Packing stars in fullerenes

Tomislav Došlić
Faculty of Civil Engineering, University of Zagreb

Zagreb, September 2020

Joint work with Meysam Taheri-Dehkordi and Gholam Hossein Fath-Tabar of Kashan, Iran.

Joint work with Meysam Taheri-Dehkordi and Gholam Hossein Fath-Tabar of Kashan, Iran.

T. Došlić, M. Taheri-Dehkordi, G. H. Fath-Tabar, Packing stars in fullerenes, *Journal of Mathematical Chemistry*, to appear.

Packings

A packing of a graph H in a graph G is a collection of vertex-disjoints subgraphs of G such that each component is isomorphic to H.

Packings

A packing of a graph H in a graph G is a collection of vertex-disjoints subgraphs of G such that each component is isomorphic to H.

A packing of H in G is perfect if it is a spanning subgraph of G.

Packings

A packing of a graph H in a graph G is a collection of vertex-disjoints subgraphs of G such that each component is isomorphic to H.

A packing of H in G is perfect if it is a spanning subgraph of G.

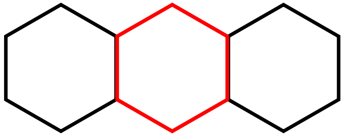
Any matching in G can be viewed as a packing of K_2 in G.

Packings

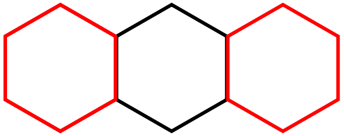
A packing of a graph H in a graph G is a collection of vertex-disjoints subgraphs of G such that each component is isomorphic to H.

A packing of H in G is perfect if it is a spanning subgraph of G.

Any matching in G can be viewed as a packing of K_2 in G.



G



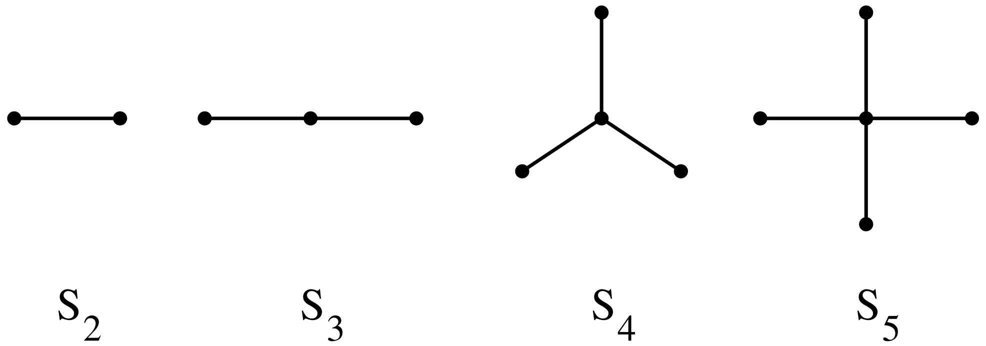
G

Stars

A star S_n is a complete bipartite graph $K_{1,n-1}$ with one of the classes of size 1.

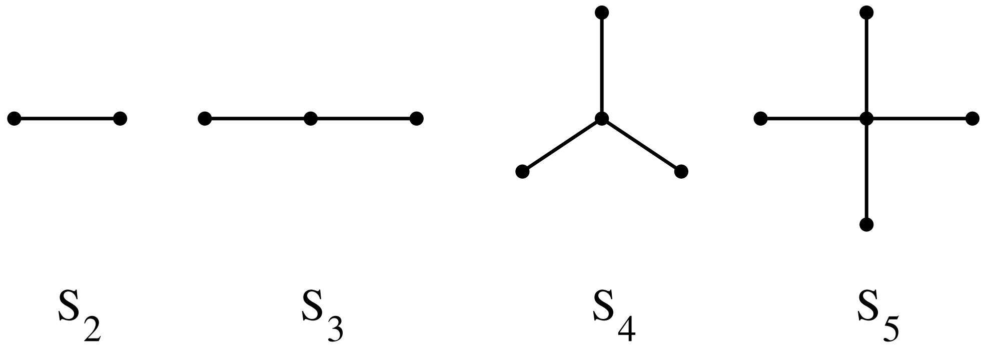
Stars

A star S_n is a complete bipartite graph $K_{1,n-1}$ with one of the classes of size 1.



