Construction of fullerenes and Pogorelov polytopes

Nikolai Erokhovets
Lomonosov Moscow State University
erochovetsn@hotmail.com

Joint work with

Victor M. Buchstaber

International Conference
«Graphs and Groups, Representations and Relations»

August 8, 2018
Novosibirsk State University

Polytopes

A (convex) polytope P is a bounded intersection of a finite number of closed halfspaces:

$$P = \{\boldsymbol{x} \in \mathbb{R}^n \colon \langle \boldsymbol{a}_i, \boldsymbol{x} \rangle + b_i \geqslant 0, i = 1, \ldots, m\}.$$

If this representation is irredundant, then facets are intersections of P with corresponding hyperplanes.

Equivalently, P is a convex hull of finite number of points:

$$P = \mathrm{Conv}(\boldsymbol{v}_1, \ldots, \boldsymbol{v}_N)$$

If this representation is irredundant, then the points are vertices.

Polytopes

- By definition $\dim(P) = \dim \operatorname{aff}(P)$. An n-dim polytope we call an *n-polytope*.
- A face of P is an intersection of P with a supporting hyperplane leaving P in one closed halfspace.
- 0-dim faces are vertices, 1-dim faces are edges, codim-1 faces are facets.
- An n-polytope P is simple, if any its vertex belongs to exactly n facets.
- Polytopes P and Q are combinatorially equivalent, if there is a bijection between their sets of faces respecting the inclusion relation.
- A combinatorial polytope is a class of combinatorial equivalent polytopes.
- In what follows by a polytope we mean a combinatorial polytope.

Graphs of 3-polytopes

Vertices and edges of a polytope P form a graph $G(P)$.

Theorem (E. Steinitz, 1922)

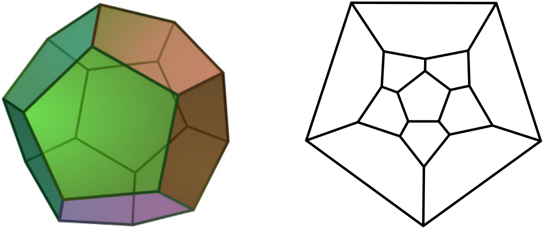
A graph G is a graph of some 3-polytope iff it has at least 4 edges, is simple, planar and 3-connected, that is deletion of at most two arbitrary vertices leaves it connected.

Theorem (H. Whitney, 1932)

An embedding of the graph $G(P)$ of a simple 3-polytope into the 2-dimensional sphere is combinatorially unique.

Shlegel diagrams

A rectilinear plane realization of $G(P)$ is given by a Shlegel diagram – a projection of P to one of its facets F from a point outside P near F.



Cyclically k-connected graphs

Definition

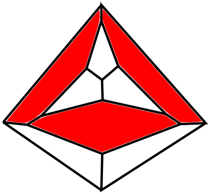
A 3-valent simple graph is said to be cyclically k-edge connected (ck-connected) provided no two circuits can be separated by cutting fewer than k edges. Also by definition K_4 is $c3$-connected, but not ck-connected for $k > 3$.

A ck-connected graph is called strongly cyclically k-edge connected (c^*k-connected), if in addition any separation of the graph by cutting k edges leaves one component that is a simple circuit of k edges.

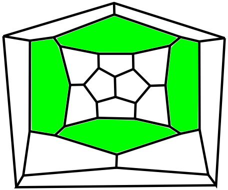
We say that a polytope is ck- or c^*k-connected, if its graph has this property. K_4 is the graph of 3-simplex Δ^3.

k-belts

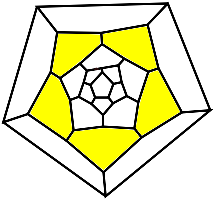
A k-belt of a simple 3-polytope P is a cyclic sequence of facets with empty common intersection such that two of these facets intersect iff they follow each other.



3-belt



4-belt



5-belt

Any simple 3-polytope has a 3-, 4-, or 5-belt.

k-belts and cyclic edge-connectivity

- Any simple 3-polytope is $c3$-connected and at most c^*5-connected.
- A simple 3-polytope is ck-connected iff it has no r-belts for $r < k$ and $P \neq \Delta^3$ for $k > 3$.
- It is c^*k-connected iff in addition any k-belt surrounds a facet (is trivial).

Flag polytopes

Definition

A simple polytope is called flag if any its set of pairwise intersecting facets has a nonempty intersection.

