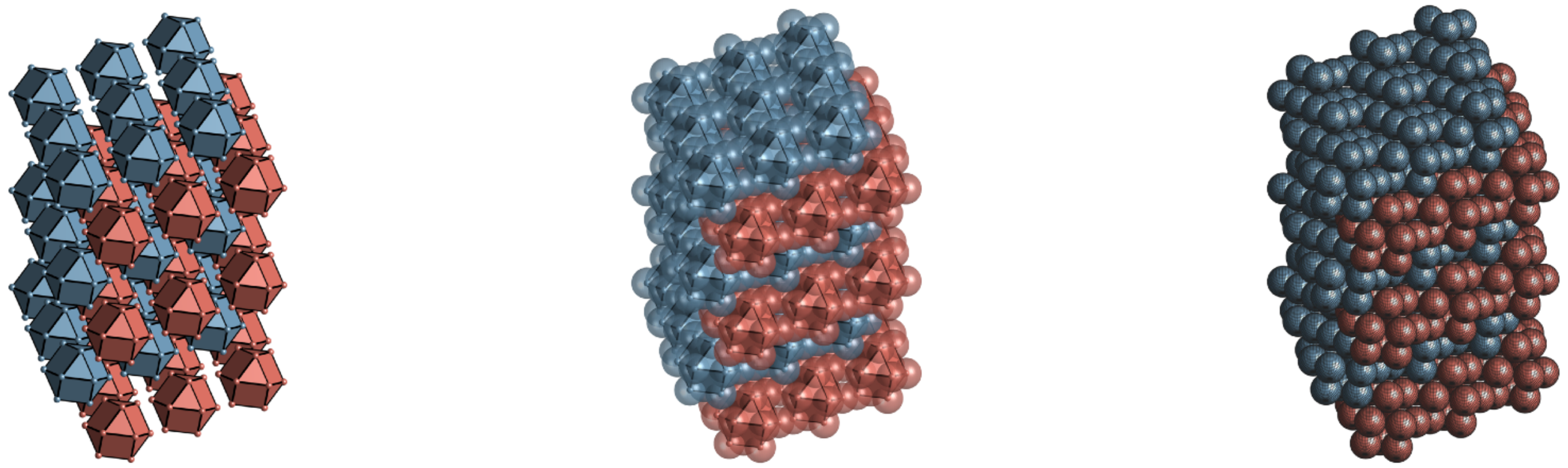


- Densest space group packing





$P\bar{1} \mid (2\ 2\ 2\ 2) \mid 0.68352... \approx \frac{12}{13}\frac{\pi}{\sqrt{18}}$



Global Cuboctahedral Molecule Packing Maximiser

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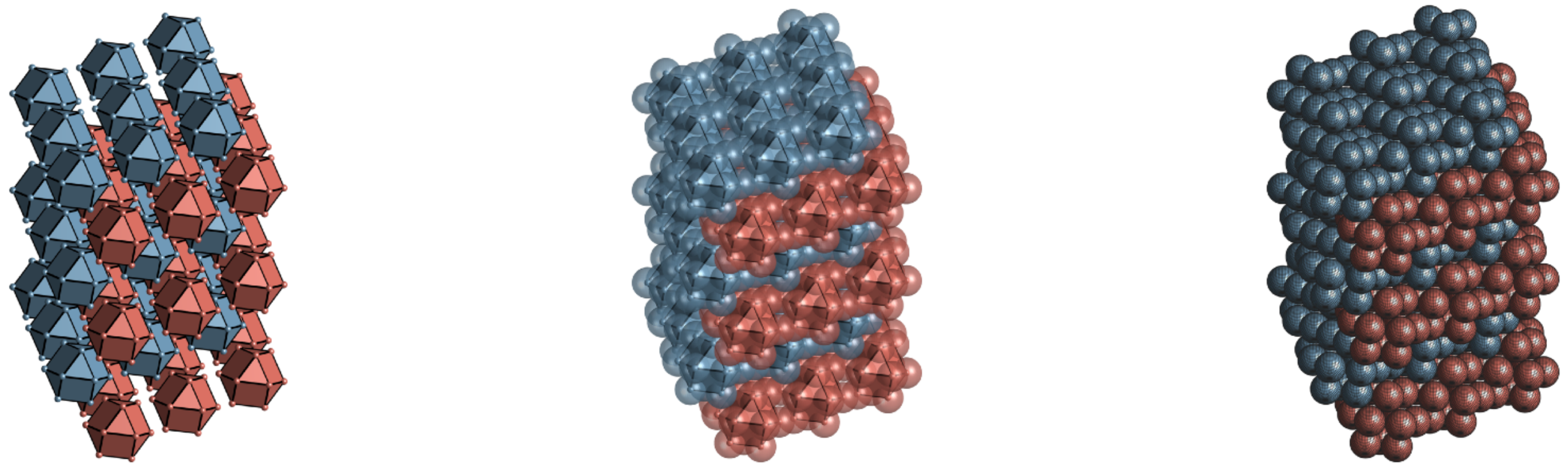

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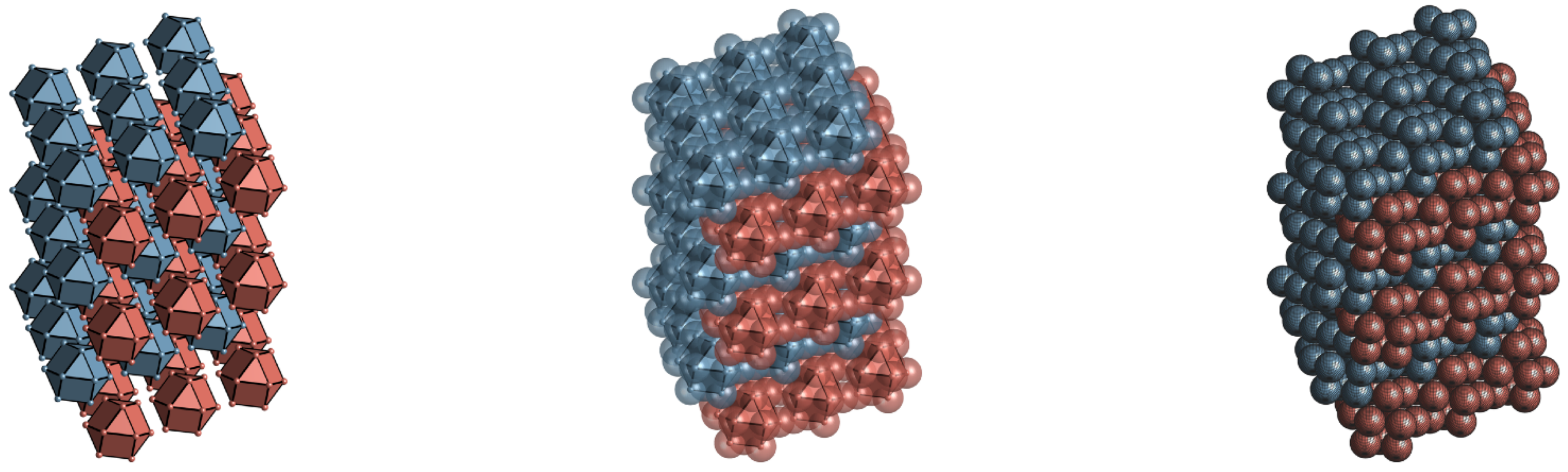

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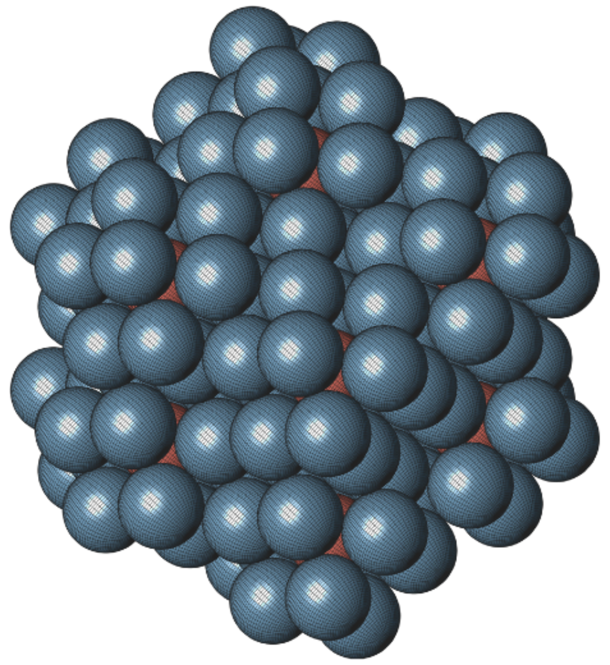
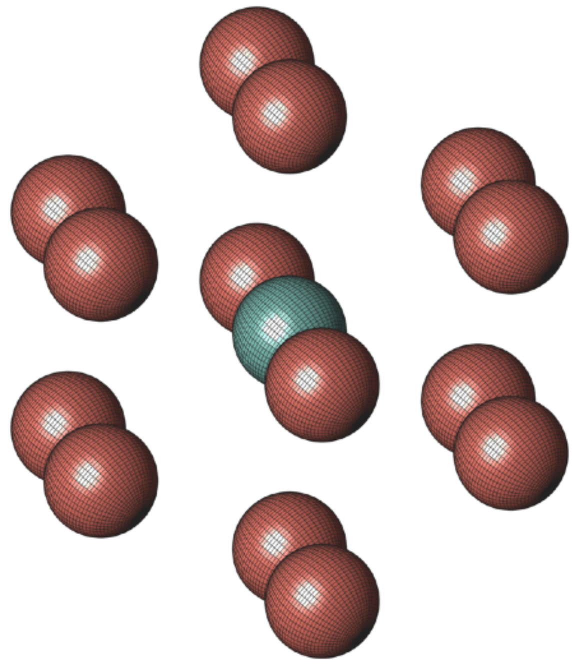