Stars

A star S_n is a complete bipartite graph $K_{1,n-1}$ with one of the classes of size 1.



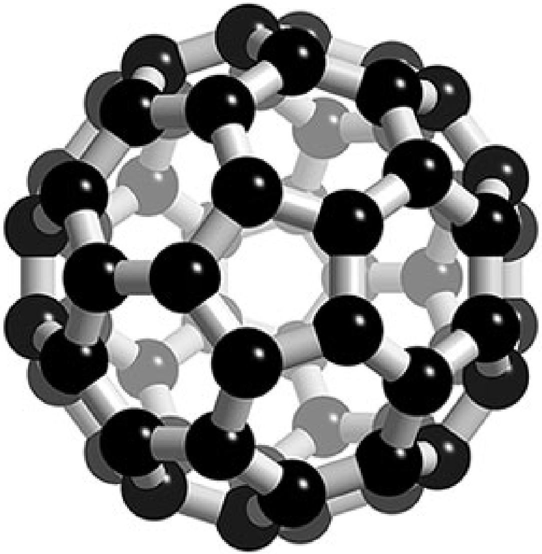
In this talk, a star means a copy of $K_{1,3}$, unless stated otherwise.

Fullerenes

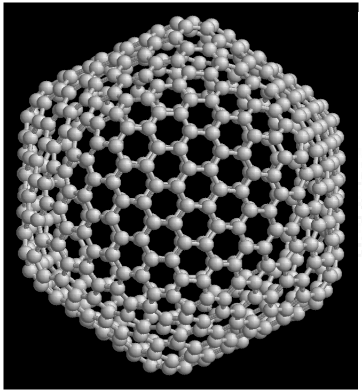
A fullerene is a polyhedral molecule consisting only of carbon atoms and containing only pentagonal and hexagonal faces.

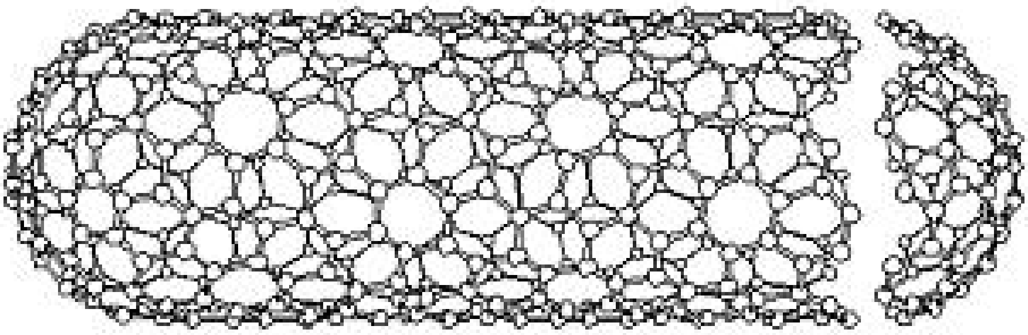
Fullerenes

A fullerene is a polyhedral molecule consisting only of carbon atoms and containing only pentagonal and hexagonal faces.



More fullerenes



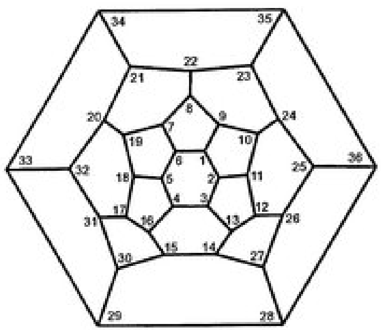


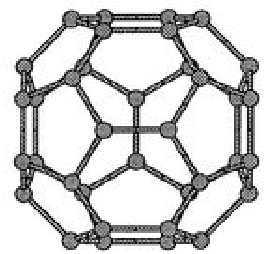
Fullerene graphs

A fullerene graph is a planar, 3-regular and 3-connected graph, twelve of whose faces are pentagons and any remaining faces are hexagons.

