

Densest plane group packings of regular polygons

Miloslav Torda*

*Leverhulme Research Centre for Functional Materials Design, University of Liverpool, Liverpool, UK and
Department of Computer Science, University of Liverpool, Liverpool, UK*

John Y. Goulermas† and Vitaliy Kurlin‡

Department of Computer Science, University of Liverpool, Liverpool, UK

Graeme M. Day§

School of Chemistry, University of Southampton, Southampton, UK

Packings of regular convex polygons (n -gons) that are sufficiently dense have been studied extensively in the context of modeling physical and biological systems as well as discrete and computational geometry. Former results were mainly regarding densest lattice or double-lattice configurations. Here we consider all 2-dimensional crystallographic symmetry groups (plane groups) by restricting the configuration space of the general packing problem of congruent copies of a compact subset of the 2-dimensional Euclidean space to particular isomorphism classes of the discrete group of isometries. We formulate the plane group packing problem as a nonlinear constrained optimization problem. By means of the Entropic Trust Region Packing Algorithm that approximately solves this problem, we examine some known and unknown densest packings of various n -gons in all 17 plane groups and state conjectures about common symmetries of the densest plane group packings for every n -gon.

I. INTRODUCTION

Understanding the packing properties of crystalline solids has important implications for solid state physics modeling [1], materials science [2, 3], and biophysics [4]. In 2-dimensional Euclidean space, crystal structures based on the densely packed representations of a molecule by a regular convex polygon (n -gon) were found to be adequate models for virus structures [5] or self-assembly of organic molecules on metal surfaces [6]. Compared to the densest packings, lower density but higher symmetry crystal structures of complex noncovalent molecular systems on surface substrates [7], monolayer covalent organic frameworks [8], or 2-dimensional crystallization of proteins on lipid monolayers [9] can also be regarded as densest packings, although among a particular isomorphism class of periodic structures.

Moreover, the crystallization problem and the disc packing problem are identical in the Euclidean space of dimensions 2 for some energy potentials [10, 11]. Thus, fast ways of identifying dense packings could accelerate predictions of molecular crystal structures, where the usual approach is to search for the lowest energy configurations [12].

The packing problem is well-studied in discrete and computational geometry. Substantial consideration has been given to densest lattice [13, 14] and double-lattice packings [15, 16] as special cases of the general densest packing configurations. On the other hand, little is

known about densest packings when configurations are restricted to the remaining isomorphism classes of discrete groups of isometries of the 2-dimensional Euclidean space.

We examine the densest packings of various n -gons where the packing configurations are restricted to one of the 17 isomorphism classes of the discrete group of isometries of the 2-dimensional Euclidean space containing a lattice subgroup, in literature also referred to as plane groups or wallpaper groups. Fig. 2 illustrates plane group packings on densest $p2$, $p2gg$, pg , $p3$ and $p1$ configurations of a pentagon, heptagon, enneagon, and dodecagon. We consider finding the densest plane group packing as a nonlinear, constrained, and bounded optimization problem. Using the Entropic Trust Region Packing Algorithm [17], developed specifically to search for densest crystal-

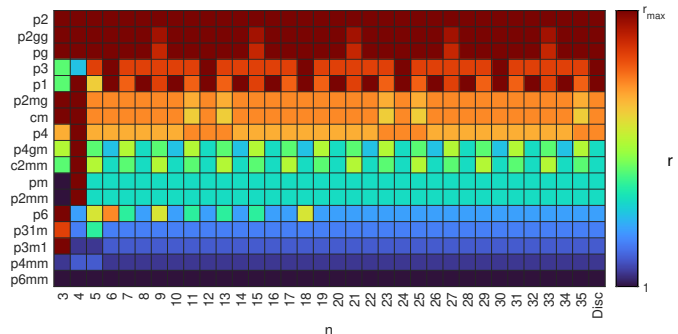


FIG. 1: The colored rank table of plane groups in relation to the number of vertices n of an n -gon. For every $n = 3, \dots, 35$ plane groups are ordered according to densities in Table I, and a color is assigned based on rank r ranging from 1 to r_{max} . The value of r_{max} depends on a specific n -gon.

* miloslav.torda@liverpool.ac.uk

† j.y.goulermas@liverpool.ac.uk

‡ vitaliy.kurlin@liverpool.ac.uk

§ G.M.Day@soton.ac.uk

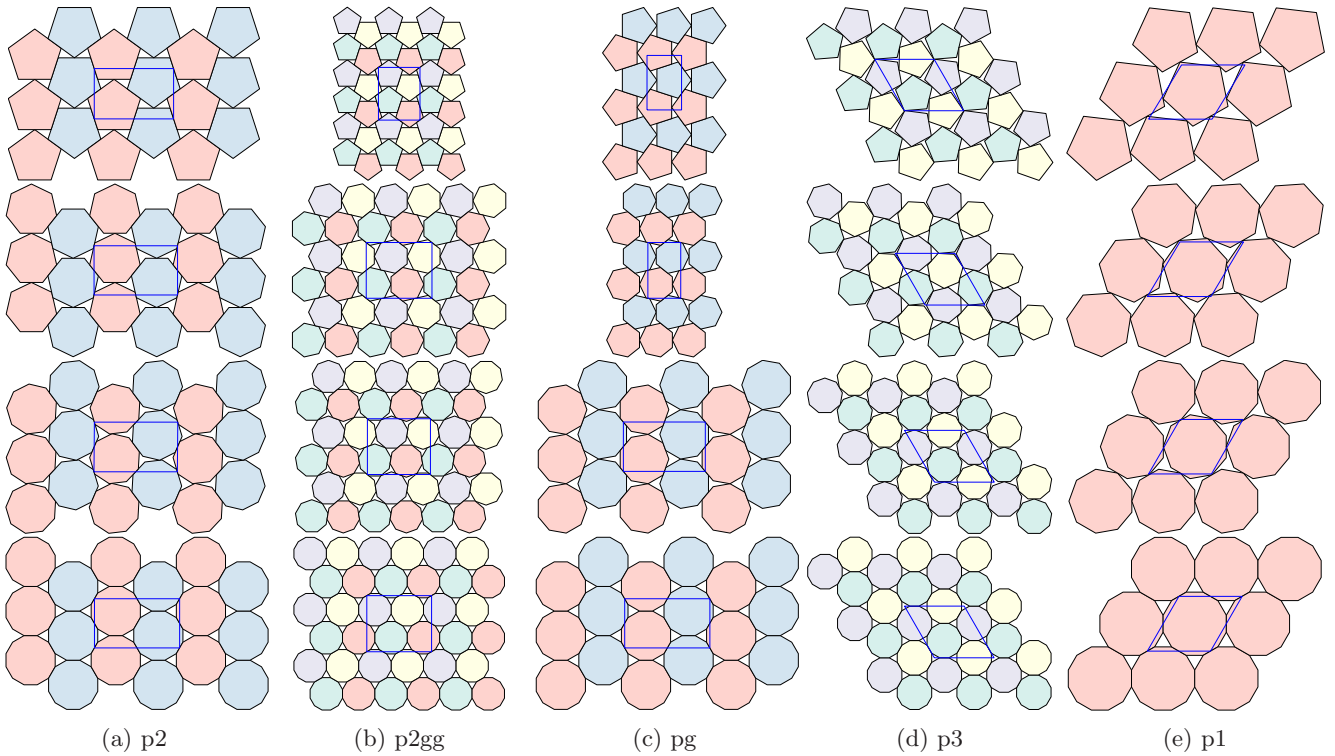


FIG. 2: Densest configurations of (from top to bottom) pentagon, heptagon, enneagon and dodecagon in plane groups $p2$, $p2gg$, pg , $p3$, and $p1$ with the following densities: pentagon in $p2/p2gg/pg \approx 0.92131$, $p3 \approx 0.87048$ and $p1 \approx 0.81725$; heptagon in $p2/p2gg/pg \approx 0.89269$, $p3 \approx 0.88085$ and $p1 \approx 0.86019$; enneagon in $p2 \approx 0.90103$, $p2gg \approx 0.89989$, $pg \approx 0.89860$ and $p3/p1 \approx 0.88773$; dodecagon in $p2/p2gg/pg/p3/p1 \approx 0.92820$. The blue parallelogram denotes the primitive cell of the respective configuration. Colors represent symmetry operations modulo lattice translations.

