# Supplementary Information: A simple solution to the problem of self-assembling cubic diamond crystals

## SI SAT-assembly clauses

| Id | Clauses | Boolean expression |
|---|---|---|
| (i) | $C^{\text{int}}_{c_i,c_j,c_k}$ | $\neg x^{\text{int}}_{c_i,c_j} \vee \neg x^{\text{int}}_{c_i,c_k}$ |
| (ii) | $C^{\text{pcol}}_{s,p,c_k,c_l}$ | $\neg x^{pcol}_{s,p,c_k} \vee \neg x^{\text{pcol}}_{s,p,c_l}$ |
| (iii) | $C^{L}_{l,s_i,o_i,s_j,o_j}$ | $\neg x^{L}_{l,s_i,o_i} \vee \neg x^{L}_{l,s_j,o_j}$ |
| (iv) | $C^{\text{lint}}_{l_i,k_i,l_j,k_j,c_i,c_j}$ | $(x^{A}_{l_i,k_i,c_i} \wedge x^{A}_{l_j,k_j,c_j}) \implies x^{\text{int}}_{c_i,c_j}$ |
| (v) | $C^{\text{LS}}_{l,s,o,c,k}$ | $x^{L}_{l,s,o} \implies \left(x^{A}_{l,k,c} \iff x^{\text{pcol}}_{s,\phi_o(k),c}\right)$ |
| (vi) | $C^{\text{all s.}}_{s}$ | $\bigvee_{\forall l,o} x^{L}_{l,s,o}$ |
| (vii) | $C^{\text{all c.}}_{c}$ | $\bigvee_{\forall s,p} x^{\text{pcol}}_{s,p,c}$ |

Table S1: SAT clauses and variables.

The color interaction is given by binary variables $x^{\text{int}}_{c_i,c_j}$ which are 1 if color $c_i$ is compatible with color $c_j$ and 0 otherwise. The patch coloring for each PP species is described by binary variables $x^{\text{pcol}}_{s,p,c}$ which are 1 if patch $p$ of species $s$ has color $c$ and 0 otherwise. The arrangement of the particle species in the lattice is described by $x^{L}_{l,s,o}$ which is 1 if the position $l$ is occupied by a PP of species $s$ in the specific orientation $o$. The mapping $\phi_o(k) = p$ for a given orientation $o$ means that PP's patch $p$ overlaps with slot $k$ in a given lattice position. The variable $x^{A}_{l,k,c}$ is 1 if slot $k$ of lattice position $l$ is occupied by a patch with color $c$ and 0 otherwise. The clauses and variables are defined for all possible combinations of colors $c \in [1, N_c]$, patches $p \in [1, N_p]$, slots $k \in [1, N_p]$, PP species $s \in [1, N_s]$, orientations $o \in [1, N_o]$ (see Table S4), and lattice positions $l \in [1, L]$. The target topology of the unit cell is encoded in a table (e.g. Table S2) that specifies which positions $l_i, l_j \in [1, L]$ are neighbors. Each position $l_i$ is assigned four slots (numbered from 1 to 4 in Tables in Section SII), and the table specifies which slots of which positions are neighbors in the topology. A patchy particle is placed into each position such that its patches overlap with the slots, as given by its assigned orientation $o$. Clauses $C^{\text{lint}}$ are defined only for slots $k_i, k_j$ that are in contact in neighboring lattice positions $l_i, l_j$. For a given $s$, clause $C^{\text{all s.}}_{s}$ is defined as a list of $x^{L}_{l,s,o}$ for all possible values of $l$ and $o$, joined by disjunctions. Clause $C^{\text{all c.}}_{c}$ is defined analogously. The SAT problem is a conjunction of all clauses. The color interaction matrix is given by the indices of the $x^{\text{int}}_{c_i,c_j}$ that are true in the found solution, and the coloring (which particle species is assigned which color) is given by the indices of variables $x^{\text{pcol}}_{s,p,c}$ that are true. We first define the SAT problem using the topology of CD lattice as given in Table S2. For each identified solution, we formulate a new SAT problem with additional new clauses that require $x^{\text{int}}_{c_i,c_j}$ and $x^{\text{pcol}}_{s,p,c}$ variables that correspond to the identified solution are true. We then reformulate clauses $C^{L}$ to correspond to the HD topology (Table S3). If such a SAT problem is satisfiable, we discard the solution and repeat the process, until we find a solution that satisifies CD topology but does not satisify the HD topology.