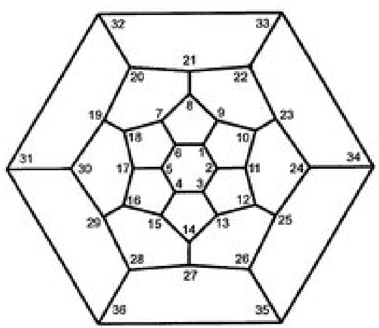
Fullerene graphs

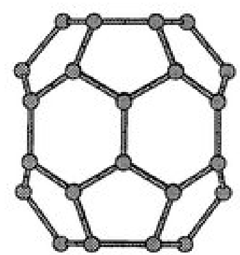
A fullerene graph is a planar, 3-regular and 3-connected graph, twelve of whose faces are pentagons and any remaining faces are hexagons.





36:14 ($\mathbf{1}$ D_{2d} 0.0)

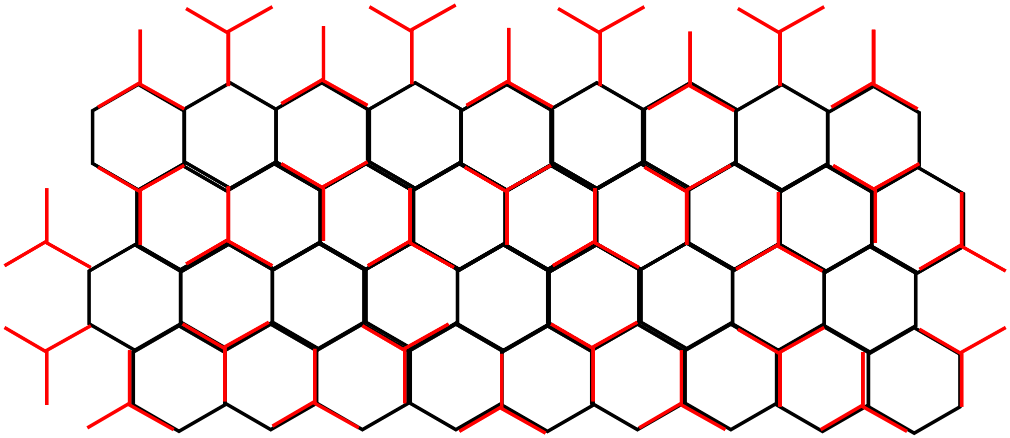




36:15 ($\mathbf{2}$ C_{6v} 11.6)

Hexagonal lattice

Hexagonal lattice



Necessary conditions for fullerenes

Proposition

If there exists a perfect packing of stars in a fullerene graph G, then

- the number of vertices of G must be divisible by 4, and
- -1 must be an eigenvalue of $A(G)$.

Main lemma

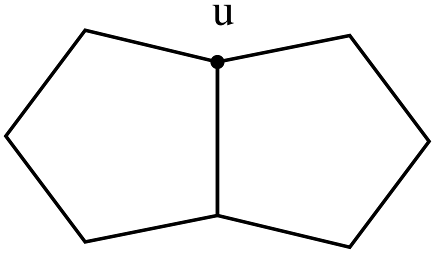
Lemma

A vertex u in a fullerene graph G shared by two pentagons cannot be the center of a star in a perfect packing of stars in G.

Main lemma

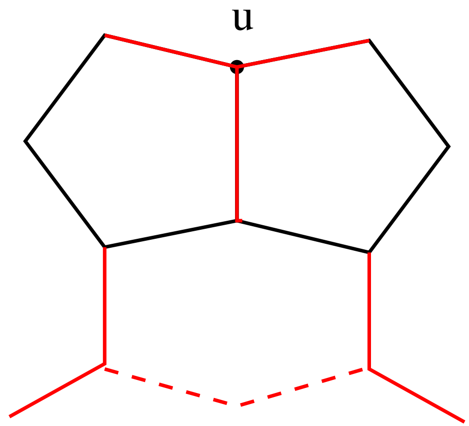
Lemma

A vertex u in a fullerene graph G shared by two pentagons cannot be the center of a star in a perfect packing of stars in G.