lographic symmetry group packings of arbitrary dimension, we successfully recover approximations of known densest lattice and double-lattice packing configurations including a disc, regarded as a limiting n -gon when the number of vertices approaches infinity. Additionally, we obtained the previously unknown highest density packings of the n -gons for all 17 plane groups and n equal to 3, 4, \dots , 25, 30, 35, 36, 37, 39, 42, 55, 89.

Our experiments suggest the following relationships between symmetries of n -gons and shared symmetries of their respective densest plane group packing configurations divided into three classes. In the $p2/p2gg/pg/p3/p1$ plane group class,

1. except for centrally non-symmetric n -gons containing a 3-fold rotational symmetry with number of vertices higher or equal to 9, densities of the densest $p2$, $p2gg$ and pg configurations are equal,
2. for centrally symmetric n -gons, densities of the densest $p2$, $p2gg$, pg and $p1$ configurations are equal,
3. for centrally non-symmetric n -gons containing a 3-fold rotational symmetry, densities of the densest $p3$ and $p1$ configurations are equal,

4. for centrally symmetric n -gons containing a 3-fold rotational symmetry, densities of the densest $p2$, $p2gg$, pg , $p3$ and $p1$ configurations are equal,

in the $p2mg/cm/p4$ plane group class,

1. except for n -gons with vertices equal to $12k - 1$ and $12k + 1$, where k is an integer, densities of densest $p2mg$ and cm configurations are equal,
2. for all n -gons with 12-fold rotational symmetry, densities of the densest $p2mg$, cm and $p4$ configurations are equal,

and in the $p4gm/c2mm/pm/p2mm$ plane group class,

1. densities of the densest pm and $p2mm$ configurations are equal for all n -gons,
2. for centrally symmetric n -gons, densities of the densest pm , $p2mm$, and $c2mm$ configurations are equal,
3. for n -gons containing a 4-fold rotational symmetry, densities of the densest pm , $p2mm$, $c2mm$ and $p4gm$ configurations are equal,

Consequently, the densest known packings of a pentagon and a heptagon have higher symmetries than that of a double-lattice configuration.

Fig. 1 visually summarizes our results. For each n -gon, all groups are ranked according to the density of the respective densest plane group packing, either obtained experimentally or extrapolated from the rankings of n -gons with similar symmetries. For instance, the ranking of densities of a 33-gon is based on rankings of 9-gon, 15-gon, 21-gon and 39-gon.

The manuscript is organized in the following way. Section II introduces the plane group packing and the underlying densest plane group packing problem. In Section III, we present the densest plane group packings of regular n -gons. We examine the symmetries of packing configurations in distinct plane group classes based on symmetries of densest plane group packings of a disc. Section IV summarizes our experimental results in the form of multiple conjectures about common symmetries of the densest plane group packings of n -gons for arbitrary n .

II. PLANE GROUP PACKING

We consider the 2-dimensional Crystallographic Symmetry Group (CSG) G , which is a discrete subgroup of the group of isometries of the 2-dimensional Euclidean space containing a lattice subgroup. The parallelogram spanned by the generators of the lattice L associated with CSG G is called the primitive cell and is denoted by U_L . An asymmetric unit is a subset of the primitive cell such that the whole 2-dimensional Euclidean space is filled when the CSG symmetry operations are applied.

It has to be noted that the term CSG has two distinct meanings in literature; one referring to an actual group and the other to a group isomorphism class. We refer to isomorphism classes of 2-dimensional CSGs as plane groups. All 2-dimensional CSGs are classified into 17 plane groups. Each class is assigned to one of the four maximal crystallographic point group conjugacy classes, referred to as the crystal system. In all the following, we use the International Union of Crystallography plane group notation [18].

Given a 2-dimensional CSG G , an element of a plane group \mathcal{G} , and a polygon K whose centroid lies in the asymmetric unit of G , by a CSG packing \mathcal{K}_G , we mean a collection of non-overlapping orbits of K with respect to the G -action on the Euclidean plane.

Since a CSG packing \mathcal{K}_G is a periodic system of rotated and translated copies of polygon K , following the formula for the density of packing of a periodic system [19], the density of a CSG packing has a simple closed form expression

$$\rho(\mathcal{K}_G) = \frac{N \text{area}(K)}{\text{area}(U_L)},$$

where N is the number of symmetry operations in CSG G modulo translations by the lattice associated with G , U_L is the primitive cell, and $\text{area}(\cdot)$ denotes area.

Given a plane group \mathcal{G} and a polygon K , the densest plane group packing of K is a CSG packing $\mathcal{K}_{G_{\max}}$ that maximizes packing density over the whole isomorphism class \mathcal{G} . Formally expressed,

$$\mathcal{K}_{G_{\max}} = \underset{\mathcal{K}_G \in \mathcal{G}}{\text{argmax}} \rho(\mathcal{K}_G).$$

Here we search not only over the whole plane group \mathcal{G} but also over all rotations and translations of K , whose centroid lies in the asymmetric unit of G such that the resulting configuration is a CSG packing.

Fig. 2 presents examples of the densest plane group packings of a pentagon, heptagon, enneagon, and dodecagon in plane groups $p2$, $p2gg$, pg , $p3$, and $p1$.

We consider the densest plane group packing as a nonlinear, constrained, and bounded optimization problem. We transform this problem via stochastic relaxation [20] to the problem of estimation of a probability distribution with the probability mass concentrated on the maxima of the optimization landscape. The 2-dimensional lattice group L associated with a CSG induces a quotient space \mathbb{R}^2/L , which is homeomorphic to a 2-dimensional torus. Therefore, we define a parametric family of probability distributions based on the multivariate von Mises distribution [21], the Extended Multivariate von Mises distribution (EMvM), and perform a stochastic trust region search on the functional space induced by this family of toroidal probability distributions where the Kullback-Leibler divergence [22] defines the trust region radius. The resulting Entropic Trust Region Packing Algorithm (ETRPA) is a variant of the natural gradient method [23].

At the first iteration, N samples are drawn from a uniform distribution on an n -dimensional torus. The number of samples used and dimensionality of torus depend on the crystal system of the plane group where the search is performed. For instance, in the case of the $p2$ group there are six configuration parameters, two for fractional coordinates of the polygon's centroid in the asymmetric unit, one for the angle of rotation of the polygon, and three parameters defining the shape of the primitive cell, that is lengths of lattice generators and an angle between them. For a 6-dimensional torus, the dimensionality of the EMvM parametric space is $p = 72$, and number of samples drawn at each iteration is set such that $\frac{p}{N} < 0.07$, meaning that for the search in $p2$ group $N = 1040$. An overlap constraint violation is evaluated for each sampled configuration, and for configurations with no intersections between polygons packing density is computed. Afterwards, a new batch of samples is generated from the EMvM based on distribution parameters estimates of the largest increase in density and lowest constraint violation. This process is repeated until the algorithm converges to a point distribution or after 8000 iterations.