Proposition

Let P be a simple 3-polytope. Then the following conditions are equivalent:

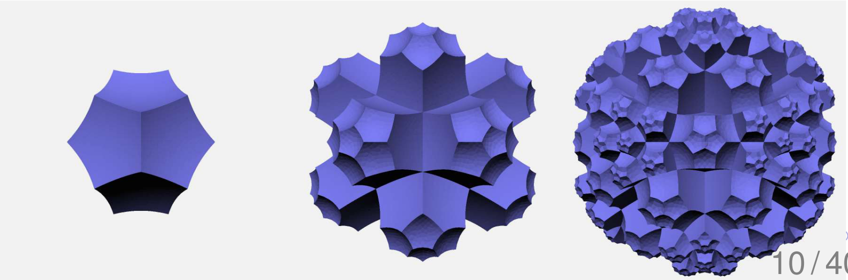
- P is flag;
- $P \neq \Delta^3$ and P has no 3-belts;
- P is c4-connected.

Pogorelov polytopes

A Pogorelov polytope is a combinatorial 3-polytope that can be realized as a bounded polytope in Lobachevsky (hyperbolic) space $\mathbb{L}^3$ with right dihedral angles.

Theorem (A.V. Pogorelov, 1967, E.M. Andreev, 1970)

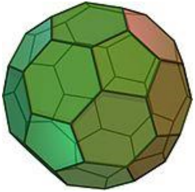
A 3-polytope P is a Pogorelov polytope iff it is a flag polytope without 4-belts (that is c5-conected). Moreover, the realization is unique up to isometries.



Fullerenes

A (mathematical) fullerene is a simple 3-polytope with all facets 5- and 6-gons.

Buckminsterfullerene C_{60}



Truncated icosahedron

Results by T. Došlić (1998, 2003) imply

Theorem

Any fullerene is a Porogelov polytope.

Notation

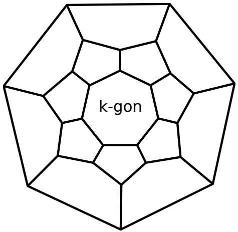
We will call

- c^*3-connected polytopes simple* polytopes;
- c^*4-connected polytopes flag* polytopes;
- c^*5-connected polytopes Pogorelov* polytopes;

Theorem (V.M. Buchstaber, N. Yu. Erokhovets, 2015)

- *Any simple* 3*-polytope with* 5*-,* 6*- and one* 7*-gonal facet is a Pogorelov polytope.*
- *Any simple* 3*-polytope with* 5*-,* 6*- and one* 4*-gonal facet is a flag* polytope.*

k-barrels (Lobell polytopes)



- a k-barrel is known as a Löbel polytope $R(k)$ by A.Yu. Vesnin (1987);
- graph of the k-barrel is a biladder on $2k$ vertices by N. Robertson, P.D. Seymour, R. Thomas (2017);
- the k-barrel is a Pogorelov* polytope for $k \geqslant 5$;
- the 5-barrel is the dodecahedron;
- the 6-barrel is a fullerene.

The Four Colour Problem and Pogorelov polytopes

3-polytopes

Simple $\supset$ simple* $\supset$ flag $\supset$ flag* $\supset$ Pogorelov $\supset$ Pogorelov*

Theorem (G.D. Birkhoff, 1913)

The Four Colour Problem for planar graphs can be reduced only to Pogorelov* polytopes.

- Each Hamiltonian cycle gives a 4-coloring of a simple 3-polytope.
- F. Kardoš (2014) proved that any fullerene has a Hamiltonian cycle.
- H. Walther (1965) gave an example of a Pogorelov polytope without Hamiltonian cycles (his example is not Pogorelov*).

Toric topology: canonical correspondence

simple polytope P^n facets $\mathcal{F}_P = (F_1, \ldots, F_m)$	$\longrightarrow$	moment-angle manifold $\mathcal{Z}_P^{m+n}$ canonical T^m-action real m-a manifold $\mathbb{R}\mathcal{Z}_P$ canonical $\mathbb{Z}_2^m$-action
characteristic function $\Lambda\colon \mathcal{F} \to \mathbb{Z}^n$	$\longrightarrow$	quasitoric manifold $M^{2n}(P,\Lambda) = \mathcal{Z}_P/T^{m-n}(\Lambda)$ canonical T^n-action
$\mathbb{Z}_2$-characteristic function $\Lambda_2\colon \mathcal{F} \to \mathbb{Z}^n$	$\longrightarrow$	small cover $R^n(P,\Lambda) = \mathbb{R}\mathcal{Z}_P/\mathbb{Z}_2^{m-n}(\Lambda_2)$ canonical $\mathbb{Z}_2^n$-action

$$\mathcal{Z}_P/T^m = \mathbb{R}\mathcal{Z}_P/\mathbb{Z}_2^m = M(P,\Lambda)/T^n = R(P,\Lambda_2)/\mathbb{Z}_2^n = P^n$$

combinatorics of polytopes $\longleftrightarrow$ algebraic topology of manifolds

Theorem (F. Fan, J. Ma, X. Wang, 2015)