Main lemma

Main lemma



Star-forbidden graphs

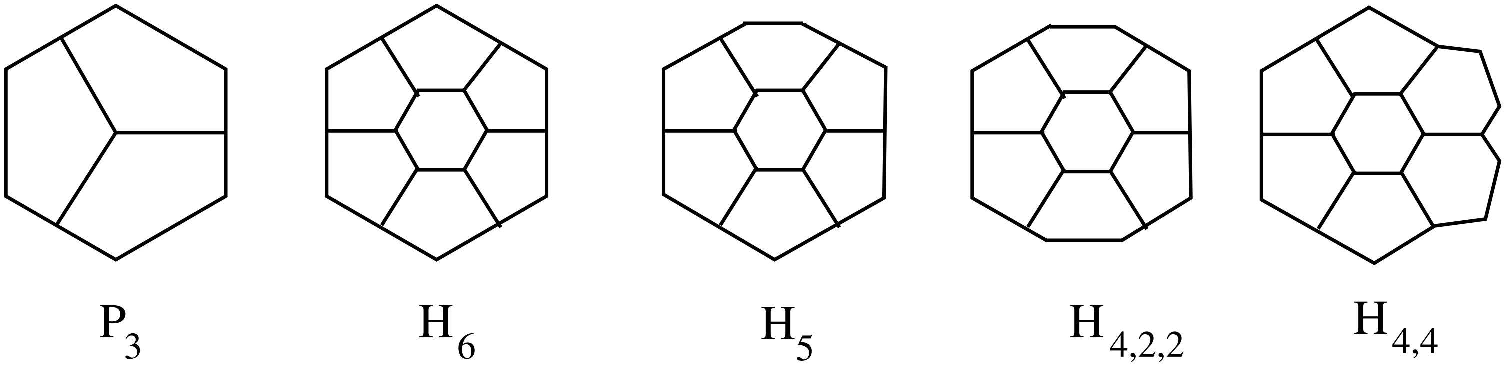
A graph F is H-forbidden in a class $\mathcal{G}$ if no graph $G \in \mathcal{G}$ having F as a subgraph has a perfect H-packing.

Star-forbidden graphs

A graph F is H-forbidden in a class $\mathcal{G}$ if no graph $G \in \mathcal{G}$ having F as a subgraph has a perfect H-packing.

Proposition

Following graphs are star-forbidden in fullerene graphs:



Negative results

Negative results

Proposition

$C_{20} : I_h$ does not have a perfect star-packing.

Negative results

Proposition

$C_{20} : I_h$ does not have a perfect star-packing.

Proposition

Narrow nanotubes C_{10n} and C_{12n} do not have perfect star-packings.

Negative results

Proposition

$C_{20} : I_h$ does not have a perfect star-packing.

Proposition

Narrow nanotubes C_{10n} and C_{12n} do not have perfect star-packings.

Proposition

Let G be a fullerene graph on less than 40 vertices. Then G does not have a perfect star-packing.

Negative results

Proposition

$C_{20} : I_h$ does not have a perfect star-packing.

Proposition

Narrow nanotubes C_{10n} and C_{12n} do not have perfect star-packings.

Proposition

Let G be a fullerene graph on less than 40 vertices. Then G does not have a perfect star-packing.

Proposition

Buckyball $C_{60} : I_h$ does not have a perfect star-packing.

Finally something positive

Finally something positive

Proposition

$C_{40} : D_{5h}$ is the unique smallest fullerene having a perfect star-packing.