complementary packing with density $\frac{1}{13}\frac{\pi}{\sqrt{18}}$



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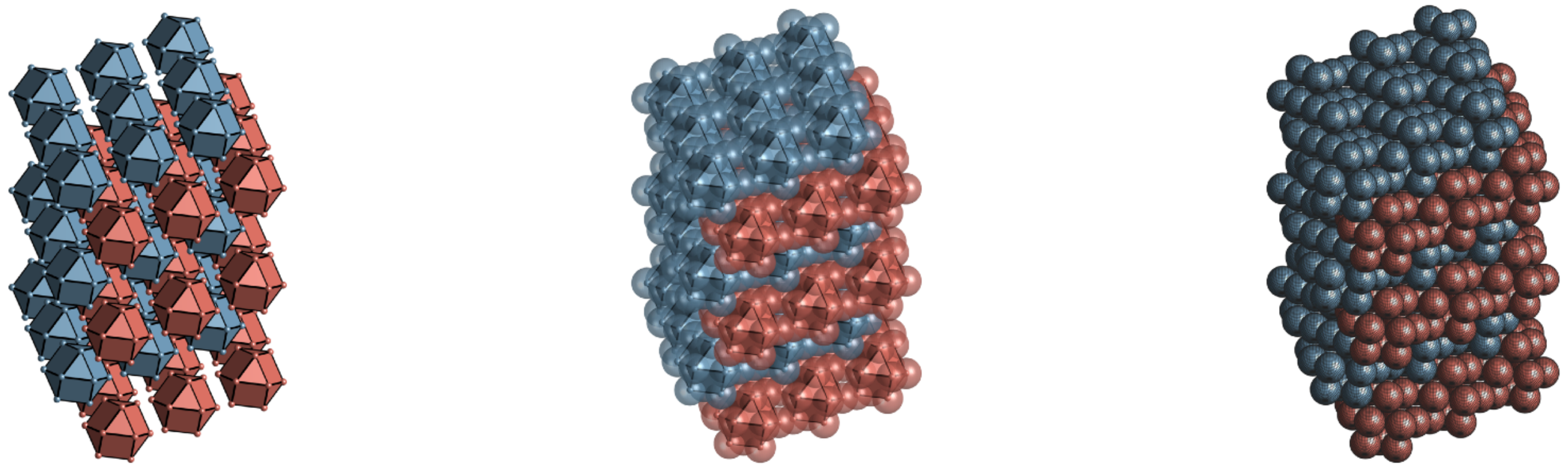

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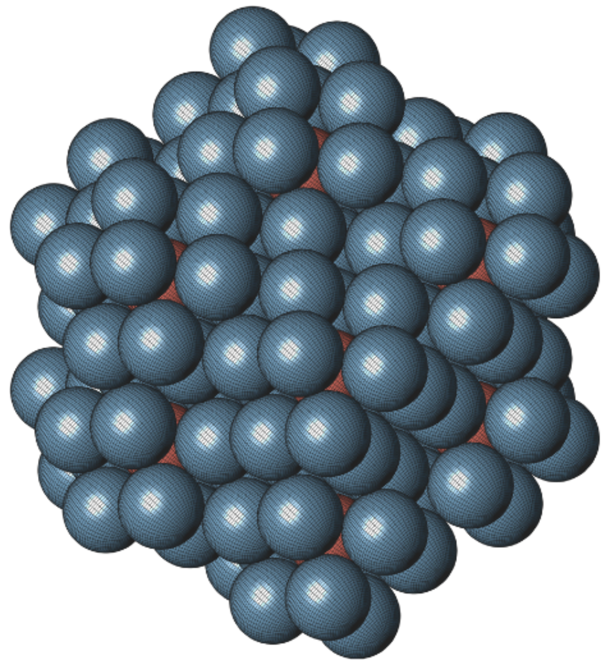

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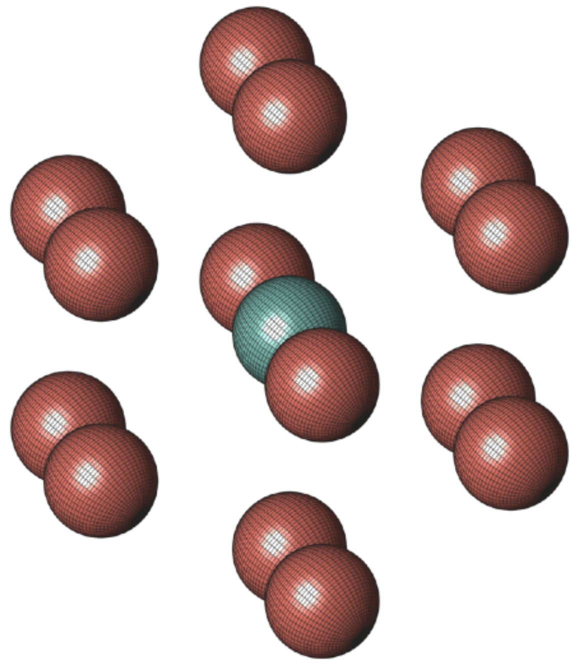
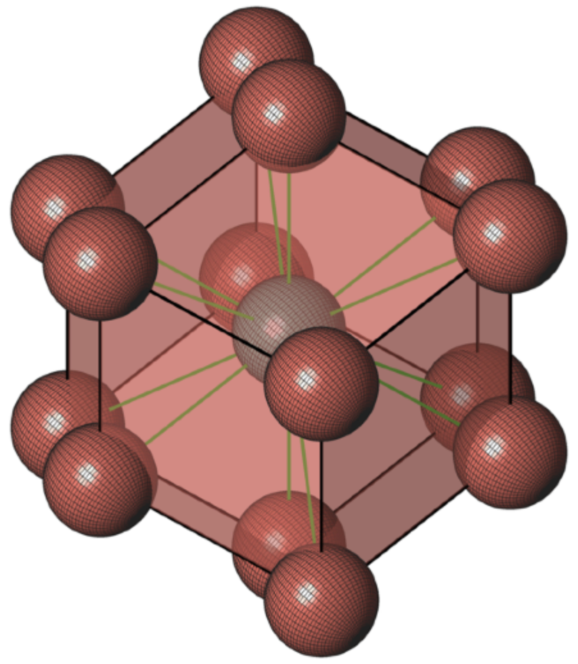


Vertices of a rhombic dodecahedron



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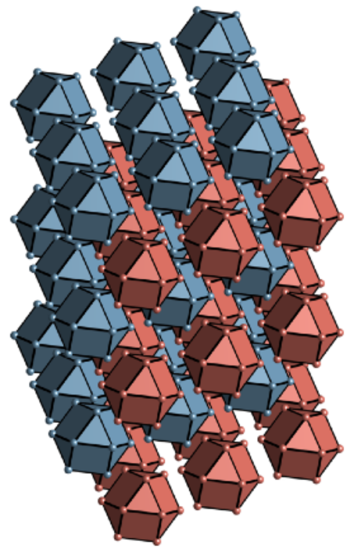

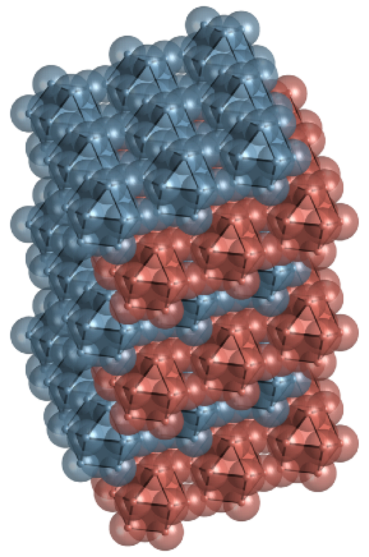

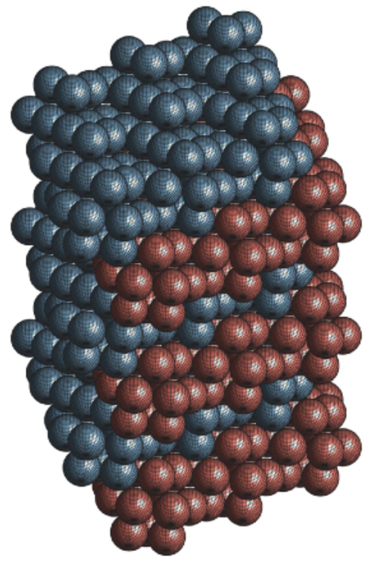

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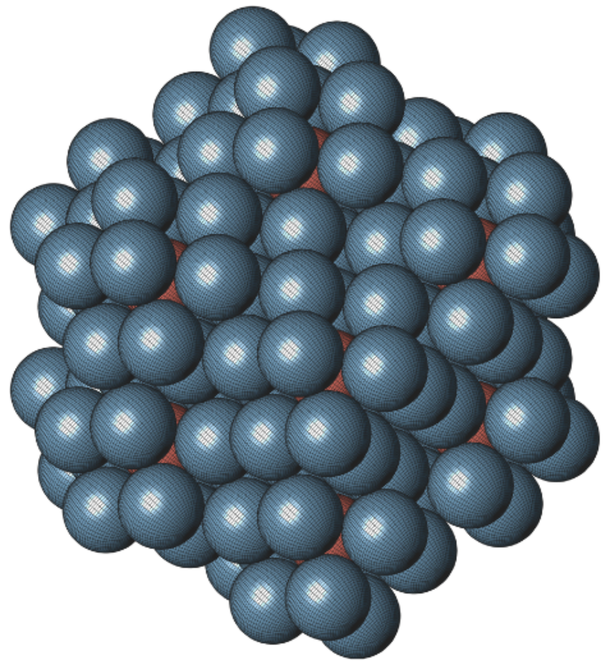