Let P be a Pogorelov polytope, Q be any simple 3-polytope, and R be $\mathbb{Z}$ or a field. Then any isomorphism of graded rings

$$H^*(\mathcal{Z}_P, R) \simeq H^*(\mathcal{Z}_Q, R)$$

implies a combinatorial equivalence $P \simeq Q$.

Any colouring $\xi\colon \mathcal{F} \to \{1, 2, \ldots, k\}$ of facets of a simple n-polytope P with $k \leqslant n+1$ such that adjacent facets have different colours defines a characteristic function $\Lambda(\xi)$:

$$\Lambda(F_i) = e_{\xi(F_i)}$$

where $(e_1, \ldots, e_n)$ is the standard basis in $\mathbb{Z}^n$ and $e_{n+1} = e_1 + \cdots + e_n$.

Similarly the $\mathbb{Z}_2$-characteristic function $\Lambda_2(\xi)$ is defined.

Corollary of the Four Colour Theorem

Any 3-polytope P admits a characteristic and a $\mathbb{Z}_2$-characteristic function.

- Any Pogorelov polytope P realized in the Lobachevsky space $\mathbb{L}^3$ defines a right-angled Coxeter group $G(P)$ generated by reflexions in its faces.
- A $\mathbb{Z}_2$-characteristic function Λ_2 defines a homomorhism $G(P) \to \mathbb{Z}_2^m$ whose kernel $K(\Lambda_2)$ acts freely on $\mathbb{L}^3$.
- The factorspace $\mathbb{L}^3/K(\Lambda_2)$ is a hyperbolic manifold.
- Such manifolds were introduced by A.Yu.Vesnin in 1987.
- $\mathbb{L}^3/K(\Lambda_2)$ is homeomopric to $R(P,\Lambda_2)$.

Theorem (V.M. Buchstaber, N. Erokhovets, M. Masuda, T.E. Panov, S. Park, 2017)

Let P be a Pogorelov polytope, Q be any simple 3-polytope, R be $\mathbb{Z}$ or any field, and Λ_P, Λ_Q be characteristic functions. Then the following conditions are equivalent

1. *the graded rings $H^*(M(P,\Lambda_P),R)$ and $H^*(M(Q,\Lambda_Q),R)$ are isomorphic;*
2. *the manifolds $M(P,\Lambda_P)$ and $M(Q,\Lambda_Q)$ are diffeomorphic;*
3. *the pairs (P,Λ_P) and (Q,Λ_Q) are equivalent.*

Theorem (V.M. Buchstaber, N. Erokhovets, M. Masuda, T.E. Panov, S. Park, 2017)

Let P be a Pogorelov polytope, Q be any simple 3-polytope, and $\Lambda_{P,2}$, $\Lambda_{Q,2}$ be $\mathbb{Z}_2$-characteristic functions. Then the following conditions are equivalent

1. *the graded rings $H^*(R(P,\Lambda_{P,2}),\mathbb{Z}_2)$ and $H^*(M(Q,\Lambda_{Q,2}),\mathbb{Z}_2)$ are isomorphic;*
2. *the manifolds $M(P,\Lambda_{P,2})$ and $M(Q,\Lambda_{Q,2})$ are diffeomorphic;*
3. *the pairs $(P,\Lambda_{P,2})$ and $(Q,\Lambda_{Q,2})$ are equivalent.*

Small covers from colourings

Let P and Q be two simple n-polytopes and χ_P, χ_Q be their colourings into at most $n+1$ colours.

Pairs (P, χ_P) and (Q, χ_Q) are equivalent, if there is a combinatorial equivalence $c\colon \mathcal{F}_P \to \mathcal{F}_Q$ and a transposition $\sigma \in S_{n+1}$ such that $\sigma \circ \chi_P = \chi_Q \circ c$.