Finally something positive

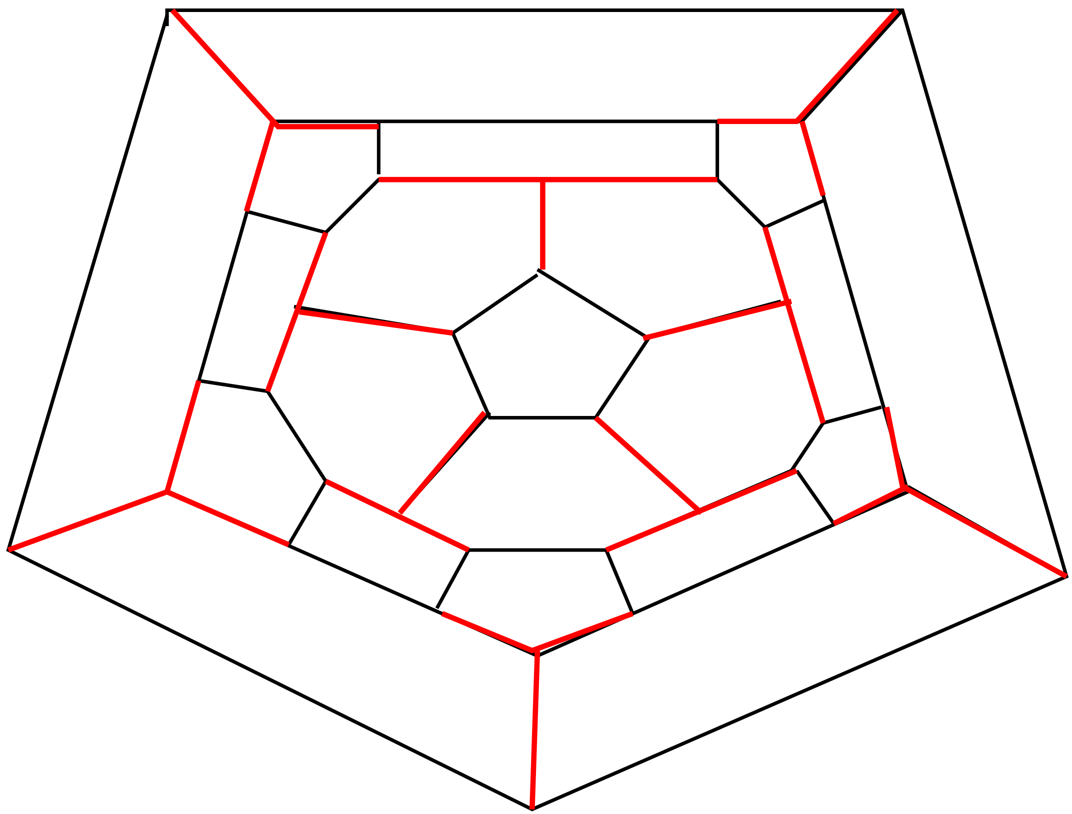
Proposition

$C_{40} : D_{5h}$ is the unique smallest fullerene having a perfect star-packing.

Proposition

There are only three fullerene graphs on at most 60 vertices having a perfect star-packing: $C_{40} : D_{5h}$, $C_{48} : D_6$, and $C_{56} : 649$.