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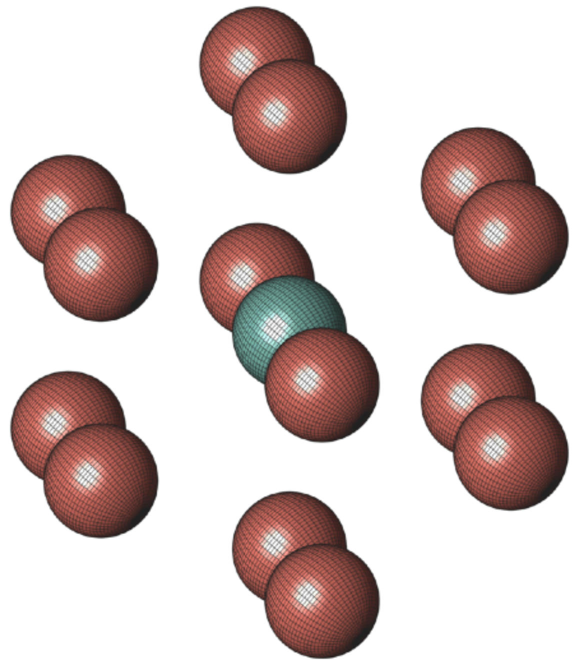

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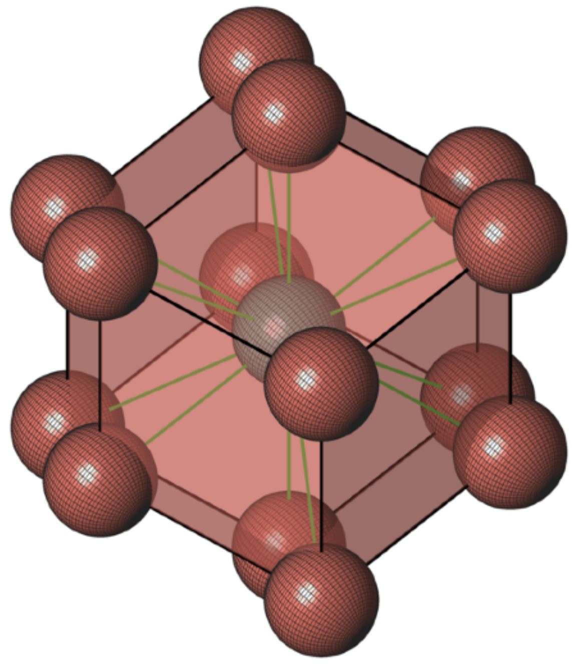
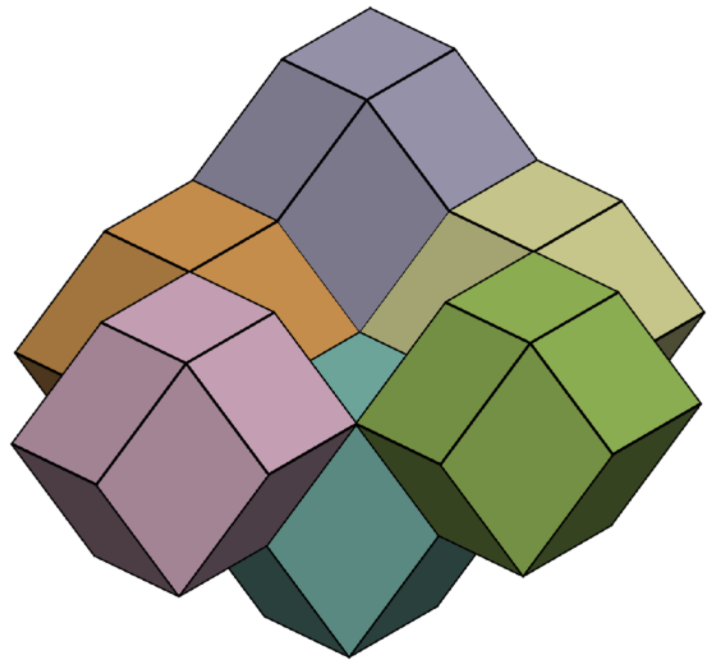
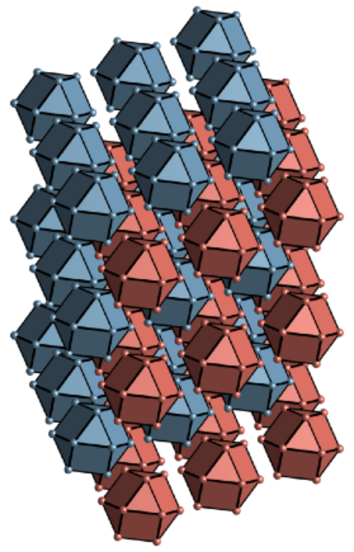


rhombic dodecahedral honeycomb





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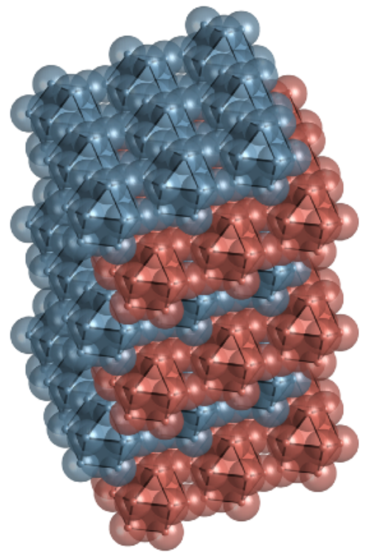

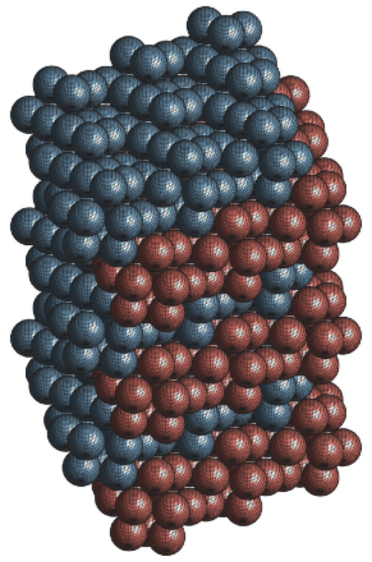

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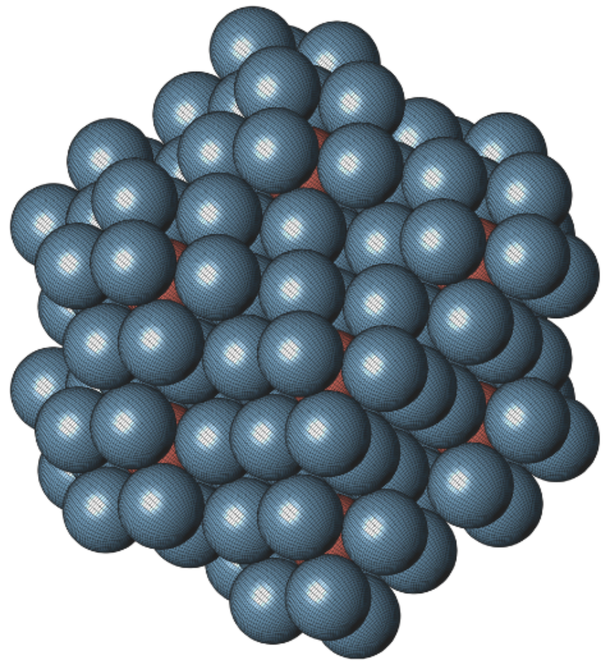

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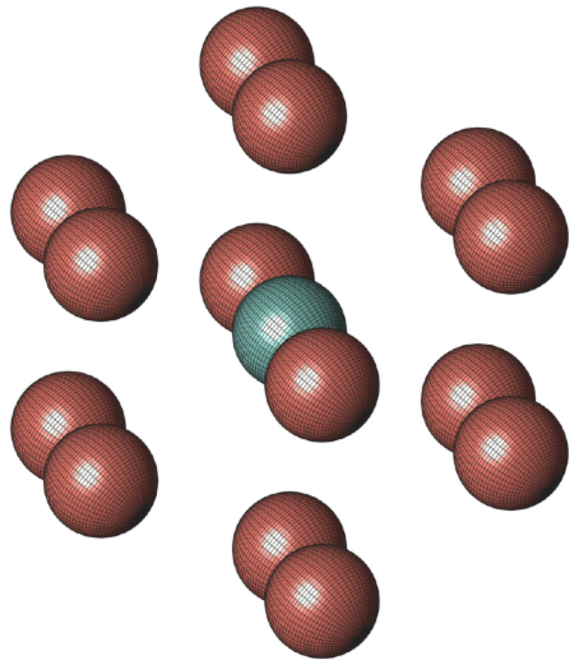

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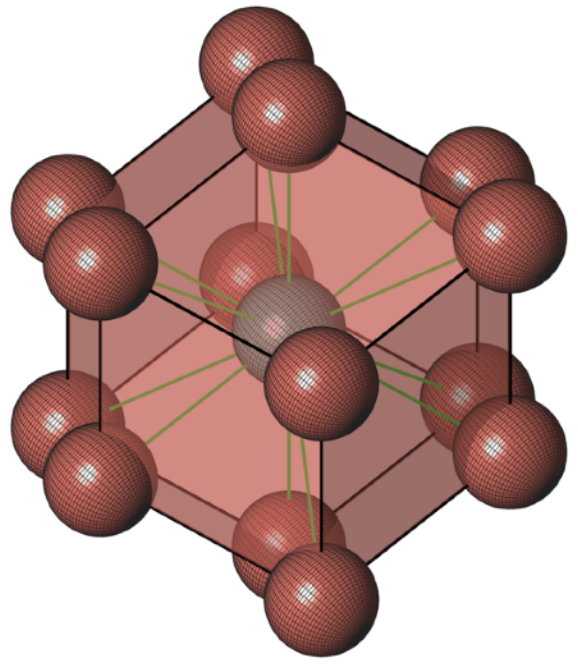