There are two main benefits of ETRPA. First, the search does not depend on initial configurations, a caveat of many stochastic search methods. The initial sampling from the uniform distribution on an n -dimensional

	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	Disc ^a	
p2	.99999	.99999	.92131	.99999	.89269	.90616	.90103	.91371	.90766	.92820	.90437	.90746	.90471	.90901	.90692	.91622	.90595	.90733	.90577	.90789	.90683	.91211	.90642	.90689	
p2 _{gg}	.99999	.99999	.92131	.99999	.89269	.90616	.89989	.91371	.90766	.92820	.90437	.90746	.90403	.90901	.90692	.91622	.90595	.90733	.90536	.90789	.90683	.91211	.90642	.90689	
pg	.99999	.99999	.92131	.99999	.89269	.90616	.89860	.91371	.90766	.92820	.90437	.90746	.90369	.90901	.90692	.91622	.90595	.90733	.90523	.90789	.90683	.91211	.90642	.90689	
p3	.66666	.77376	.87048	.99999	.88085	.87665	.88773	.88775	.89896	.92820	.90005	.89722	.90017	.89950	.90348	.91622	.90379	.90218	.90349	.90300	.90500	.91211	.90513	.90689	
p1	.66666	.99999	.81725	.99999	.86019	.90616	.88773	.91371	.88912	.92820	.89383	.90746	.90017	.90901	.89947	.91622	.90084	.90733	.90349	.90789	.90284	.91211	.90341	.90689	
p2 _{mg}	.99999	.99999	.85410	.85714	.84226	.86555	.83419	.83722	.83116	.86156	.83306	.83823	.83993	.84856	.84215	.84346	.84189	.84571	.84052	.84068	.83929	.84662	.83952	.84178	
cm	.99999	.99999	.85410	.85714	.84226	.86555	.83419	.83722	.82795	.86156	.83212	.83823	.83993	.84856	.84215	.84346	.84189	.84571	.84052	.84068	.83865	.84662	.83916	.84178	
p4	.71281	.99999	.84211	.81776	.84219	.85031	.83030	.83004	.83780	.86156	.83691	.83527	.83765	.84613	.84190	.83945	.84177	.84367	.83971	.83933	.84072	.84662	.84061	.84178	
p4 _{gm}	.69615	.99999	.71119	.74613	.76477	.82842	.76593	.77205	.77628	.80384	.77662	.77869	.78028	.79564	.78043	.78137	.78213	.79192	.78220	.78271	.78313	.78991	.78317	.78539	
c2 _{mm}	.66666	.99999	.71714	.74999	.76253	.82842	.76697	.77254	.77570	.80384	.77697	.77882	.78006	.79564	.78058	.78141	.78202	.79192	.78229	.78273	.78307	.78991	.78322	.78539	
pm	.49999	.99999	.69098	.74999	.73825	.82842	.75712	.77254	.76655	.80384	.77193	.77882	.77530	.79564	.77754	.78141	.77911	.79192	.78025	.78273	.78111	.78991	.78177	.78539	
p2 _{mm}	.49999	.99999	.69098	.74999	.73825	.82842	.75712	.77254	.76655	.80384	.77193	.77882	.77530	.79564	.77754	.78141	.77911	.79192	.78025	.78273	.78111	.78991	.78177	.78539	
p6	.99999	.72193	.75933	.85714	.75740	.76438	.78535	.76932	.77293	.79560	.77254	.77326	.77997	.77425	.77536	.78533	.77523	.77536	.77863	.77571	.77622	.78181	.77616	.77734	
p3 _{1m}	.74999	.66323	.70166	.71999	.72084	.71565	.73410	.71653	.72182	.74613	.72205	.72380	.73087	.72583	.72735	.72825	.72787	.72698	.72996	.72662	.72722	.73320	.72725	.72900	
p3 _{m1}	.99999	.49742	.53854	.66666	.57196	.57980	.63041	.58887	.59164	.61880	.59535	.59664	.61359	.59851	.59921	.61081	.60029	.60071	.60915	.60139	.60166	.60807	.60211	.60459	
p4 _{mm}	.57735	.49999	.55537	.52148	.51446	.56854	.52443	.53314	.54240	.53589	.54144	.53607	.53385	.54604	.53500	.53725	.54014	.53792	.53994	.53783	.53683	.54211	.53716	.53901	
p6 _{mm}	.49999	.46410	.49372	.47999	.49025	.48235	.48940	.48305	.47750	.49742	.47995	.48454	.48724	.48518	.48675	.48550	.48660	.48548	.48664	.48542	.48409	.48880	.48418	.48600	

^a We consider the disc as a limiting n -gon where the number of vertices n approaches infinity.

TABLE I: Densities of the densest plane group packing configurations of n -gons obtained by ETRPA for $n = 3, 4, \dots, 25$. The densities are truncated at the 5th decimal place.

torus provides a satisfactory overview of the optimization landscape induced by the configuration space. Second, by performing the search on an n -dimensional torus, we cover problematic instances when the optimal solution lies on the boundary.

To further improve the accuracy of the approximate solutions, after the initial run of the ETRPA search, we perform a refining process by creating progressively smaller ϵ -neighbourhoods around the best solution found and employ ETRPA with new boundaries defined by the ϵ -neighbourhoods. To prevent the escape of the optimal solution from the ϵ -neighbourhood, if a solution with higher density than in previous runs is found, the ϵ -neighbourhood is not decreased only centered on this solution. Otherwise, the ϵ -neighbourhood is decreased. The lowering of ϵ is repeated 30 times.

It has to be noted that the entropic trust region is not a physical simulation since particles in the system are allowed to overlap during the search. A detailed treatment of ETRPA is presented for the interested reader in [17].

III. RESULTS

Using the ETRPA, we recovered known as well as obtained previously unknown densest packings of n -gons for $n = 3, 4, \dots, 25, 30, 35, 36, 37, 39, 42, 55, 89$ in all 17 plane groups, including a disc regarded as a limiting n -gon when the number of vertices n approaches infinity. The densities of the densest configurations obtained in our experiments for $n = 3, 4, \dots, 25$ are shown in Table I [24]. All the values are truncated at the fifth decimal place.

In the following paragraphs, we examine these configurations classified according to the disc's densest plane group packings. Since the symmetry group of a circle contains symmetries of all n -gons, our results indicate that the 24-fold rotational symmetry of an n -gon is sufficient to constitute the optimal plane group configurations of a disc and further suggests a relationship with the plane group symmetries. Notably, for the

packing densities to be equal in the plane group class $p2/p2gg/pg/p3/p1$, 2-fold and 3-fold rotational symmetries are necessary, examined in Section III A. In the class $p2mg/cm/p4$, a 4-fold rotational and a local 3-fold symmetry is necessary, examined in Section III B, and in the class $p4gm/c2mm/pm/p2mm$, a 4-fold rotational symmetry is necessary, examined in Section III C. In the context of the crystallographic restriction theorem [25], which states that periodic crystals can only have 2-fold, 3-fold, 4-fold, and 6-fold rotational symmetries, minimal rotational symmetry containing all preceding is 12-fold. However, a 12-fold rotational symmetry of an n -gon does not cover a local 8-fold rotational symmetry that is present in a disc's optimal $p4mm$ packing, as demonstrated in Section III D. Therefore, minimal symmetry containing the symmetries mentioned earlier is a 24-fold rotational symmetry.