$C_{40} : D_{5h}$

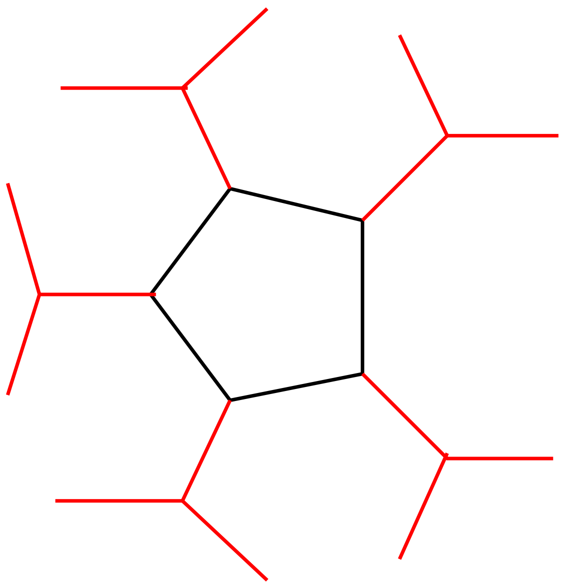


$P0$ and $P1$ packings

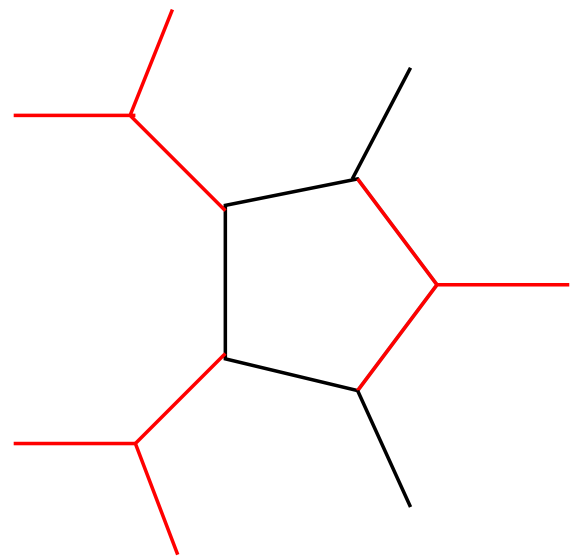
A star-packing in a fullerene graph G is of type $P0$ if no center of a star lies on a pentagon. Otherwise it is of type $P1$.

$P0$ and $P1$ packings

A star-packing in a fullerene graph G is of type $P0$ if no center of a star lies on a pentagon. Otherwise it is of type $P1$.



P_0



P_1

$C_{80} : I_h$

$C_{80} : I_h$

Proposition

$C_{80} : I_h$ is the unique smallest fullerene having a perfect star-packing of type $P0$.

$C_{80} : I_h$

Proposition

$C_{80} : I_h$ is the unique smallest fullerene having a perfect star-packing of type $P0$.

Theorem

A fullerene graph F_{8m} on $4m$ vertices has a perfect star-packing of type $P0$ if and only if it arises from a fullerene graph F_{2m} via chamfering transformation.

$C_{80} : I_h$

Proposition

$C_{80} : I_h$ is the unique smallest fullerene having a perfect star-packing of type $P0$.