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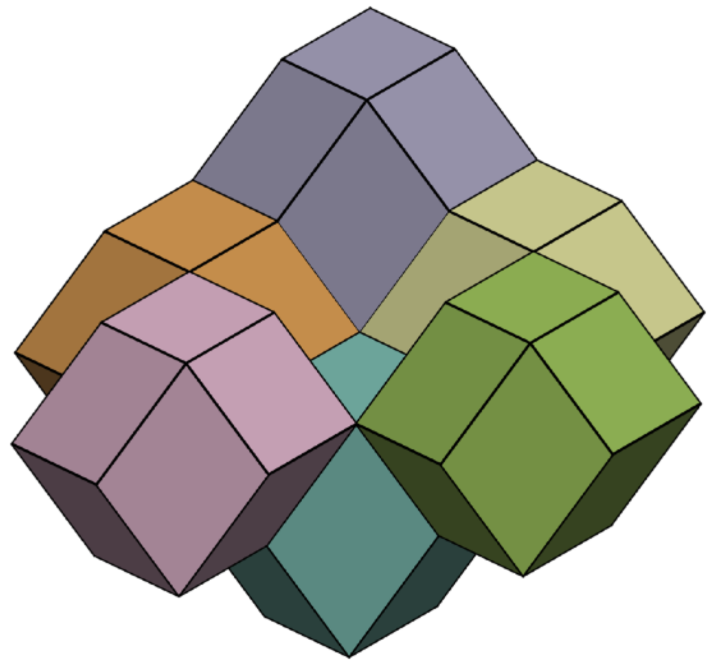
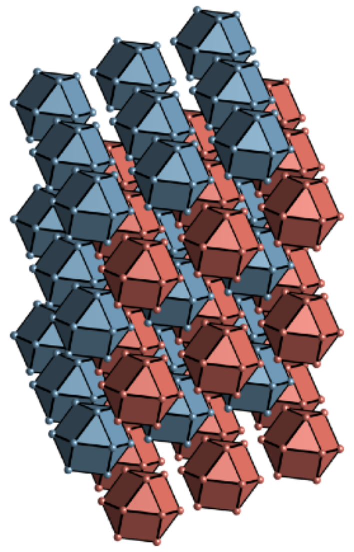


dual honeycomb

tetrahedral–octahedral honeycomb



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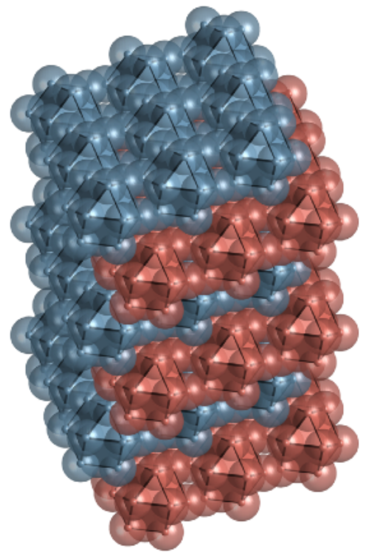

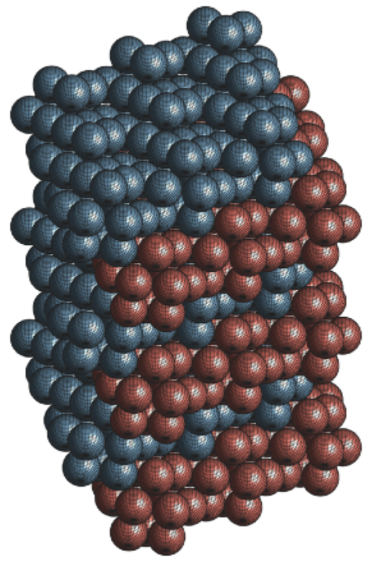

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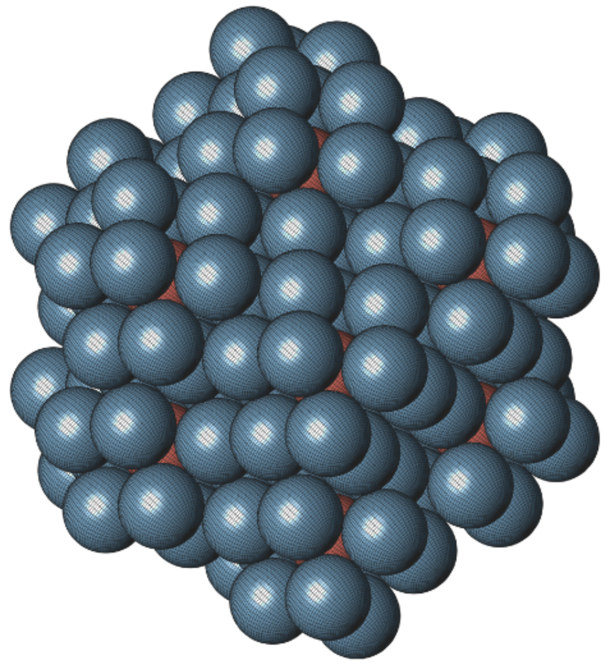

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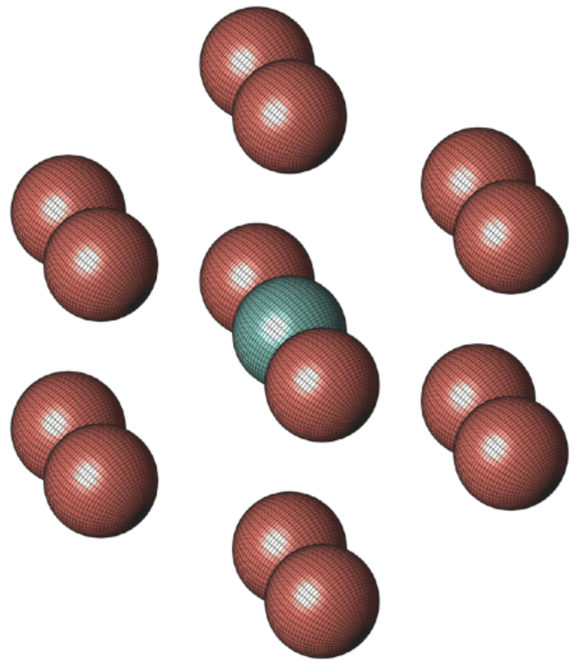
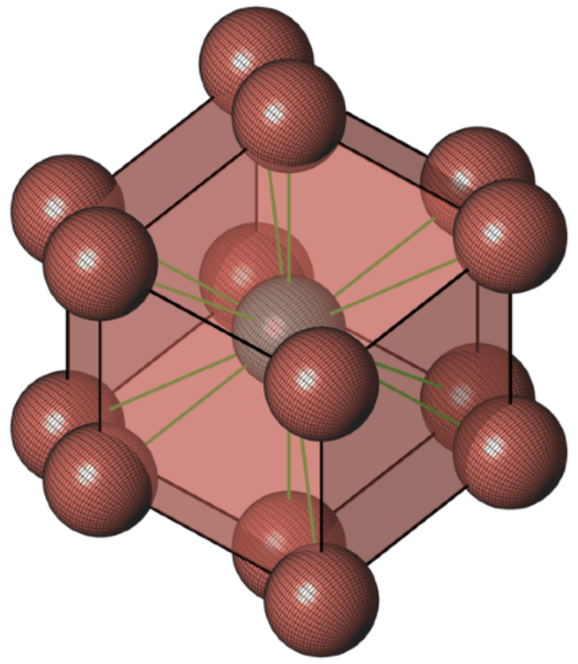
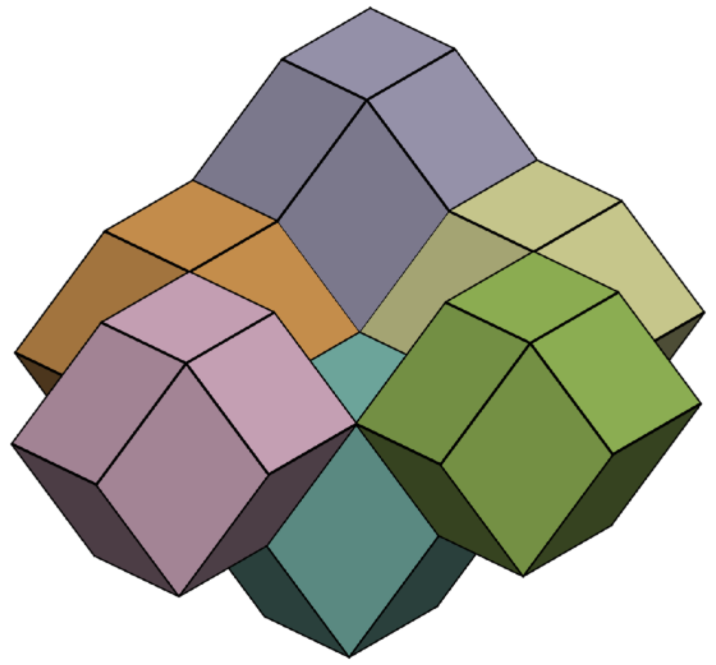


Vertices of a rhombic dodecahedron



rhombic dodecahedral honeycomb



dual honeycomb

tetrahedral–octahedral honeycomb

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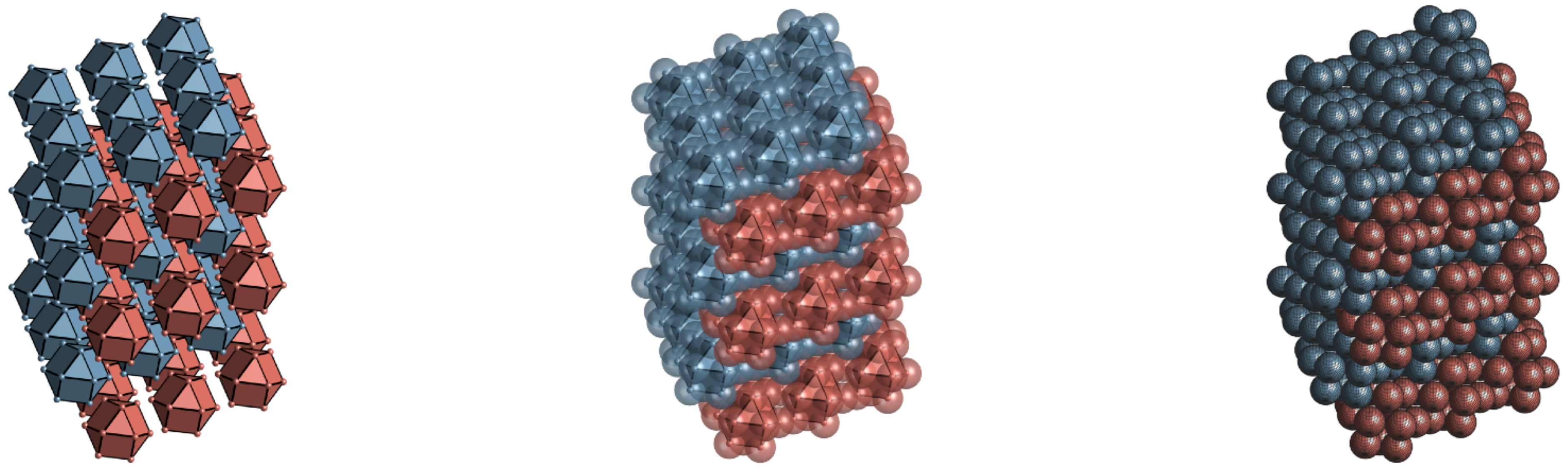