A. Densest $p2$, pg , $p2gg$, $p3$, and $p1$ packings

It is known that the packing density of the densest packing of a disc is $\frac{\pi}{\sqrt{12}} \approx 0.9068996\dots$ [14]. This density was attained as the densest plane group packing of a disc in groups $p2$, $p2gg$, pg , $p3$, and $p1$.

The highest packing densities among all plane groups were observed in the plane group $p2$ for all examined n -gons. The $p2$ group is sometimes referred to as a double lattice since it can be viewed as a collection of two lattices related by a 2-fold rotational symmetry.

Our results are consistent with known densest packings of polygons, that is, the uniform triangular, square, and hexagonal tilings, densest known packing of a pentagon [16], heptagon [15], octagon [26], enneagon [27], and disc [28]. Moreover, given that the double lattice packing is at least locally optimal for convex polygons in the space of all packings [29] and that the plane group packings are inherently periodic, our results support the optimality of $p2$ packing among all plane group packings.

Additionally, for the space of plane group packing configurations, we experimentally verified the conjecture

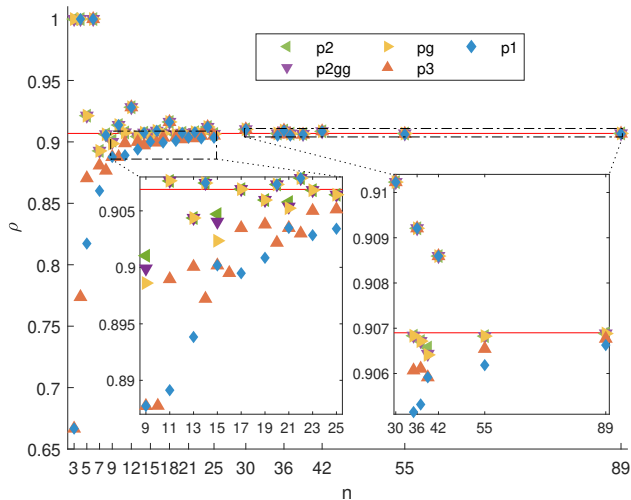


FIG. 3: Densities of the densest packings of examined n -gons in the $p2/p2gg/pg/p3/p1$ plane groups class. The red line denotes the density of the densest disc packing in this plane group class.

that the densest $p2$ packing of the heptagon is less than any other shape [30]. The extremality of the heptagon can be generalized to all n -gons since the $p2$ packing density converges to the optimal packing density of a disc when the number of vertices is increased, as is shown in Fig. 3. Moreover, our results suggest that for every n -gon such that $n > 6k + 1 = m$ and $k \in \mathbb{N}$ the densest $p2$ n -gon packing is strictly higher than the densest $p2$ m -gon packing.

Further, our results show that for some n -gons, the densest plane group packings in groups $p2$, $p2gg$, and pg are equal. Thus the densest known configurations of pentagon and heptagon have higher symmetry than a double lattice, and these configurations can be realized using a glide reflection instead of a rotation by π around the center of symmetry of the $p2$ group. This observation holds for every n -gon we examined, where the number of vertices n of a given n -gon is not equal to $3k$ where $k = 2, 3, \dots$

It is known that the group $p2gg$ has three maximal non-isomorphic subgroups, one with $p2$ symmetry and two with pg symmetry [18]. Due to the mirror symmetry of n -gons and the equality of densest $p2$ and pg configurations, in the densest $p2gg$ configuration, the $p2$ subgroup induces an additional pg symmetry, and the glide reflection plane of one of the pg subgroups induces an additional $p2$ symmetry. Thus, the densest $p2gg$ configuration coincides with the densest $p2$ and pg configurations in these cases.

The only instances where the equality between maximal densities in groups $p2$, $p2gg$, and pg does not hold is for n -gons with 3-fold but no central symmetry where $n \geq 9$. The lowest densities of these three packing configurations were attained in the pg group. Furthermore, any densest pg configuration of an n -gon can be easily con-

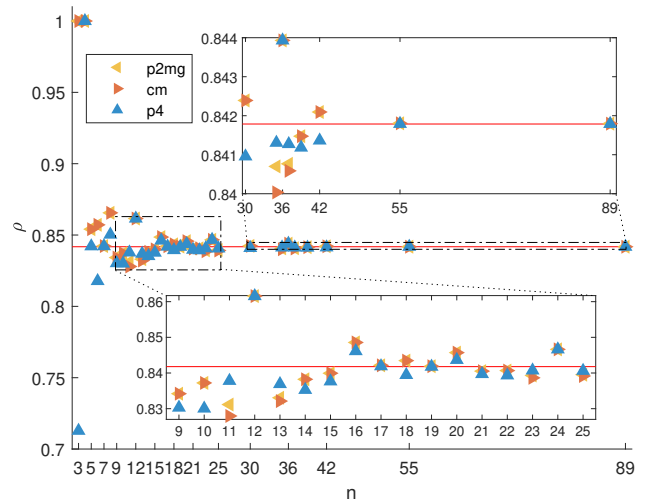


FIG. 4: Densities of the densest packings of examined n -gons in the $p2mg/cm/p4$ plane groups class. The red line denotes the density of the in this plane group class.

verted to a $p2gg$ and $p2$ packing with the same density, which means that the densest pg packings for a fixed n can serve as a lower bound for $p2$ and $p2gg$ densest packings. In fact, this lower bound was attained as densest $p2$ and $p2gg$ packings for all but centrally non-symmetric n -gons containing a 3-fold rotational symmetry and $n \geq 9$. The additional symmetry operations in $p2gg$ group and the additional degree of freedom of the $p2$ crystal system (oblique) allow for higher density packing than that of pg in these cases.

The densest packing of a convex compact subset of the 2-dimensional Euclidean space with central symmetry is that of a lattice packing [31]. In the crystallographic setting, it is the plane group $p1$, which is a group containing only lattice translations. Moreover, any lattice packing of a centrally symmetric convex polygon can be easily converted to a $p2$ packing with the same density [32], meaning that for centrally symmetric n -gons, densities of the densest $p1$ and $p2$ packings are equal. Indeed, in our experiments, the densest $p2$ packings of centrally symmetric n -gons attained the same approximate highest density as in $p1$. Moreover, we obtained the same densities as in the densest $p2gg$ and pg packings. These observations suggest that optimal packings of centrally symmetric polygons can also be realized as either two lattices related to each other by a glide reflection or as four lattices related to each other by two glide reflections and 2-fold rotational symmetry. Consequently, optimal packings of centrally symmetric n -gons have higher symmetry than that of a lattice or double lattice packing.