Buchstaber, Panov, 2016

Pairs $(P, \Lambda(\chi_P))$ and $(Q, \Lambda(\chi_Q))$ are equivalent iff pairs (P, χ_P) and $(Q, \chi(Q)$ are equivalent.

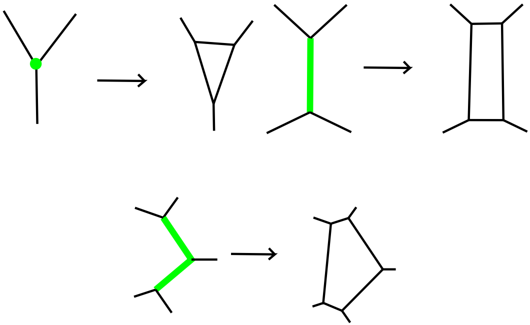
Corollary

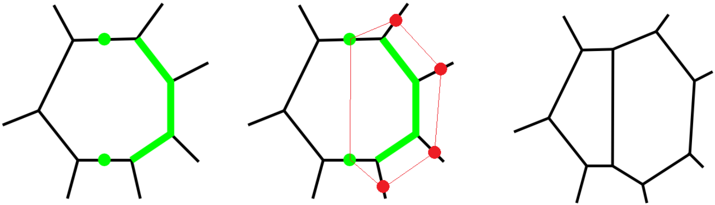
Hyperbolic 3-manifolds defined from colourings are diffeomorphic iff the pairs (P, χ_P) and (Q, χ_Q) are equivalent.

Construction of simple 3-polytopes

Theorem (V. Eberhard, 1891)

A 3-polytope P is simple iff it is can be obtained from the simplex Δ^3 by a sequence of operations of cutting off a vertex, an edge, or two adjacent edges by one hyperplane.

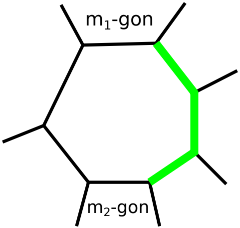




Let F be a k-gonal face of a simple 3-polytope P.

- choose s subsequent edges of F;
- rotate the supporting hyperplane of F around the axis passing through the midpoints of adjacent two edges (one on each side);
- take the corresponding hyperplane truncation.

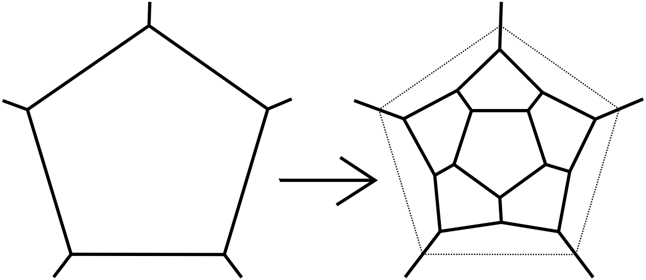
We call it (s, k)-truncation. This is a combinatorial operation.



If the facet F is adjacent to an m_1 and m_2-gons by edges next to cutted one, then we also call the corresponding operation an $(s, k; m_1, m_2)$-truncation.

Connected sum along k-gonal facets

A connected sum of two simple 3-polytopes P and Q along k-gonal facets F and G is a combinatorial analog of glueing of two polytopes along congruent facets perpendicular to adjacent facets.



Connected sum with the dodecahedron along 5-gons.

Construction of simple* polytopes

Let P be a simple* polytope different from Δ^3 and $\Delta^2 \times I$. Then an (s,k)-truncation gives a simple* polytope iff it is not a cutting off a vertex of a triangle.

Proposition

- A simple 3-polytope P is simple* iff either $P = \Delta^3$, or $P = \Delta^2 \times I$, or is a vertex cut of $\Delta^2 \times I$, or can be obtained from these polytopes by a sequence of vertex, edge, or $(2,k)$-truncations, $k \geqslant 6$, different from cutting off a vertex of a triangle.
- A simple 3-polytope P is simple* iff either $P = \Delta^3$, or P obtained from a flag polytope by simultaneous cutting off any number of disjoint vertices, or P is obtained from $\Delta^2 \times I$ by simultaneous cutting off any number of vertices of one 3-gon.

Construction of flag polytopes

Let P be a flag polytope. Then an (s, k)-truncation gives a flag polytope iff $1 \leqslant s \leqslant k - 3$.

Theorem (A. Kotzig, 1967; V. Volodin, 2012)

A simple 3-polytope is flag iff it can be obtained from the cube I^3 by a sequence of (s, k)-truncations, $1 \leqslant s \leqslant k - 3$.