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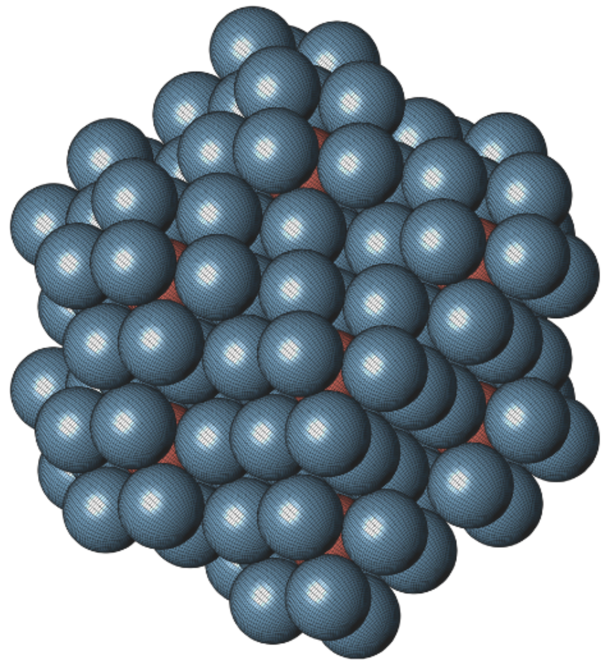

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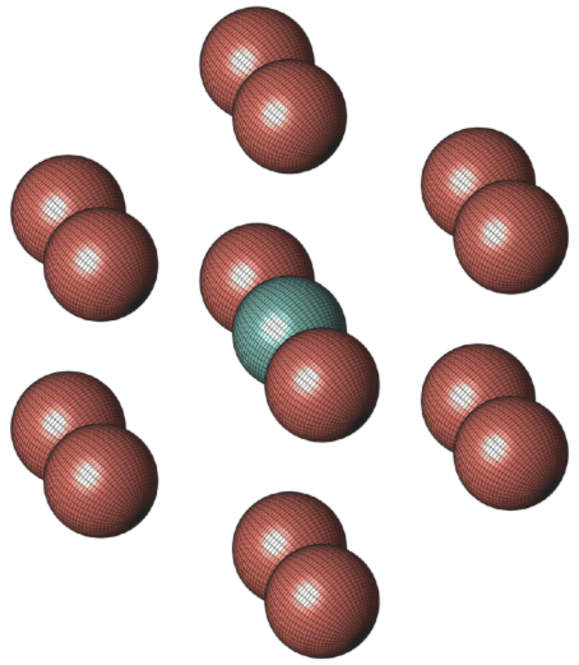

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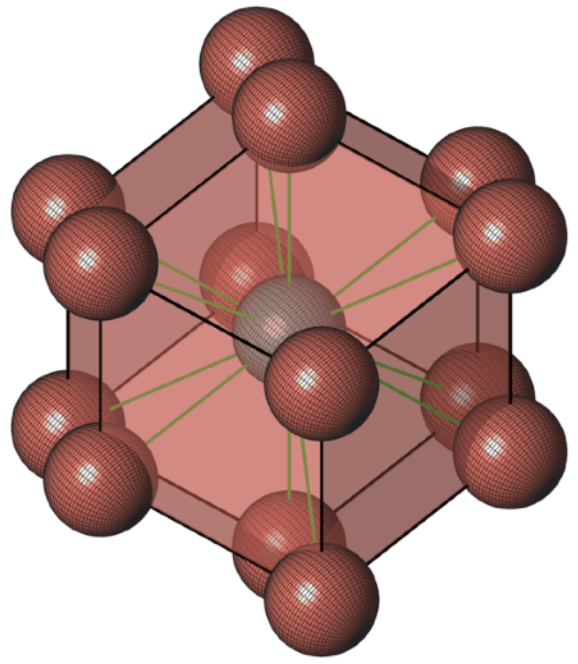
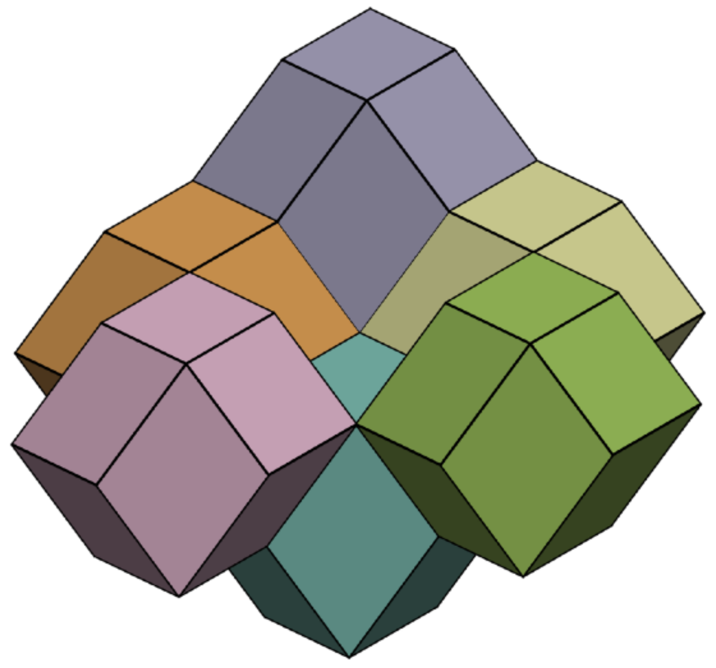


rhombic dodecahedral honeycomb



dual honeycomb

tetrahedral–octahedral honeycomb

- What is the takeaway?
- Two levels of locally maximal close packing configurations:

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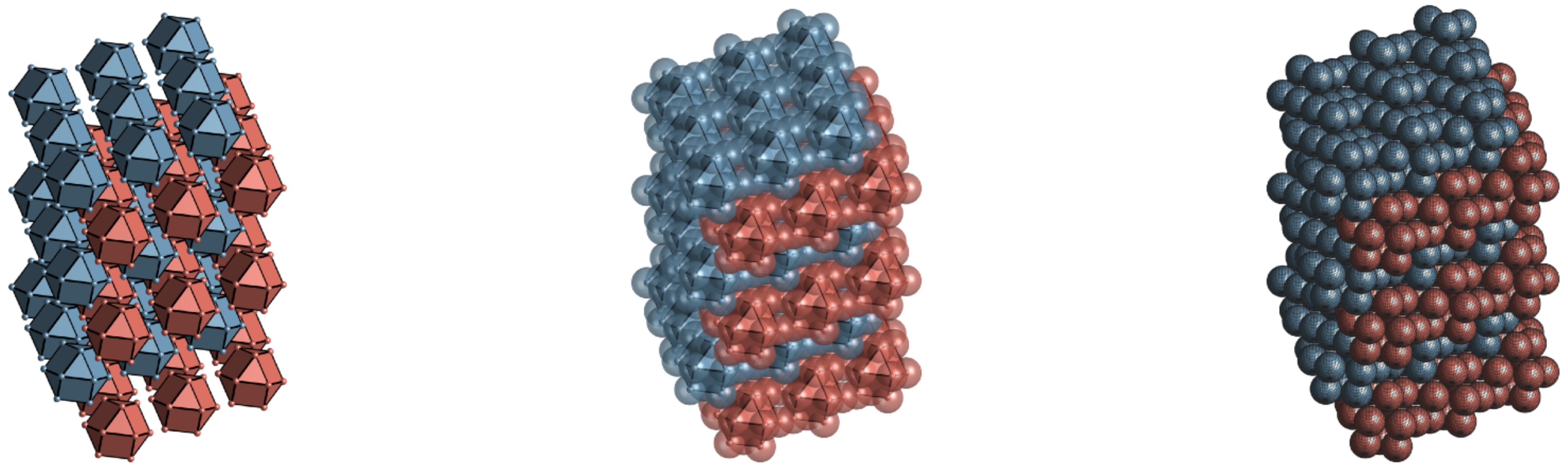

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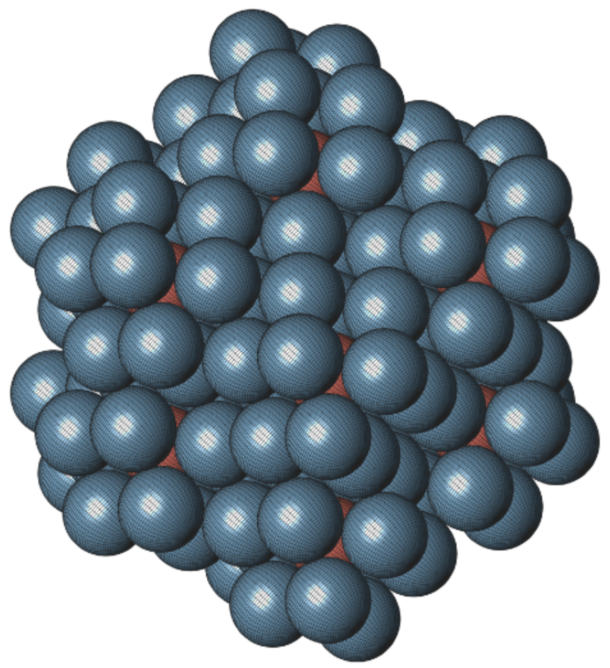