Concerning the densest $p3$ and $p1$ packings of n -gons with 3-fold rotational symmetry, our results show that the densities in these instances are equal. Moreover, combining 2-fold and 3-fold rotational symmetries for n -gons, where the number of vertices n is divisible by 6,

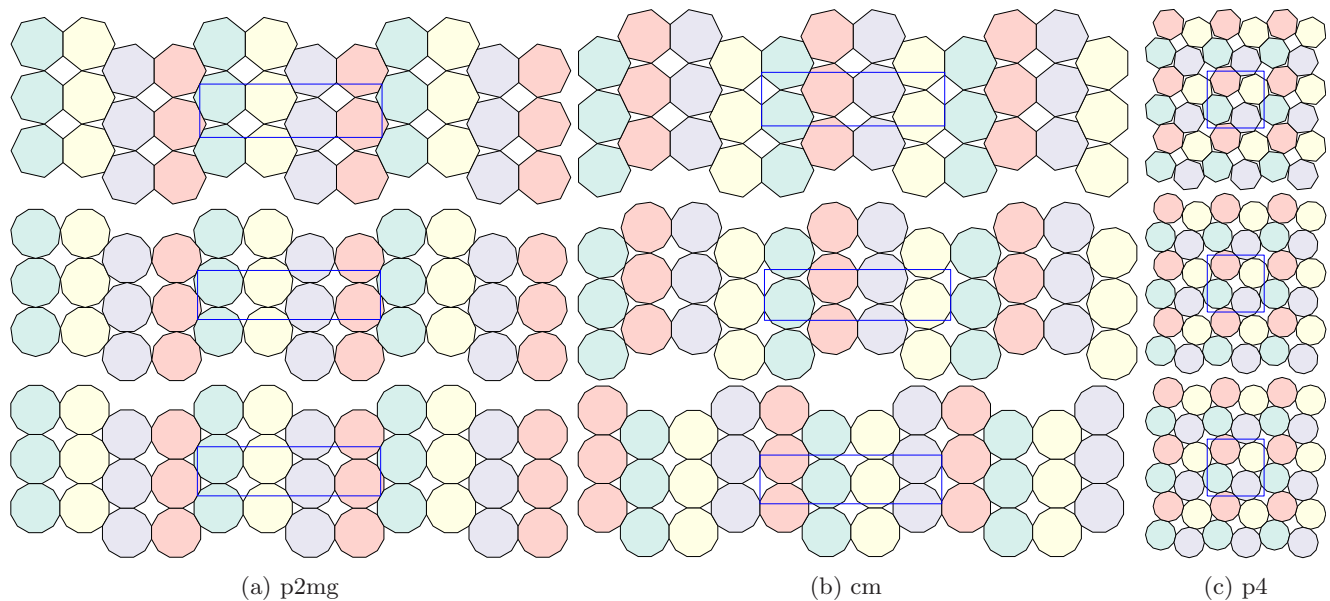


FIG. 5: Densest configurations of (top) heptagon, (middle) endecagon and (bottom) dodecagon in plane groups $p2mg$, cm , and $p4$ with the following densities: heptagon in $p2mg/cm \approx 0.84226$ and $p4 \approx 0.84219$; endecagon in $p2mg \approx 0.83116$, $cm \approx 0.82795$ and $p4 \approx 0.83780$; dodecagon in $p2mg/cm/p4 \approx 0.86156$. The blue parallelogram denotes the primitive cell of the respective configuration. Colors represent symmetry operations modulo lattice translations.

the densities of the densest packings in groups $p2$, $p2gg$, pg , $p3$, and $p1$ are equal. Consequently, in our experiments, the symmetries of optimal packing configurations of n -gons with a 6-fold rotational symmetry coincided with the symmetries of optimal packing configurations of a disc.

Additionally, it is known that the densest $p1$ packing of a regular triangle has the lowest density among all densest $p1$ configurations of 2-dimensional convex shapes [13]. Combined with the observation that for n -gons without central symmetry, densities of the densest $p3$ packings are greater or equal to their respective densest $p1$ packing densities and supported by the convergence of densest $p3$ packing densities to the optimal packing density of a disc, shown in Fig. 3, suggests that the regular triangle also minimizes the maximum density in the group $p3$.

B. Densest $p2mg$, cm , and $p4$ packings

The packing densities of a disc in plane groups $p2mg$, cm , and $p4$ are equal, with a density of approximately 0.8938363. Our results suggest this is also true for n -gons with 12-fold rotational symmetry. The difference between these $p2mg/cm$, and $p4$ packing configurations is that the $p4$ and $p2mg/cm$ packing configurations are not isometric, as can be observed by visual comparison in the example of a dodecagon in Fig. 5. However, there is a local 3-fold rotational symmetry of dodecagonal trimers and 4-fold rotational symmetry of dodecagonal tetramers present in $p2mg$, cm and $p4$ configurations.

The densities of densest $p2mg$ and cm packings are

equal for all n -gons we examined except for those where the number of vertices is close to a polygon with 12-fold rotational symmetry. Precisely, for $12k - 1$ and $12k + 1$, where $k \in \mathbb{N}$. In fact, they are isometric. On the other hand, for centrally symmetric n -gons there are at least two non-isometric densest $p2mg$ configurations shown on the example of decagon in Fig. 6. Consequently, for centrally symmetric n -gons without 4-fold rotational symmetry there exist densest non-isometric $p2mg$ and cm configurations with equal density.

Visually comparing the heptagon $p2mg$ and cm packings in Fig. 5, the structure of both packing configurations is similar in that the mirror symmetry planes of polygons are orthogonal to the mirror symmetry planes

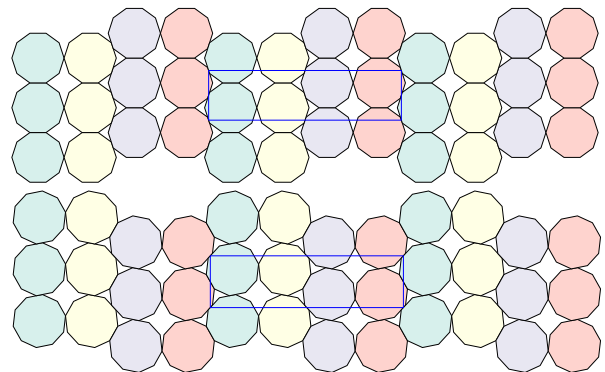


FIG. 6: Two non-isomorphic densest $p2mg$ packings of a decagon obtained by ETRPA with packing density of approximately 0.83722.