Theorem

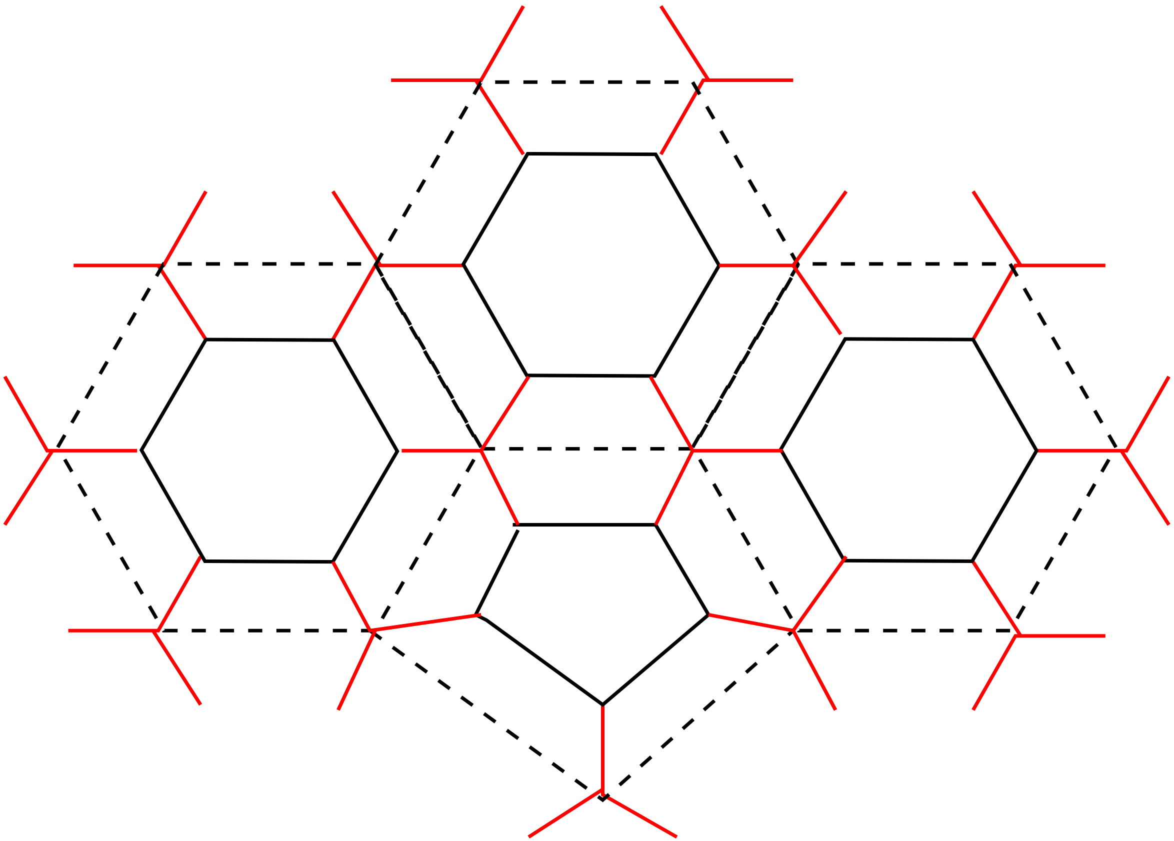
A fullerene graph F_{8m} on $4m$ vertices has a perfect star-packing of type $P0$ if and only if it arises from a fullerene graph F_{2m} via chamfering transformation.

Corollary

The fraction of fullerenes that have a perfect star-packing is bounded away from zero.

Chamfering transformation

Chamfering transformation



$(k,6)$-fullerene graphs

A $(k,6)$-fullerene graph is a planar, 3-regular and 3-connected graph, with only k-gonal and hexagonal faces.

$(k,6)$-fullerene graphs exist only for $k = 3,\ 4,\ 5$.

$(k,6)$-fullerene graphs

A $(k,6)$-fullerene graph is a planar, 3-regular and 3-connected graph, with only k-gonal and hexagonal faces.

$(k,6)$-fullerene graphs exist only for $k = 3,\ 4,\ 5$.

Theorem

All $(3,6)$-fullerene graphs have perfect star-packings.

Context

Context

- (Perfect) k-codes

Context

- (Perfect) k-codes
- k-independence

Context

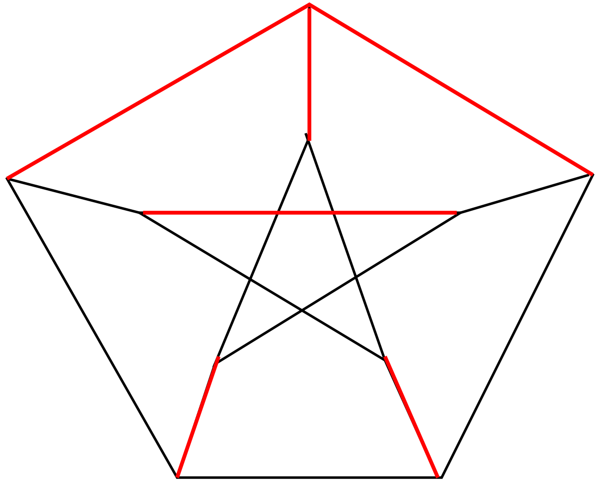
- (Perfect) k-codes
- k-independence
- Efficient domination

Context

- (Perfect) k-codes
- k-independence
- Efficient domination
- Perfect pseudo-matchings

Context

- (Perfect) k-codes
- k-independence
- Efficient domination
- Perfect pseudo-matchings



Perfect pseudo-matchings in fullerenes

Perfect pseudo-matchings in fullerenes

Theorem

Every fullerene graph on n vertices has a perfect pseudo-matching of size at most $\frac{n}{2} - 2$.