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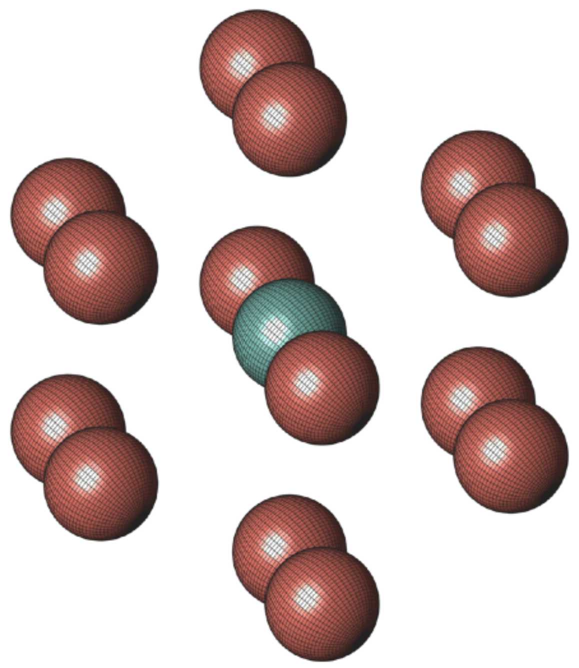

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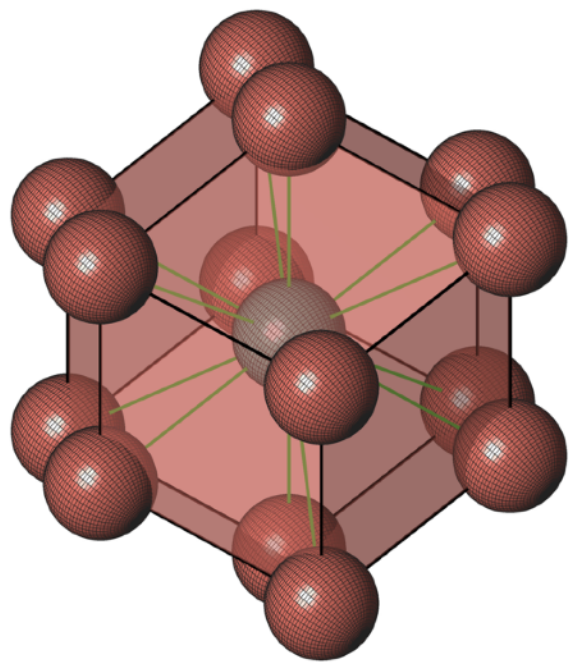
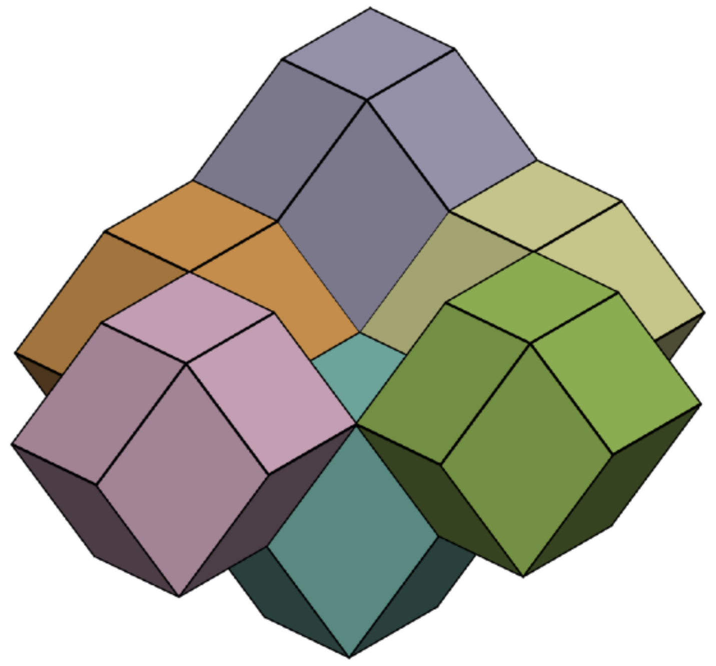


rhombic dodecahedral honeycomb



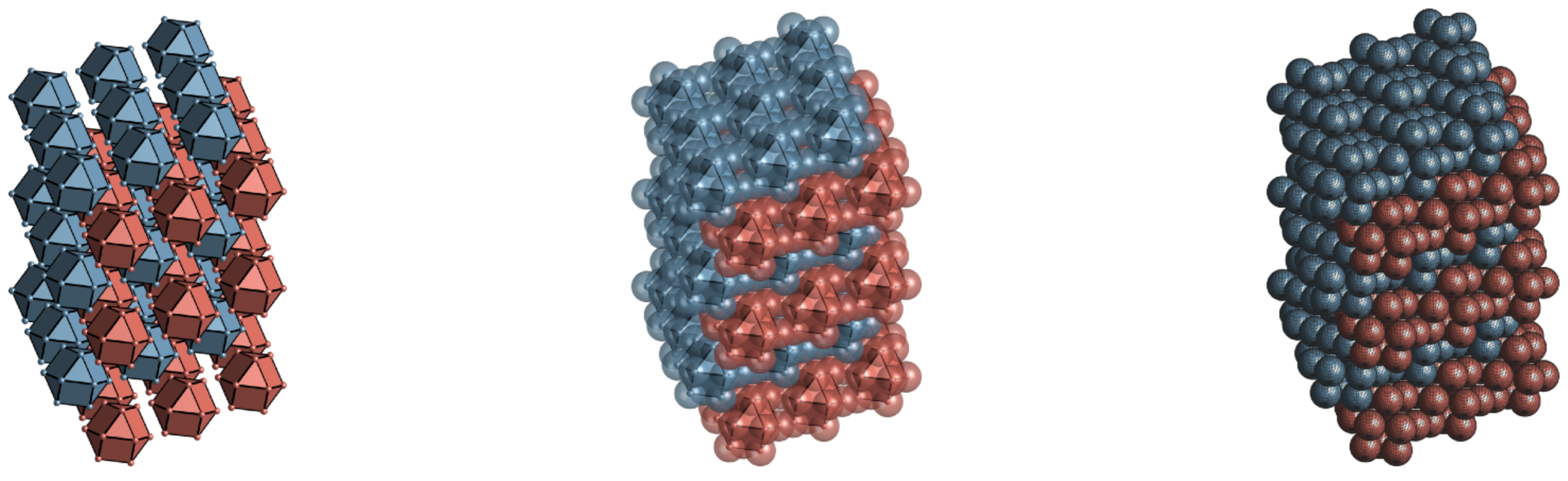
dual honeycomb

tetrahedral–octahedral honeycomb

- What is the takeaway?
- Two levels of locally maximal close packing configurations:

1. Atomic – Locally maximal dense packings between atoms of different molecules, where each atom touches seven atoms from neighbouring molecules.

$P\bar{1} \,|\, (2\ 2\ 2\ 2) \,|\, 0.68352... \approx \frac{12}{13}\frac{\pi}{\sqrt{18}}$



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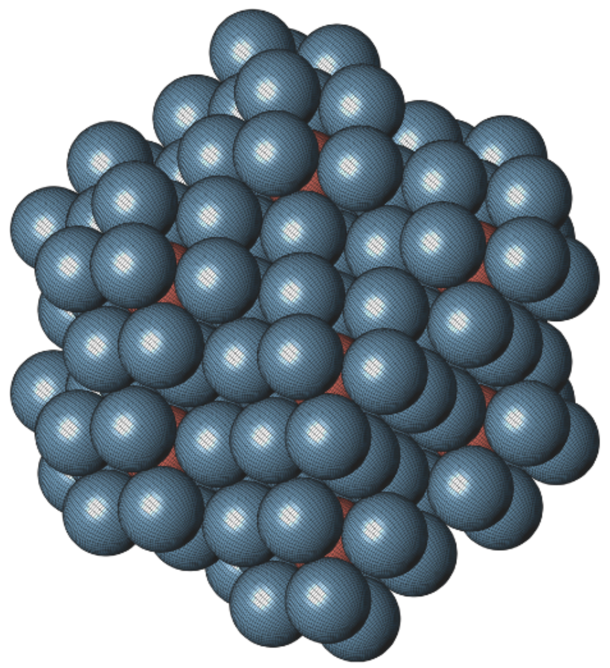

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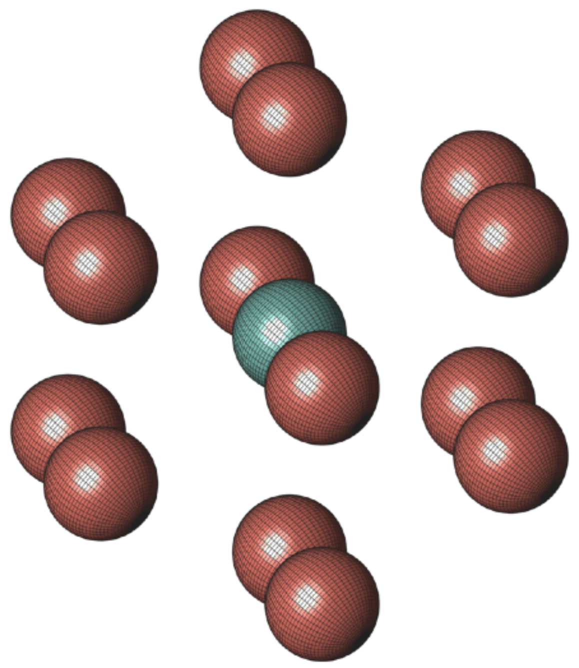