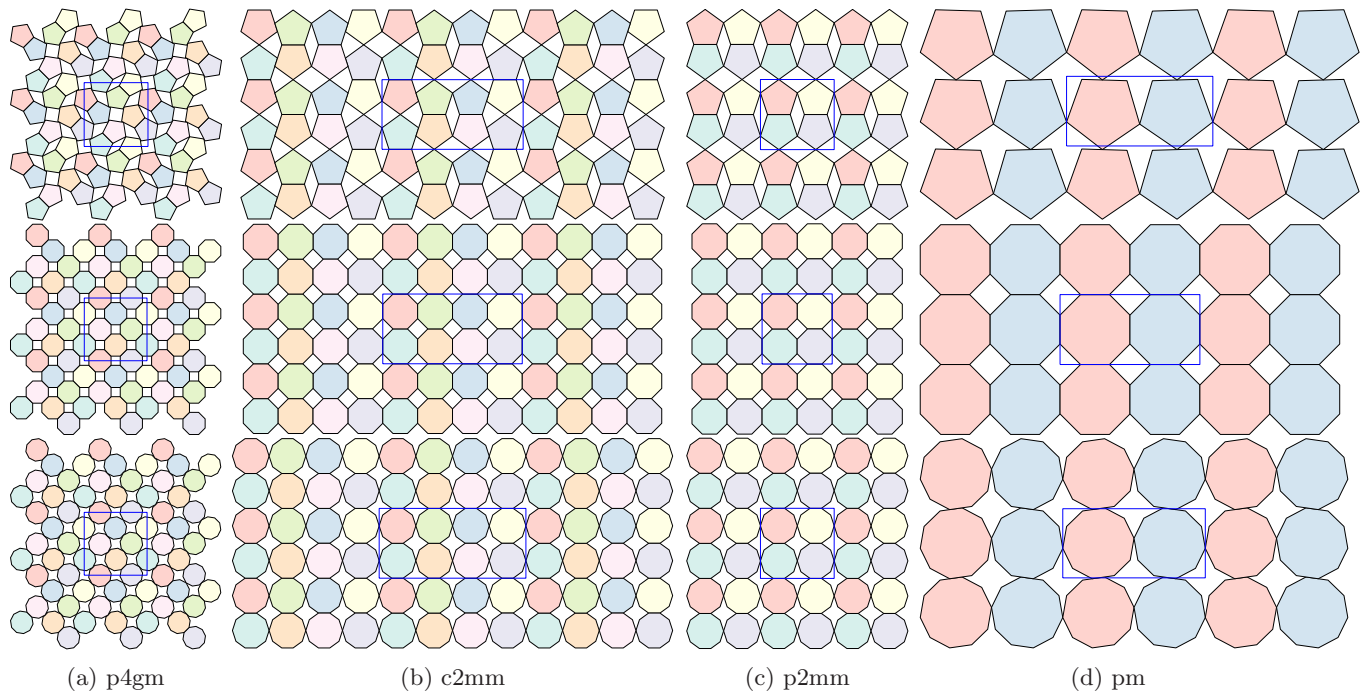


FIG. 7: Densest configurations of (top) pentagon, (middle) octagon and (bottom) decagon in plane groups $p4gm$, $c2mm$, $p2mm$ and pm with the following densities: pentagon in $p4gm \approx 0.71119$, $c2mm \approx 0.71714$ and $p2mm/pm \approx 0.69098$; octagon in $p4gm/c2mm/p2mm/pm \approx 0.82842$; decagon in $p4gm \approx 0.77205$ and $c2mm/p2mm/pm \approx 0.77254$. The blue parallelogram denotes the primitive cell of the respective configuration. Colors represent symmetry operations modulo lattice translations.

of the cm group. This is not the case for the $p2mg$ packing configuration of the endecagon where the planes of mirror symmetries of polygons are parallel to the $p2mg$ mirror symmetry planes of reflection. In fact, it is not hard to convert the densest cm packings in Table I to $p2mg$ packings of equal density, indicating that the densest cm packing configurations of n -gons are lower or equal to the densest $p2mg$ packing configurations. The $12k - 1$ or $12k + 1$ symmetry of the polygon where $k \in \mathbb{N}$ allows for a slightly higher density in $p2mg$ group than in the cm group.

Furthermore, the densities of the densest $p2mg/cm$ packings are greater or equal to $p4$ packings with equality for n -gons with 12-fold rotational symmetry, except in cases of n -gons with $12k - 1$ and $12k + 1$ symmetries, where densest $p4$ packing densities are above corresponding $p2mg/cm$ packing densities. These intricacies

of $p2mg/cm/p4$ packing configurations are visually presented as a colored rank table in Fig. 1.

The highest packing density in groups $p2mg$ and cm was attained by the triangle and square where both polygons tile the 2-dimensional Euclidean plane, and the highest density $p4$ packing configuration was attained by one of the uniform tilings by a square. The lowest packing density in plane groups $p2mg$ and cm was observed in the case of endecagon. The lowest density $p4$ packing was attained by the triangle, although higher than the densities of the densest packings of the triangle in the $p1$ and $p3$ plane groups. From the convergence of n -gon packings to the densest $p2mg/cm/p4$ configurations of a disc, presented in Fig. 4, it is reasonable to assume that the lowest densest packing in this plane group class is attained by the endecagon in $p2mg/cm$ and triangle in $p4$ for all n -gons.

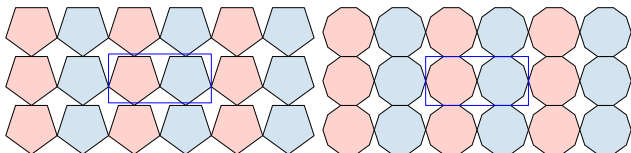


FIG. 8: Manually constructed pm packings of a (left) pentagon and (right) decagon from their respective densest $p2mm$ packing configurations with approximately equal density as their $p2mm$ counterparts presented in Fig. 7.

C. Densest $p4gm$, $c2mm$, pm , and $p2mm$ packings

Densest disc packings in groups $p4gm$, $c2mm$, pm , and $p2mm$ have an equal packing density of 0.7853981, constituting another class of plane groups. The equality between packing density in this plane group class was also true when a 4-fold rotational symmetry was present in an n -gon. In fact, all four configurations are isometric, as seen in the example of an octagon in Fig. 7.

For all examined n -gons, the densities of the densest

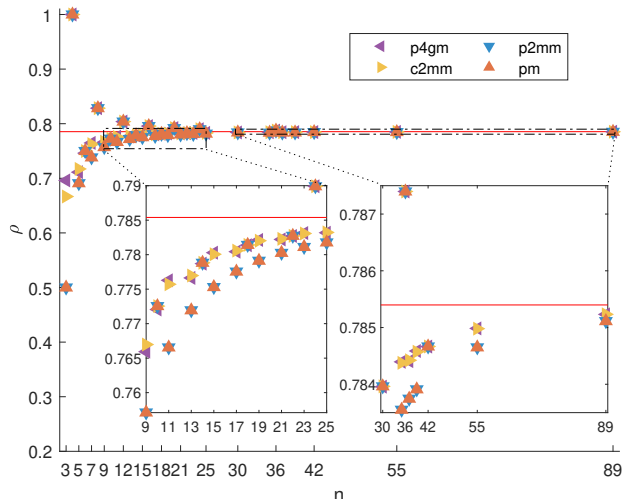


FIG. 9: Densities of the densest packings of examined n -gons in the $p4gm/c2mm/p2mm/pm$ plane groups class. The red line denotes the density of the densest disc packing in this plane group class.

$p2mm$ and pm packings are equal. Visually comparing the $p2mm$ and pm , the densest packings in Fig. 7, the configurations are clearly non-isometric except for n -gons with 4-fold rotational symmetry. However, the densest $p2mm$ packing of an arbitrary n -gon can be easily converted to a pm packing of the same density as is demonstrated in Fig. 8. This construction suggests that for n -gons without 4-fold rotational symmetry, the pm density landscape contains at least two non-isometric global maxima and provides multiple densest pm packing configurations. These rewritten pm configurations are isometric to their corresponding densest $p2mm$ packings for n -gons with central symmetry.

The difference between these two alternative densest pm configurations for centrally symmetric n -gons can be observed by noticing contact edge length. The total length of edges with non-zero contact of the decagon in Fig. 8 with its surrounding decagons is clearly higher when compared to the manually constructed configuration in Fig. 7. In the example of the pentagon, the polygons in the pm configuration in Fig. 7 are slightly rotated compared to Fig. 8 where one of the edges of pentagons is parallel to the basic vector of the primitive cell.

Further, our results suggest that for n -gons with a central symmetry, the densities of densest $c2mm$, $p2mm$, and pm packings are equal. In fact, there are configurations where all three packing configurations are isometric. Moreover, given a $p2mm/pm$, it is possible to construct a $c2mm$ structure with the same density. However, these $c2mm$ packings are not optimal for centrally non-symmetric n -gons.