Perfect pseudo-matchings in fullerenes

Theorem

Every fullerene graph on n vertices has a perfect pseudo-matching of size at most $\frac{n}{2} - 2$.

Problem

Find the smallest size of a perfect pseudo-matching for a given fullerene graph.

Packing other small graphs in fullerenes

Packing other small graphs in fullerenes

Theorem

Let G be a fullerene graph on $14n$ vertices arising from a fullerene graph on $2n$ vertices *via* the **capra** septupling transformation. Then there is a perfect packing of $S(K_{1,3})$ in G.

Packing other small graphs in fullerenes

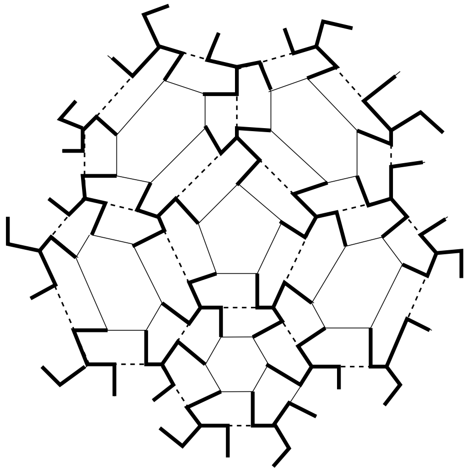
Theorem

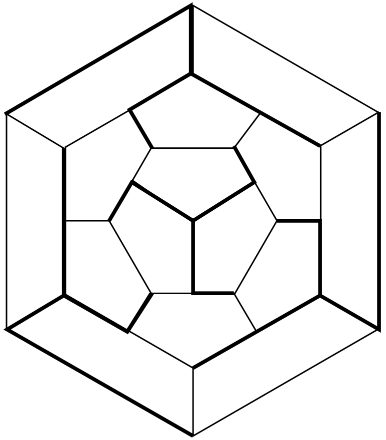
Let G be a fullerene graph on $14n$ vertices arising from a fullerene graph on $2n$ vertices *via* the **capra** septupling transformation. Then there is a perfect packing of $S(K_{1,3})$ in G.

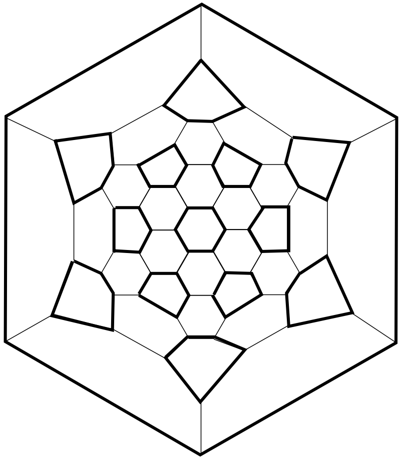
Theorem

A fullerene graph G has a perfect $\{C_5, C_6\}$-packing if and only if it is a leapfrog fullerene.

Packing other small graphs in fullerenes







Open problems

Open problems

- Existence of perfect star-packings in fullerenes on $8n + 4$ vertices.

Open problems

- Existence of perfect star-packings in fullerenes on $8n + 4$ vertices.

- Perfect star-packings in $(4, 6)$-fullerenes.

Open problems

- Existence of perfect star-packings in fullerenes on $8n + 4$ vertices.

- Perfect star-packings in $(4, 6)$-fullerenes.

- Other packings in classical and generalized fullerenes.

Open problems

- Existence of perfect star-packings in fullerenes on $8n+4$ vertices.
- Perfect star-packings in $(4,6)$-fullerenes.
- Other packings in classical and generalized fullerenes.
- Enumerative aspects.

Open problems

- Existence of perfect star-packings in fullerenes on $8n + 4$ vertices.
- Perfect star-packings in $(4, 6)$-fullerenes.
- Other packings in classical and generalized fullerenes.
- Enumerative aspects.
- $\cdots$

Thank you!