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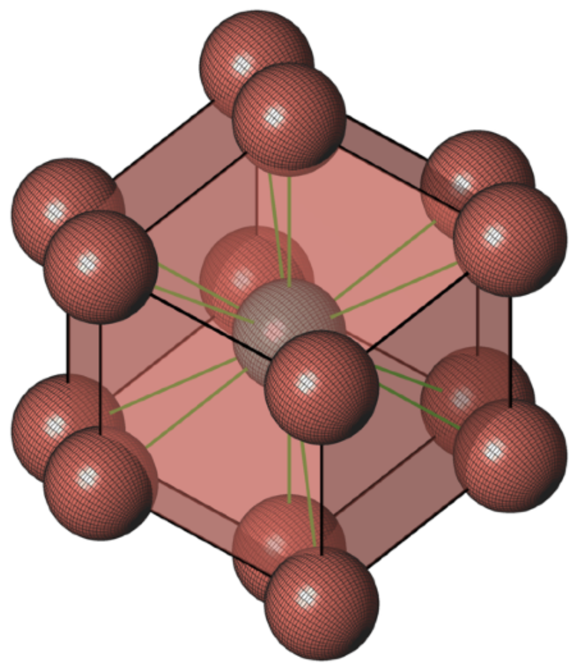
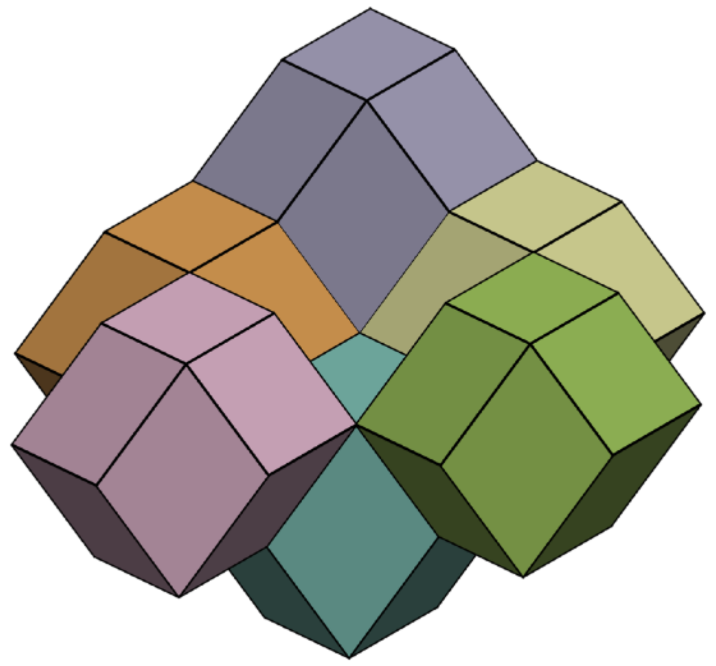


rhombic dodecahedral honeycomb



dual honeycomb

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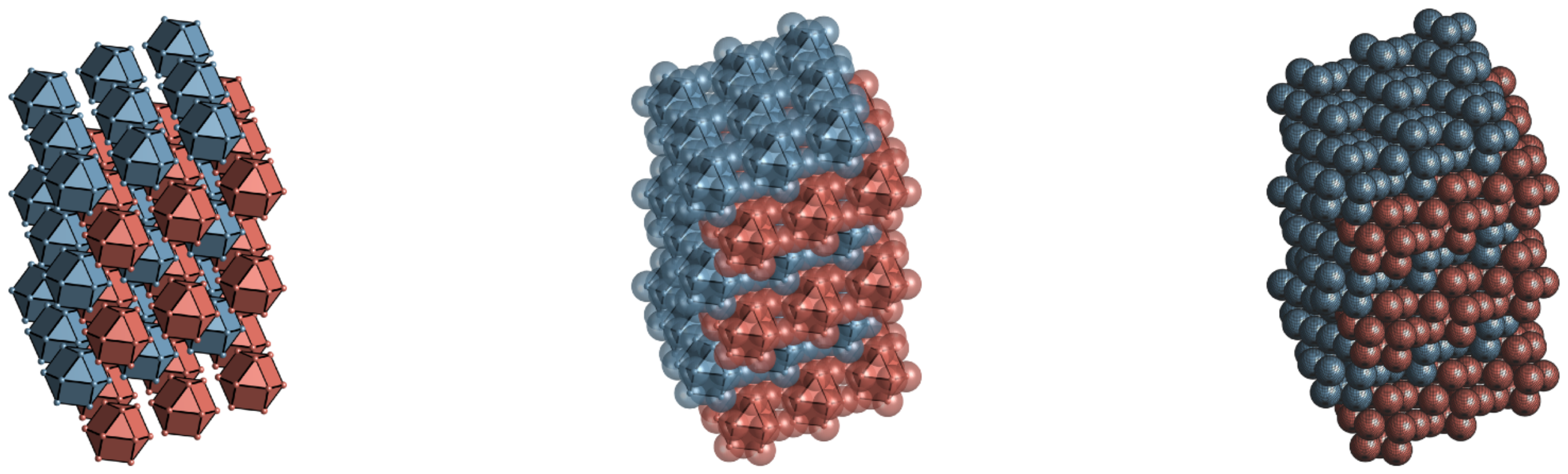
- Two levels of locally maximal close packing configurations:

  1. Atomic – Locally maximal dense packings between atoms of different molecules, where each atom touches seven atoms from neighbouring molecules.

  2. Molecular – Locally maximal dense packings between molecules, where each molecule touches 14 surrounding molecules, giving each molecule a molecular coordination number of 14.

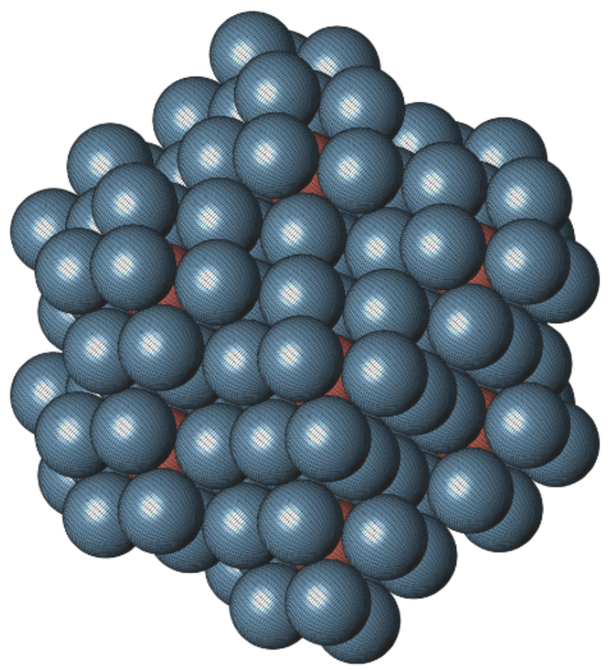
$P\bar{1} \mid (2\ 2\ 2\ 2) \mid 0.68352... \approx \frac{12}{13}\frac{\pi}{\sqrt{18}}$



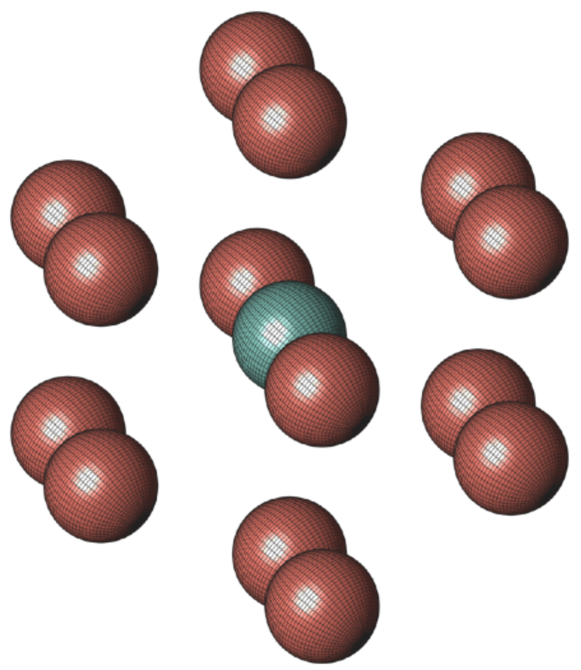
Global Cuboctahedral Molecule Packing Maximiser

- How do we know it is the global maximum?
- By construction our cuboctahedral molecule model is a collection of equal spheres with centres on the twelve vertices of a cuboctahedron,

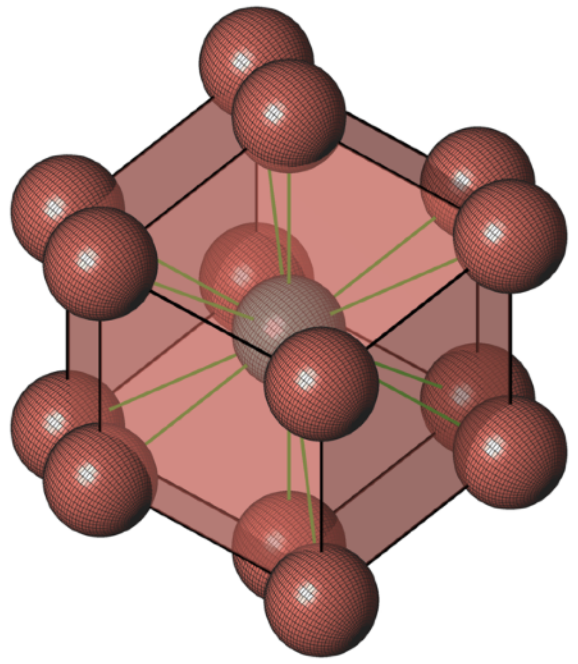
$P1 \mid (\circ) \mid 0.68352\ldots \approx \frac{12}{13}\frac{\pi}{\sqrt{18}}$