The densest $p4gm$ packings in our experiments are higher for all centrally non-symmetric n -gons than their corresponding $p2mm/pm$ packings. On the other hand, comparing $p4gm$ and $c2mm$ configurations, n -gons with

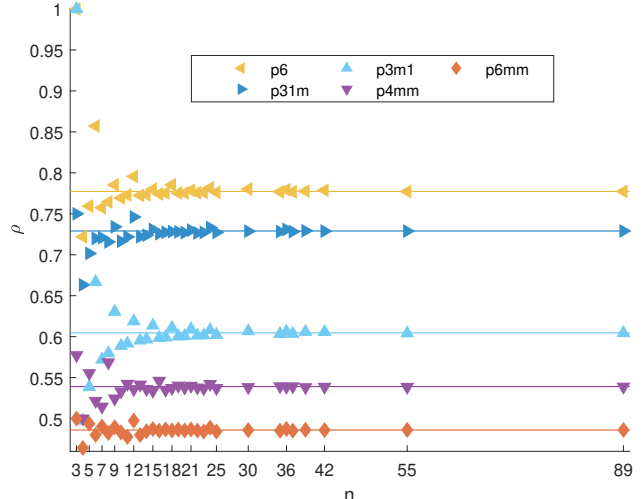


FIG. 10: Densities of the densest packings of examined n -gons in the $p6/p31m/p3m1/p4mm/p6mm$ plane groups class. The coloured lines denote the density of the corresponding densest plane group disc packings.

a $4k-1$ fold rotational symmetry attained slightly higher packing densities in the $p4gm$ group than in $c2mm$, and for n -gons with a $4k+1$ fold rotational symmetry $c2mm$ packings were higher than those in $c2mm$. For centrally symmetric n -gons, the $p4gm$ densest packings were lower or equal to their $c2mm/p2mm/pm$ densest configurations.

The lowest densities of the densest $p4gm$, $c2mm$, $p2mm$, and pm packings were attained in the case of the regular triangle, and uniform square tilings attained the highest densities in all four plane groups. From the evolution of densities as the number of vertices increases, presented in Fig. 9, it is reasonable to assume that the extremal values of densities of densest $p4gm$, $c2mm$, $p2mm$, and pm packings among n -gons are attained for the regular triangle and square.

D. Densest $p6$, $p31m$, $p3m1$, $p4mm$, and $p6mm$ packings

The last class corresponds to the plane groups for which the optimal densest packings of a disc share no common symmetries. All five plane groups can be therefore regarded as separate classes by themselves. Moreover, the disc attains the lowest density values when the packing configurations are restricted to $p6$, $p31m$, $p3m1$, $p4mm$, and $p6mm$ plane groups.

Similarly to previous classes, we did not observe any clear trend with the packing density oscillating around the respective densest disc packing density. Although the densest $p6$ packing of a disc is lower than the packings in previous plane group classes we examined, this is true for all n -gons for $n > 18$, where the distance of densest n -gon $p6$ packing density to the $p6$ disc packing is suffi-

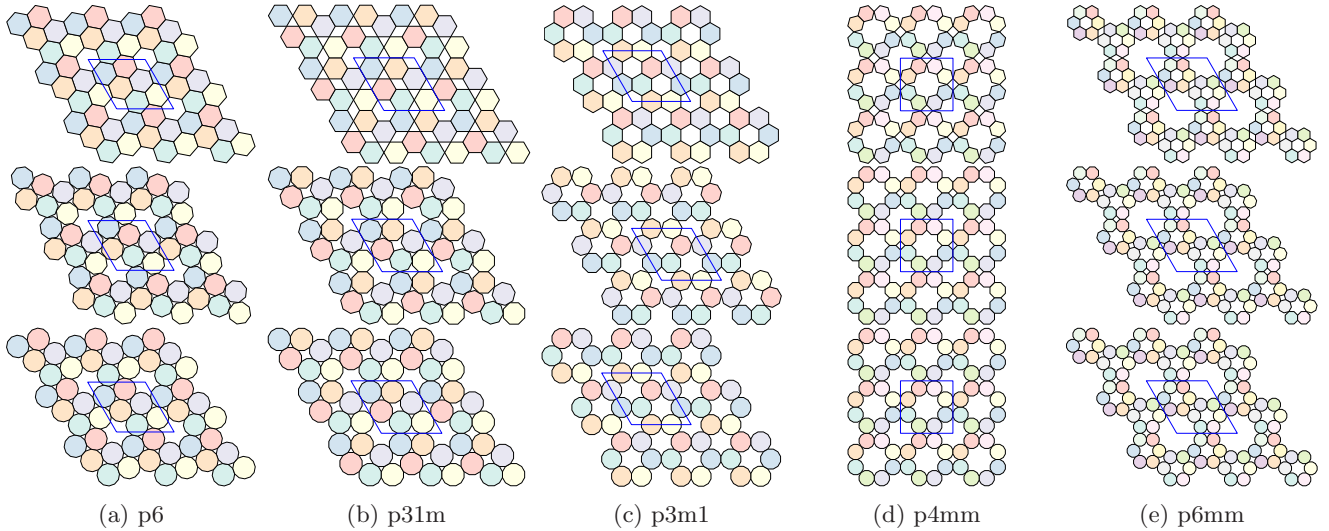


FIG. 11: Densest configurations of (from top to bottom) hexagon, octagon and dodecagon in plane groups $p6$, $p31m$, $p3m1$, $p4mm$, and $p6mm$ with the following densities: hexagon in $p6 \approx 0.85714$, $p31m \approx 0.71999$, $p3m1 \approx 0.66666$, $p4mm \approx 0.52148$ and $p6mm \approx 0.47999$; octagon in $p6 \approx 0.76438$, $p31m \approx 0.71565$, $p3m1 \approx 0.57980$, $p4mm \approx 0.56854$ and $p6mm \approx 0.48235$; dodecagon in $p6 \approx 0.79560$, $p31m \approx 0.74613$, $p3m1 \approx 0.61880$, $p4mm \approx 0.53589$ and $p6mm \approx 0.49742$. The blue parallelogram denotes the primitive cell of the respective configuration. Colors represent symmetry operations modulo lattice translations.

ciently small to be separated from the previous class. For instance, $p6$ packing configurations of 5, 9, and 18-gon have higher densities than their corresponding densest packings in the $p4gm/c2mm/p2mm/pm$ class, visually demonstrated in the colored rank table in Fig. 1.

However, we observed correspondences between the densest plane group packings in this density plane group class and previous classes. For a hexagon, we computed the following ratios of packing densities of respective densest $p2/p2gg/pg/p3/p1$, $p6$, and $p3m1$ packing configuration denoted $\mathcal{K}_{p2/p2gg/pg/p3/p1_{\max}}$, $\mathcal{K}_{p6_{\max}}$ and $\mathcal{K}_{p3m1_{\max}}$,

$$\frac{\rho(\mathcal{K}_{p2/p2gg/pg/p3/p1_{\max}})}{\rho(\mathcal{K}_{p6_{\max}})} = \frac{7}{6}$$

and

$$\frac{\rho(\mathcal{K}_{p2/p2gg/pg/p3/p1_{\max}})}{\rho(\mathcal{K}_{p3m1_{\max}})} = \frac{3}{2}.$$

By numerical comparison, these ratios approximately hold for all n -gons with 6-fold rotational symmetry in Table I.

Secondly, by comparing densest $p4mg/c2mm/pm/p2mm$ and $p4mm$ packing configurations of an octagon denoted $\mathcal{K}_{p4mg/c2mm/pm/p2mm_{\max}}$ and $\mathcal{K}_{p4mm_{\max}}$, we obtained the following packing density ratio,

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

We compared this value against ratios of densest $p4mg/c2mm/pm/p2mm$ and $p4mm$ packings in Table I

and observed an approximate equality for all n -gons with 8-fold rotational symmetry. Interestingly, a local 8-rotational symmetry is present in the octagonal octamers of the $p4mm$ packing configuration, shown in Fig.11.