Theorem (V.M. Buchstaber, N.Yu. Erokhovets, 2015)

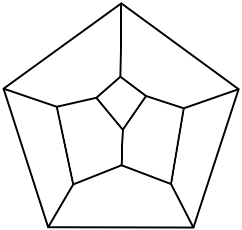
A simple 3-polytope is flag iff it can be obtained from the cube I^3 by a sequence of $(2, k)$-truncations, $k \geqslant 6$.

Construction of flag* polytopes

Let $P \neq I^3$ be a flag* polytope. Then an (s, k)-truncation gives a flag* polytope iff $1 \leqslant s \leqslant k-3$ and truncation is not a cutting off an edge of a 4-gon.

Theorem (follows from the paper by D. Barnette, 1974)

A simple 3-polytope P is flag* iff either P is the 3-cube, or the 5-gonal prism, or it can be obtained from the polytope below by cuttings off edges not lying in 4-gons, and $(2, k)$-truncations, $k \geqslant 6$.



Construction of Pogorelov and Pogolelov* polytopes

- Let P be a Pogorelov(*) polytope. Then an (s,k)-truncation gives a Pogorelov(*) polytope iff $2 \leqslant s \leqslant k-4$.
- Let P and Q be two Pogorelov polytopes. Then their connected sum along k-gonal facets is a Pogorelov polytope (but not Pogorelov*).

Theorem (D. Barnette, 1977)

- *A simple 3-polytope P is Pogorelov iff it can be obtained from q-barrels, $q \geqslant 5$, by a sequence of (s,k)-truncations, $2 \leqslant s \leqslant k-4$, and connected sums along 5-gons.*
- *A simple 3-polytope P is Pogorelov* iff it can be obtained from q-barrels, $q \geqslant 5$, by a sequence of only (s,k)-truncations, $2 \leqslant s \leqslant k-4$.*

Volumes of Pogorelov polytopes

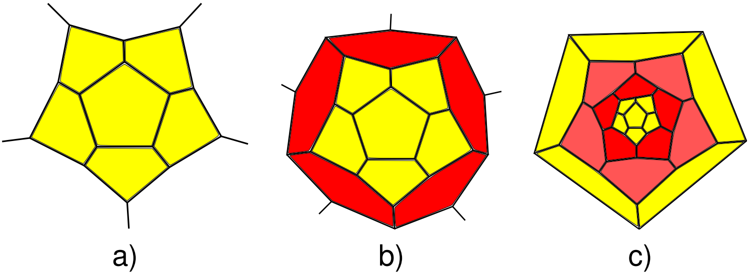
Theorem (T. Inoue, 2008)

Operations of (s, k)*-truncation,* $2 \leqslant s \leqslant k - 4$*, and connected sum along p-gons,* $p \geqslant 5$ *does not decrease volumes of hyperbolic polytopes.*

Theorem (V.M. Buchstaber, N.Yu. Erokhovets, 2017)

- *A q-barrel, $q \geqslant 5$, can not be obtained from a Pogorelov polytope by a $(2, k)$-truncation or a connected sum with the 5-barrel along a 5-gon;*
- *A simple 3-polytope P is Pogorelov iff either P is a q-barrel, $q \geqslant 5$, or it can be constructed from the 5- or the 6-barrel by a sequence of $(2, k)$-truncations, $k \geqslant 6$, and connected sums with the 5-barrel.*
- *A simple 3-polytope P is Pogorelov* iff either P is a q-barrel, $q \geqslant 5$, or it can be constructed from the 6-barrel by a sequence of $(2, k)$-truncations, $k \geqslant 6$.*

Family $\mathcal{F}_1$, $(5,0)$-nanotubes for $k \geqslant 1$



1. Take patch a) of the dodecahedron;
2. apply the connected sum with another copy of the dodecahedron along the central 5-gon;
3. we obtain the patch a) again;
4. make $k \geqslant 0$ steps;
5. finish to obtain the fullerene D_{5k}.

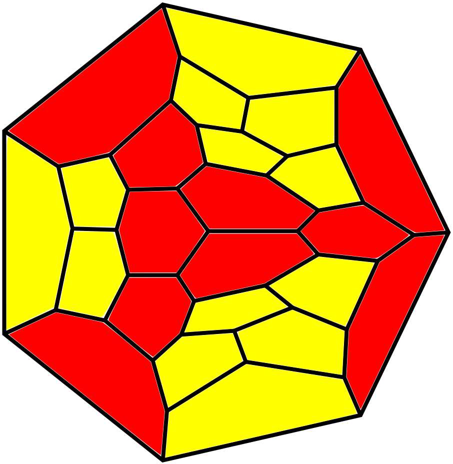
Denote by $\mathcal{P}_{57}$ the family of simple 3-polytopes with all facets 5- and 6-gons except for one face 7-gon, which is adjacent to some 5-gon.