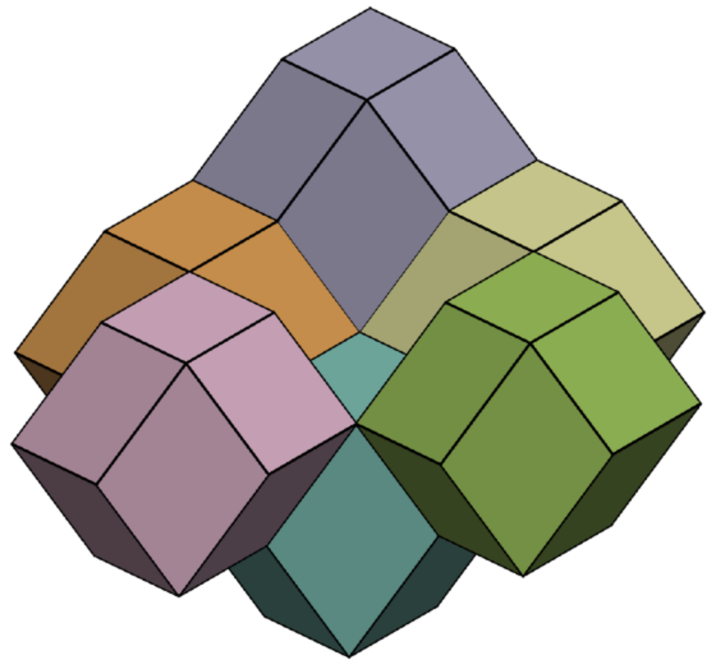
complementary packing with density $\frac{1}{13}\frac{\pi}{\sqrt{18}}$



Vertices of a rhombic dodecahedron



rhombic dodecahedral honeycomb



dual honeycomb

tetrahedral–octahedral honeycomb

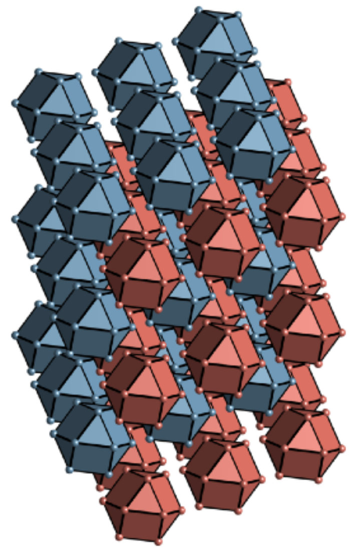
- What is the takeaway?
- Two levels of locally maximal close packing configurations:

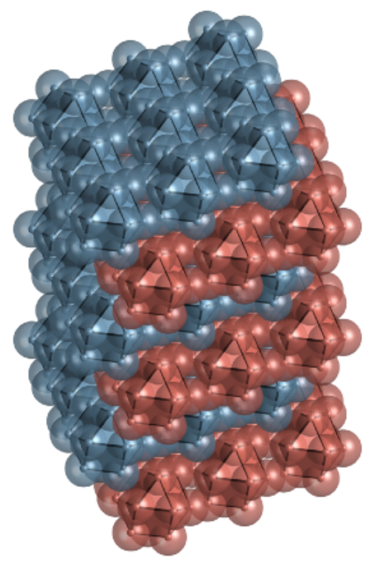
  1. Atomic – Locally maximal dense packings between atoms of different molecules, where each atom touches seven atoms from neighbouring molecules.

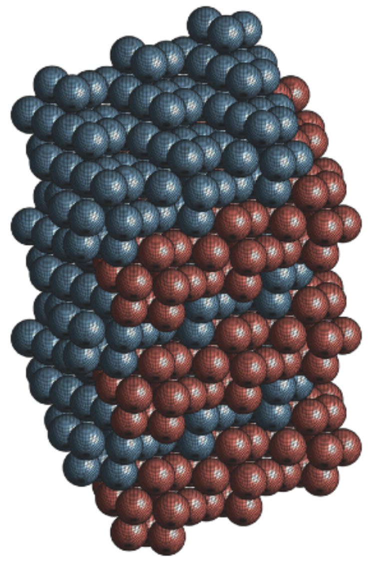
  2. Molecular – Locally maximal dense packings between molecules, where each molecule touches 14 surrounding molecules, giving each molecule a molecular coordination number of 14.

- High atomic and molecular kissing / coordination numbers

$P\bar{1} \mid (2\ 2\ 2\ 2) \mid 0.68352\ldots \approx \frac{12}{13}\frac{\pi}{\sqrt{18}}$







What Do the Space Groups $P\bar{1}$, $P2_1$, $P2_1/c$,$C2/c$, $P2_12_12_1$ and $Pbca$ and Have in Common?

- Relatively low-symmetry subgroups of the space group $Fm\bar{3}m$

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Cambridge Structural Database
1 January 2025

CSD Space Group Statistics – Space Group Frequency Ordering

Space group frequency ranking for the 1,359,039 CSD structures for which the space group is fully defined. Statistics for enantiomorphous space groups are as reported in the CSD. 1,063,306 (78 %) structures adopt centrosymmetric space groups, 295,733 (22 %) adopt non-centrosymmetric space groups, and 222,854 (16 %) structures adopt Sohncke space groups.

Rank	*SG No.*	*Space Group*	*No. in CSD*	*% of CSD*
1	14	P21/c	461,012	33.9
2	2	P-1	342,599	25.2
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[illegible]	[illegible]	[illegible]	[illegible]	[illegible]

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CLOSEST-PACKED SPACE GROUPS AND SPACE GROUPS OF MAXIMUM DENSITY FOR ORGANIC CRYSTALS

Molecular symmetry in crystal	1	2	m	$\bar{1}$	mm	$2/m$	222	mmm
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Space groups of maximum density	none	$C2/c$ $P2_12_12$ $Pbcn$	Pmc Cmc $Pnma$	none	Fmm $Pmma$ $Pmnn$	$C2/m$ $Pbaa$ $Cmca$	$C222$ $F222$ $I222$ $Ccca$	$Cmmm$ $Fmmm$ $Immm$

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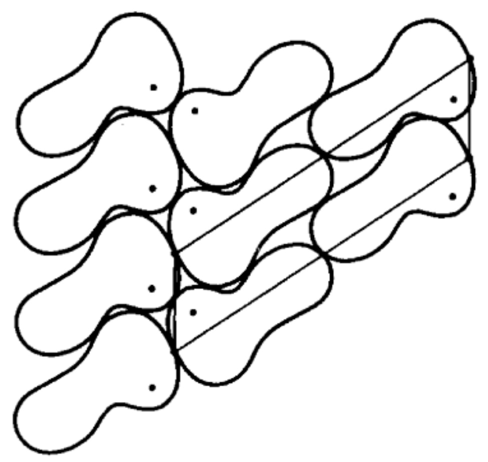

Fig. 20. Dense layer with symmetry *p2*.

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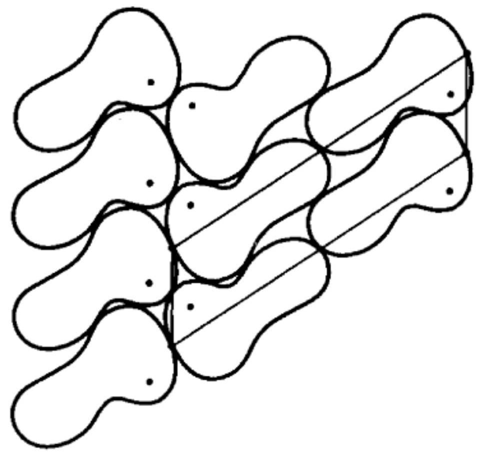

Fig. 20. Dense layer with symmetry *p2*.

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Space groups of maximum density	none	$C2/c$ $P2_12_12$ $Pbcn$	Pmc Cmc $Pnma$	none	Fmm $Pmma$ $Pmnn$	$C2/m$ $Pbaa$ $Cmca$	$C222$ $F222$ $I222$ $Ccca$	$Cmmm$ $Fmmm$ $Immm$

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Space groups of maximum density	none	$C2/c$ $P2_12_12$ $Pbcn$	Pmc Cmc $Pnma$	none	Fmm $Pmma$ $Pmnn$	$C2/m$ $Pbaa$ $Cmca$	$C222$ $F222$ $I222$ $Ccca$	$Cmmm$ $Fmmm$ $Immm$

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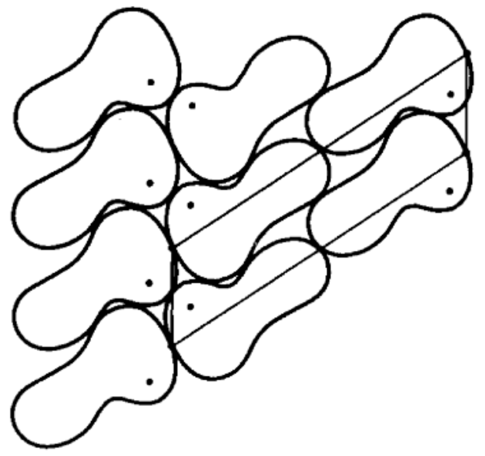

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For molecules with tetrahedral symmetry T_d, the closest packing is attainable in space group $P\bar{1}$.

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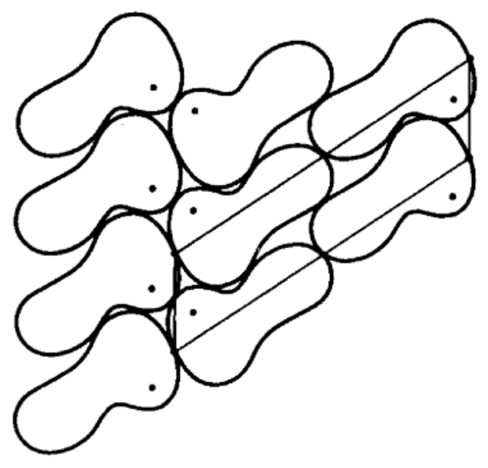

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Space groups of maximum density	none	$C2/c$, $P2_12_12$, $Pbcn$	Pmc, Cmc, $Pnma$	none	Fmm, $Pmma$, $Pmnn$	$C2/m$, $Pbaa$, $Cmca$	$C222$, $F222$, $I222$, $Ccca$	$Cmmm$, $Fmmm$, $Immm$	

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The Leverhulme Research Centre for Functional Materials Design

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THANK YOU

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THANK YOU

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Roland Púček (Ruhr University, Bochum)

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ICNS INTERNATIONAL CENTER FOR NANO-SYSTEMS
Imperial College London
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