## SII Cubic and Hexagonal diamond topologies, list of rotations, and solution

We include here the topology for a unit cell of cubic diamond crystal lattice 16-unit cell, and for hexagonal diamond lattice 32-unit cell. These cells are created by merging smaller unit cells of cubic diamond and hexagonal diamond respectively. In our prior work [1, 2], we found that any solution that satisfies the 8-unit cell of diamond crystal can also satisfy the 32-unit cell of hexagonal diamond. Hence, for the search

| Position $l_i$ | Slot $s_i$ | Position $l_j$ | Slot $s_j$ |
|---|---|---|---|
| 1 | 1 | 16 | 1 |
| 1 | 2 | 15 | 1 |
| 1 | 3 | 6 | 1 |
| 1 | 4 | 5 | 4 |
| 2 | 1 | 16 | 2 |
| 2 | 2 | 6 | 4 |
| 2 | 3 | 5 | 3 |
| 2 | 4 | 15 | 4 |
| 3 | 1 | 5 | 1 |
| 3 | 2 | 6 | 3 |
| 3 | 3 | 7 | 3 |
| 3 | 4 | 8 | 4 |
| 4 | 1 | 8 | 3 |
| 4 | 2 | 6 | 2 |
| 4 | 3 | 5 | 2 |
| 4 | 4 | 7 | 2 |
| 7 | 1 | 9 | 2 |
| 7 | 4 | 10 | 4 |
| 8 | 1 | 9 | 1 |
| 8 | 2 | 10 | 1 |
| 9 | 3 | 14 | 1 |
| 9 | 4 | 13 | 4 |
| 10 | 2 | 14 | 4 |
| 10 | 3 | 13 | 3 |
| 11 | 1 | 13 | 1 |
| 11 | 2 | 14 | 3 |
| 11 | 3 | 15 | 3 |
| 11 | 4 | 16 | 4 |
| 12 | 1 | 16 | 3 |
| 12 | 2 | 14 | 2 |
| 12 | 3 | 13 | 2 |
| 12 | 4 | 15 | 2 |

Table S2: Cubic diamond 16-unit cell topology: List of lattice positions $l_i$ and $l_j$ that are neighbors in the unit cell of the lattice and their respective slot numbers $s_i$, $s_j$ through which they are bound. The unit cell of size 16 is obtained by pasting together two unit cells of size 8.

of patchy particle solutions that can form cubic diamond, we look for solutions that satisfy a 16-unit cell, but cannot form a 32-unit hexagonal diamond cell, using the SAT-assembly approach outlined above. The list which unit cell position of the 16-unit cell cubic diamond lattice is occupied by which species of the two-particle species solution is listed in Table S5.

| Position $l_i$ | Slot $s_i$ | Position $l_j$ | Slot $s_j$ |
|---|---|---|---|
| 1 | 1 | 5 | 1 |
| 1 | 2 | 8 | 1 |
| 1 | 3 | 13 | 1 |
| 1 | 4 | 24 | 1 |
| 2 | 1 | 6 | 1 |
| 2 | 2 | 7 | 1 |
| 2 | 3 | 14 | 1 |
| 2 | 4 | 23 | 1 |
| 3 | 1 | 5 | 2 |
| 3 | 2 | 7 | 2 |
| 3 | 3 | 15 | 1 |
| 3 | 4 | 21 | 1 |
| 4 | 1 | 6 | 2 |
| 4 | 2 | 8 | 2 |
| 4 | 3 | 16 | 1 |
| 4 | 4 | 22 | 1 |
| 5 | 3 | 9 | 1 |
| 5 | 4 | 19 | 1 |
| 6 | 3 | 10 | 1 |
| 6 | 4 | 20 | 1 |
| 7 | 3 | 11 | 1 |
| 7 | 4 | 18 | 1 |
| 8 | 3 | 12 | 1 |
| 8 | 4 | 17 | 1 |
| 9 | 2 | 13 | 2 |
| 9 | 3 | 31 | 1 |
| 9 | 4 | 15 | 2 |
| 10 | 2 | 14 | 2 |
| 10 | 3 | 32 | 1 |
| 10 | 4 | 16 | 2 |
| 11 | 2 | 14 | 4 |
| 11 | 3 | 30 | 1 |
| 11 | 4 | 15 | 4 |
| 12 | 2 | 13 | 4 |
| 12 | 3 | 29 | 1 |
| 12 | 4 | 16 | 4 |
| 13 | 3 | 28 | 1 |
| 14 | 3 | 27 | 1 |
| 15 | 3 | 25 | 1 |
| 16 | 3 | 26 | 1 |
| 17 | 2 | 21 | 2 |
| 17 | 3 | 29 | 2 |
| 17 | 4 | 24 | 2 |
| 18 | 2 | 22 | 2 |
| 18 | 3 | 30 | 2 |
| 18 | 4 | 23 | 2 |
| 19 | 2 | 21 | 4 |
| 19 | 3 | 31 | 2 |
| 19 | 4 | 23 | 4 |
| 20 | 2 | 22 | 4 |
| 20 | 3 | 32 | 2 |
| 20 | 4 | 24 | 4 |
| 21 | 3 | 25 | 2 |
| 22 | 3 | 26 | 2 |
| 23 | 3 | 27 | 2 |
| 24 | 3 | 28 | 2 |
| 25 | 3 | 29 | 3 |
| 25 | 4 | 31 | 3 |
| 26 | 3 | 30 | 3 |
| 26 | 4 | 32 | 3 |
| 27 | 3 | 30 | 4 |
| 27 | 4 | 31 | 4 |
| 28 | 3 | 29 | 4 |
| 28 | 4 | 32 | 4 |