As mentioned above, these polytopes are Pogorelov polytopes.

Theorem (V.M. Buchstaber, N.Yu. Erokhovets, 2017)

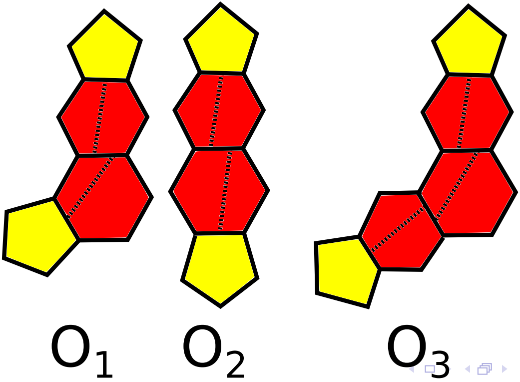
- *Any fullerene in $\mathcal{F}_1$ is either a dodecahedron, or is a connected sum of dodecahedra along 5-gons.*
- *Any fullerene not in $\mathcal{F}_1$ can be obtained from the 6-barrel by a sequence of operations of $(2,6;5,5)$-, $(2,6;5,6)$-, $(2,7;5,6)$-, $(2,7;5,5)$-truncation such that each intermediate polytope is either a fullerene or a polytope in $\mathcal{P}_{5,7}$.*

Example of a polytope in $\mathcal{P}_{5,7}$ that can not be obtained by $(2,6;5,5)$-, $(2,6;5,6)$-, $(2,7;5,6)$-, $(2,7;5,5)$-truncations and a connected sum with the dodecahedron from a fullerene or a polytope in $\mathcal{P}_{5,7}$.



Theorem (N.Yu. Erokhovets, 17)

Any polytope in $\mathcal{P}_{5,7}$ can be obtained from the 6-barrel by a sequence of operations, each operation being a connected sum with the dodecahedron, $(2,6;5,5)$-, $(2,6;5,6)$-, $(2,7;5,6)$-, $(2,7;5,5)$-truncation, or one of the operations O_1, O_2, O_3, such that each intermediate polytope is either a fullerene or a polytope in $\mathcal{P}_{5,7}$.



Remarks

- Operations O_1, O_2, O_3 are compositions of $(2,6;5,5)$-, $(2,6;5,6)$-, $(2,7;5,6)$-, $(2,7;5,5)$-truncations.
- When we apply these compositions on the intermediate steps polytopes with 5-, 6-, and at most two 7-gonal faces may appear.

N.Yu. Erokhovets,
Construction of fullerenes and Pogorelov polytopes with 5-, 6- and one 7-gonal face
Symmetry 2018, **10**, 67; doi:10.3390/sym10030067.

V.M. Buchstaber, N.Yu. Erokhovets,
Construction of families of three-dimensional polytopes, characteristic patches of fullerenes, and Pogorelov polytopes
Izvestiya: Mathematics, **81**:5 (2017), 901–972.

V.M. Buchstaber, N.Yu. Erokhovets, M. Masuda, T.E. Panov, S. Park,
Cohomological rigidity of manifolds defined by 3-dimensional polytopes
Russian Math. Surveys, 72:2 (2017),199–256

V.M. Buchstaber, T.E. Panov,
Toric Topology
AMS Math. Surv. and monographs, vol. 204, 2015. 518 pp.

V.M. Buchstaber, N.Yu. Erokhovets,
Fullerenes, Polytopes and Toric Topology
Lecture Note Series, IMS, NUS, Singapore, 2017, 67–178,
arXiv:math.CO/160902949.

F. Fan, J. Ma, X. Wang,
B-Rigidity of flag 2-spheres without 4-belt
arXiv:1511.03624.

V.M. Buchstaber and T.E. Panov,
On manifolds defined by 4-colourings of simple 3-polytopes
Russian Math. Surveys, 71:6 (2016), 1137–1139.

A.Yu. Vesnin,
Right-angled polyhedra and hyperbolic 3*-manifolds*
Russian Math. Surveys, 72:2 (2017), 335–374.

Thank You for the Attention!