Lastly, we obtained the following packing density ratios of densest $p2mg/cm/p4$, $p31m$, and $p6mm$ packing configurations of a dodecagon denoted $\mathcal{K}_{p2mg/cm/p4_{\max}}$, $\mathcal{K}_{p31m_{\max}}$ and $\mathcal{K}_{p6mm_{\max}}$,

$$\frac{\rho(\mathcal{K}_{p2mg/cm/p4_{\max}})}{\rho(\mathcal{K}_{p31m_{\max}})} = \frac{2\sqrt{3}}{3}$$

and

$$\frac{\rho(\mathcal{K}_{p2mg/cm/p4_{\max}})}{\rho(\mathcal{K}_{p6mm_{\max}})} = \sqrt{3}.$$

Compared to the $p2mg/cm/p4$, $p31m$ and $p6mm$ densities in Table I, these packing density ratios are approximately equal for all n -gons with 12-fold rotational symmetry. Additionally, by visual examination of the $p2mg/cm/p4$, $p31m$ and $p6mm$ configurations of a dodecagon in Fig. 11 and Fig. 5, all three configurations contain local 3-fold and 4-fold rotational symmetries in the dodecagonal trimers and tetramers.

Consequently, these relationships suggest that 24-fold rotational symmetry of an n -gon constitutes the optimal configurations of a disc in all plane groups. Considering that the minimal symmetry containing 6-fold, 8-fold and 12-fold rotational symmetries is 24-fold rotational symmetry and that the symmetries of densest $p2/p2gg/pg/p3/p1$, $p2mg/cm/p4$ and $p4mg/c2mm/pm/p2mm$ packings of n -gons with 12-fold

rotational symmetry coincide with the symmetries of corresponding densest plane group packings of a disc [33].

Concerning the extrema of the densest plane group packings, the regular triangle attained the highest packing density in all five plane groups, where in $p6$ and $p3m1$, we have regular triangular tilings. ETRPA obtained the lowest packing densities in our experiments in the case of a square in all five groups. The evolution of packing density as the number of vertices increases, shown in Fig. 10, suggests that the triangle and pentagon attain the extremal densities among all n -gons in this plane group class.

IV. DISCUSSION AND CONCLUSIONS

Using the ETRPA, we obtained and analyzed the densest packings in all 17 plane groups of various n -gons. Although ETRPA is a stochastic search algorithm and the plane group packing problem has multiple local and global optima, our results indicate that we indeed acquired approximations of densest n -gon packing configurations subject to CSG restrictions.

Since 2-dimensional CSGs are inherently periodic and combined with the fact that the $p2$ plane group is a local optimum in the space of all packings [29], further confirmed by our results, it can be stated that the $p2$ plane group realizes the densest plane group packings for all n -gons among all 17 plane group. Moreover, depending on the symmetries of an n -gon, the densest known packings can be realized in multiple plane groups. In the densest known configuration of a pentagon and heptagon, one of the mirror symmetry planes of the polygon is parallel to one of the primitive cell's basic vectors. This symmetry plane, in fact, coincides with one of the glide reflection planes in the $p2gg$ group and is orthogonal to the pg glide reflection plane. Thus, the densest known configurations can be realized using glide reflections in $p2gg$ and pg plane groups.

In the densest known packing configuration of the regular enneagon, the mirror symmetry plane of a polygon is slightly rotated in relation to the primitive cell basic vectors [27] and, therefore, cannot be constructed using a glide reflection. We have observed this property for all n -gons containing a 3-fold rotational symmetry but no central symmetry.

One of the methods to construct the densest double-lattice configurations of a convex polygon is based on finding the minimum area of a type of inscribed parallelogram called a half-length parallelogram [32]. In line with our results, the enneagon's diameter given by the minimum area half-length parallelogram has a non-zero slope and the local optimum corresponds to the densest pg packing, contrary to the pentagon and heptagon cases where the diameter corresponding to the global optima coincides with the mirror symmetry of both polygons [29].

An intuition why the n -gons with 3-fold rotational

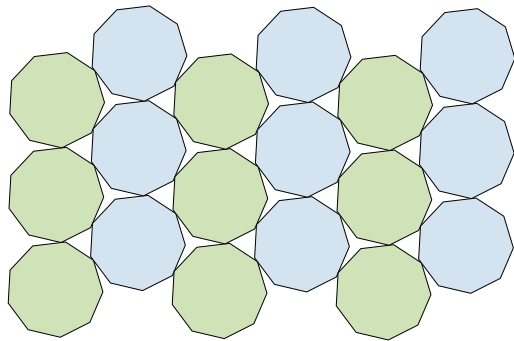


FIG. 12: $p3/p1$ packing of the enneagon with a packing density of approximately 0.87358, manually constructed from the enneagon's densest $p2$ packing configuration in Fig. 2.

symmetry are exceptional can be obtained from the optimal configuration of a disc as an approximation of the enneagon. The densest packing configuration of a disc is also referred to as a hexagonal close-packed configuration and can be constructed using the plane group $p3$ with the hexagonal crystal system. The hexagonal crystal system induces a 6-fold rotational symmetry on the crystal lattice with the 3-fold rotational symmetry as a subgroup. We observed this 6-fold rotational packing symmetry in all n -gons with 6-fold rotational symmetry.

Additionally, there is a quasi-6-fold rotational packing symmetry [34] in the densest $p2$ configurations of all centrally non-symmetric n -gons with a 3-fold rotational symmetry which is not present in densest $p2$ configurations of n -gons without 3-fold rotational symmetry. This quasi-6-fold rotational symmetry is realized by lattice translations in a $p2$ configuration. Two polygons related to each other by a lattice translation are also related by a 3-fold rotational symmetry. Moreover, because of this relation, it is possible to construct a $p3/p1$ packing, as is demonstrated on a packing with $p3$ and $p1$ symmetries constructed from the densest $p2$ packing of an enneagon in Fig. 12. Here the blue polygons are unchanged polygons from $p2$ packing of enneagon in Fig. 2. However this packing has lower density than the densest $p3/p1$ packing of an enneagon.

Since the crystallographic restriction theorem does not allow higher than 6-fold rotational symmetries in a crystal [25], our results strongly suggest that centrally non-symmetric n -gons with a 3-fold rotational symmetry are an exception to general densest plane group configuration symmetries of n -gons, and it is reasonable to state the following conjectures.

Conjecture 1 *Densities of the densest $p2$, pg , and $p2gg$ packings are equal for all, but centrally non-symmetric n -gons with 3-fold rotational symmetry and $n \geq 9$, densities of the densest $p2$, pg , $p2gg$, and $p1$ packings are equal for all centrally symmetric n -gons, and densities of the densest $p2$, pg , $p2gg$, $p1$, and $p3$ packings are equal for all n -gons containing a 6-fold rotational symmetry.*

Conjecture 2 *Densities of the densest $p2mg$ and cm packings are equal for all but n -gons with a $12k - 1$ and $12k + 1$ rotational symmetry where $k \in \mathbb{N}$ and densities of densest $p2mg$, cm , and $p4$ packings are equal for all n -gons containing a 12-fold rotational symmetry.*

Conjecture 3 *Densities of the densest pm and $p2mm$ packings are equal for all n -gons, densities of the densest $c2mm$, pm and $p2mm$ packings are equal for all centrally symmetric n -gons, and densities of the densest $p4gm$,*

$c2mm$, pm , and $p2mm$ packings are equal for all n -gons containing a 4-fold rotational symmetry.

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