Bipartizing fullerenes

Zdeněk Dvořák, Bernard Lidický and Riste Škrekovski

Charles University
University of Illinois
University of Ljubljana

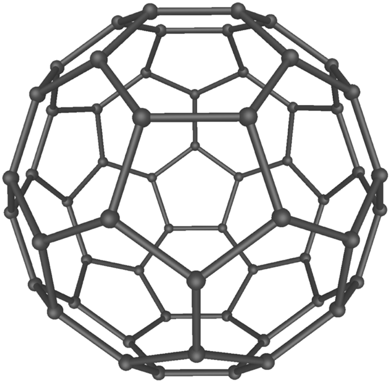
Second Postdoctoral Research Symposium
Urbana-Champaign
Jan 27 2012

What is a fulleren?

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

What is a fulleren?

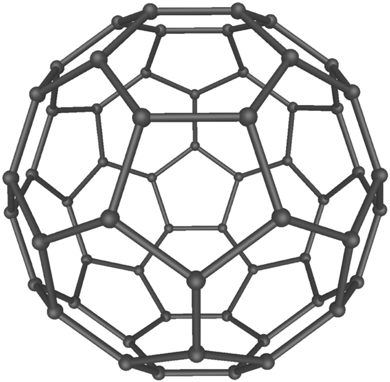
A *fullerene* is a polyhedral molecule consisting only of carbon atoms and containing only pentagonal and hexagonal faces.



buckyball (C_{60})

What is a fulleren?

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

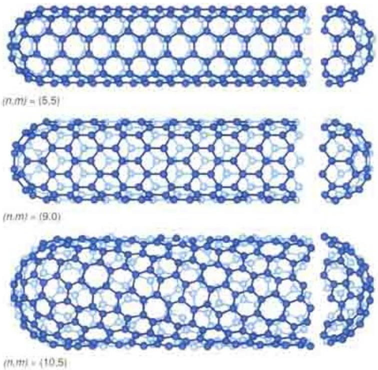


buckyball (C_{60})

soccer ball

What is a fulleren?

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



nanotubes

History

- 1965 - C_{60} first mentioned H.P. Schultz (1965)
- 70's - theoretical study (prediction) of C_{60}
- 1985 - C_{60} exists! H. Kroto, J. R. Heath, S. O'Brien, R. Curl and R. Smalley
- 1991 - possible to produce C_{60}, nanotubes
- 1996 - Nobel prize in chemistry for C_{60}

History

- 1965 - C_{60} first mentioned H.P. Schultz (1965)
- 70's - theoretical study (prediction) of C_{60}
- 1985 - C_{60} exists! H. Kroto, J. R. Heath, S. O'Brien, R. Curl and R. Smalley
- 1991 - possible to produce C_{60}, nanotubes
- 1996 - Nobel prize in chemistry for C_{60}

History

- 1965 - C_{60} first mentioned H.P. Schultz (1965)
- 70's - theoretical study (prediction) of C_{60}
- 1985 - C_{60} exists! H. Kroto, J. R. Heath, S. O'Brien, R. Curl and R. Smalley
- 1991 - possible to produce C_{60}, nanotubes
- 1996 - Nobel prize in chemistry for C_{60}

History

- 1965 - C_{60} first mentioned H.P. Schultz (1965)
- 70's - theoretical study (prediction) of C_{60}
- 1985 - C_{60} exists! H. Kroto, J. R. Heath, S. O'Brien, R. Curl and R. Smalley
- 1991 - possible to produce C_{60}, nanotubes
- 1996 - Nobel prize in chemistry for C_{60}

History

- 1965 - C_{60} first mentioned H.P. Schultz (1965)
- 70's - theoretical study (prediction) of C_{60}
- 1985 - C_{60} exists! H. Kroto, J. R. Heath, S. O'Brien, R. Curl and R. Smalley
- 1991 - possible to produce C_{60}, nanotubes
- 1996 - Nobel prize in chemistry for C_{60}

History

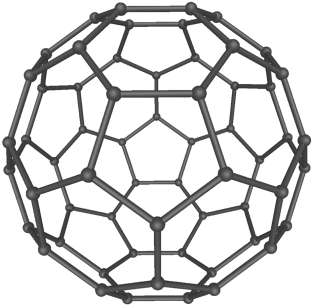
- 50's - Select manufactured the first "C_{60}" soccer ball
- 1965 - C_{60} first mentioned H.P. Schultz (1965)
- 70's - theoretical study (prediction) of C_{60}
- 1985 - C_{60} exists! H. Kroto, J. R. Heath, S. O'Brien, R. Curl and R. Smalley
- 1991 - possible to produce C_{60}, nanotubes
- 1996 - Nobel prize in chemistry for C_{60}

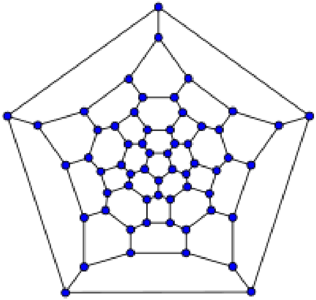
Theoretical prediction of fullerenes

- glue together pentagonal and hexagonal faces
- is the result stable?

Fullerens as graphs (in graph theory)

- atoms - vertices
- adjacency - edges
- molecule - planar graph
- 12 pentagonal faces, unbounded number of hexagonal faces





C_{60}

Stability of fullerenes predicted by graphs

Not all graphs correspond to fullerenes
(resulting molecules are not stable)

Conjecture

Stability of fullerenes corresponds to some graph property.

- number of perfect matchings
- independence number
- ....
- isolated pentagon rule - close pentagons are trouble
  - What is the distance between pentagons?

(No good correspondence is know yet)

Stability of fullerenes predicted by graphs

Not all graphs correspond to fullerenes
(resulting molecules are not stable)

Conjecture

Stability of fullerenes corresponds to some graph property.

- number of perfect matchings
- independence number
- ....
- isolated pentagon rule - close pentagons are trouble
  - What is the distance between pentagons?

(No good correspondence is know yet)

How distant?

How far can the pentagons be from each other?

Conjecture (Došlić, Vukičević)

Distance is at most $\sqrt{12n/5}$.

Theorem (Dvořák, L., Škrekovski)

Distance is at most $c\sqrt{n}$ for some constant c.

Fullerene graph can be made bipartite by removing $c\sqrt{n}$ edges.

How distant?

How far can the pentagons be from each other?

Conjecture (Došlić, Vukičević)

Distance is at most $\sqrt{12n/5}$.

Theorem (Dvořák, L., Škrekovski)

Distance is at most $c\sqrt{n}$ for some constant c.

Fullerene graph can be made bipartite by removing $c\sqrt{n}$ edges.

Our result

Theorem (Dvořák, L., Škrekovski)

Let F be a pentagonal face. There are 5 other pentagonal faces in distance at most $c\sqrt{n}$ from F.

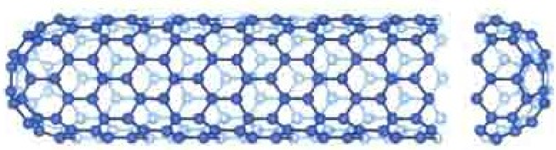
Our result

Theorem (Dvořák, L., Škrekovski)

Let F be a pentagonal face. There are 5 other pentagonal faces in distance at most $c\sqrt{n}$ from F.

Corollary (Dvořák, L., Škrekovski)

"Fullerenes look like nanotubes."



Thank you for your attention!