Table S3: Hexagonal 32-unit cell topology, obtained by joining 4 unit cell lattices. List of lattice positions $l_i$ and $l_j$ that are neighbors in the unit cell and their respective slot numbers $s_i$, $s_j$ through which they are bound

| Orientation $o$ | Mapping $\phi_o$ |
|---|---|
| 1 | (1,2,3,4) |
| 2 | (1,4,2,3) |
| 3 | (1,3,4,2) |
| 4 | (2,4,3,1) |
| 5 | (2,1,4,3) |
| 6 | (2,3,1,4) |
| 7 | (4,1,3,2) |
| 8 | (4,2,1,3) |
| 9 | (4,3,2,1) |
| 10 | (3,1,2,4) |
| 11 | (3,4,1,2) |
| 12 | (3,2,4,1) |

Table S4: List of orientations $o$ for a PP with a tetrahedral symmetry of patch positions. Each orientation determines a mapping $\phi_o$, which specifies which patches overlap with patches in the original position before applying the rotation. The first mapping for $o = 1$ corresponds to no rotation.

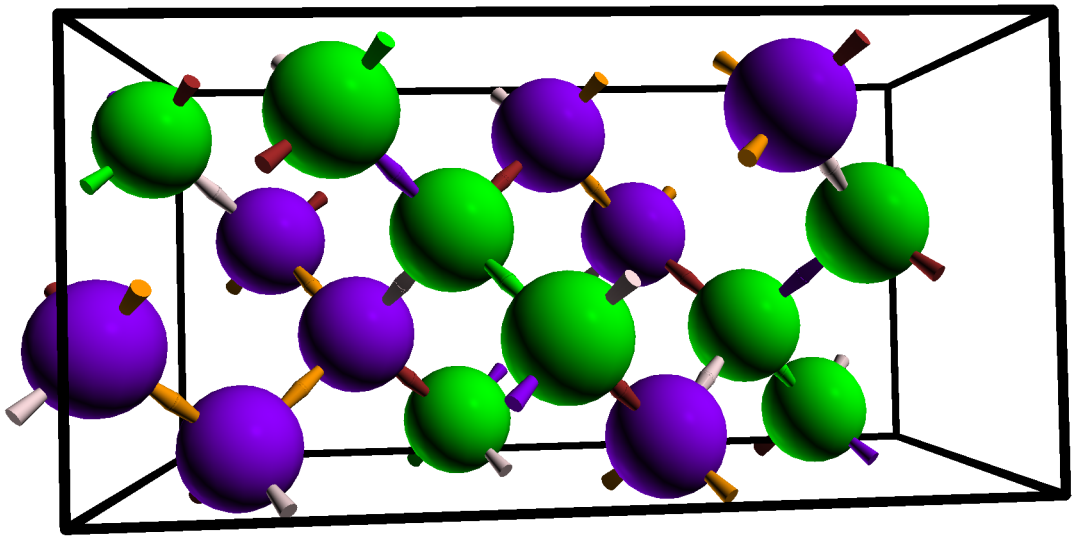

Figure S1: The 16-unit cell of cubic diamond lattice, with the respective positions occupied by particles of species 1 (green) or 2 (violet). The file with coordinates of the respective positions is available on the zenodo archive provided in the main text.

| Lattice position $l$ | Particle Species | Orientation $o$ |
|---|---|---|
| 1 | 2 | 3 |
| 2 | 1 | 9 |
| 3 | 1 | 12 |
| 4 | 2 | 12 |
| 5 | 1 | 10 |
| 6 | 1 | 2 |
| 7 | 2 | 9 |
| 8 | 2 | 6 |
| 9 | 1 | 7 |
| 10 | 2 | 2 |
| 11 | 2 | 8 |
| 12 | 1 | 1 |
| 13 | 1 | 3 |
| 14 | 1 | 12 |
| 15 | 2 | 1 |
| 16 | 2 | 12 |

Table S5: List of particle species and their orientations $o$ that are assigned to the 16-unit cubic diamond lattice cell for the two-species solution. The orientations are set so that the particles in neighboring positions are arranged such that complementary patches are in contact.

# References


[1] F. Romano, J. Russo, L. Kroc, and P. Šulc. Designing patchy interactions to self-assemble arbitrary structures. *Physical Review Letters*, 125(11):118003, 2020.

[2] J. Russo, F. Romano, L. Kroc, F. Sciortino, L. Rovigatti, and P. Šulc. SAT-assembly: A new approach for designing self-assembling systems. *Journal of Physics: Condensed Matter*, 2022.