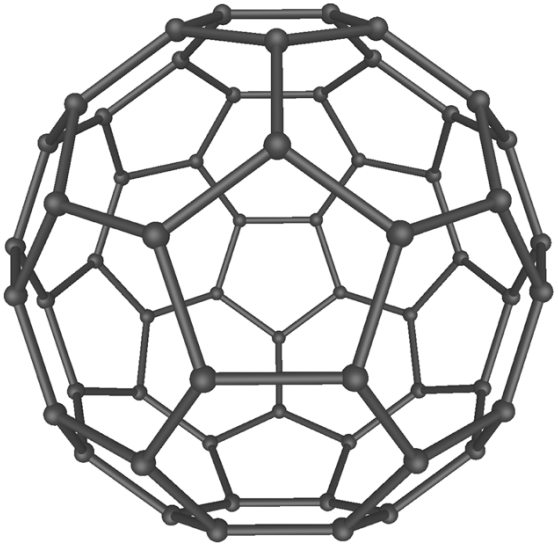


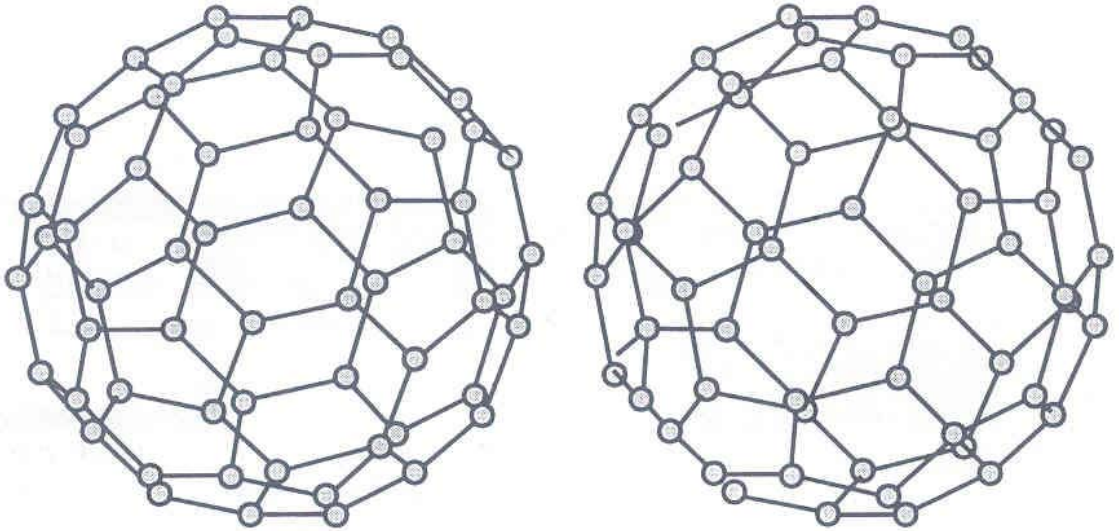
Introduction to Fullerene

PHY 891
May 8, 2009

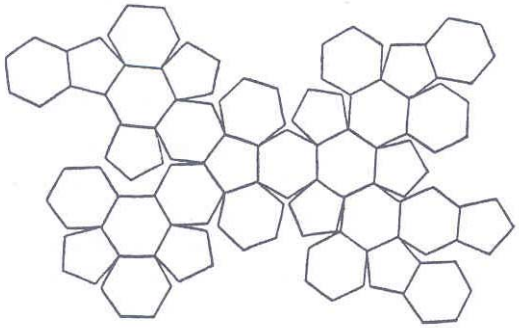
Kritsada Kittimanapun

Outline

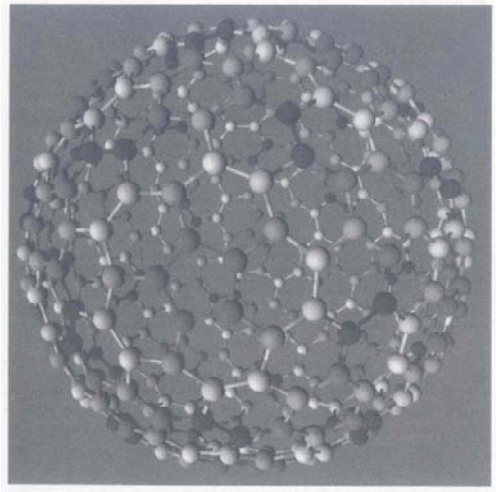
- Historical Introduction
- Fullerene structure
- Electronic structure
- Electrical conductivity
- Specific heat
- Conclusion

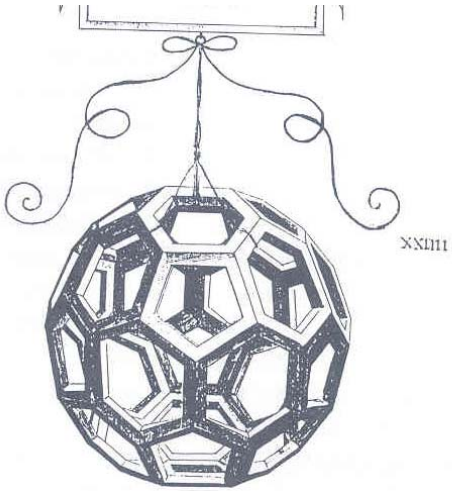


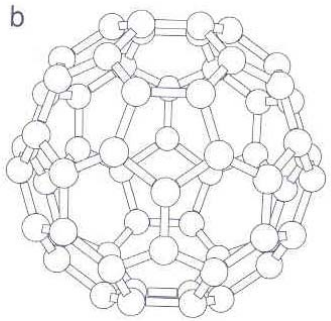
Historical introduction

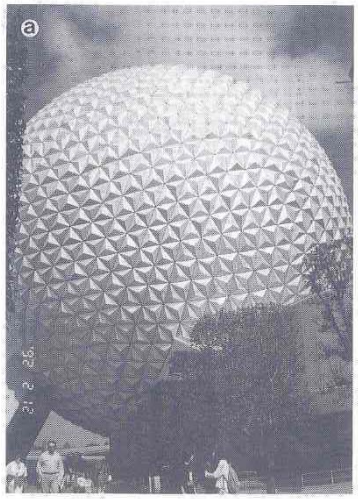


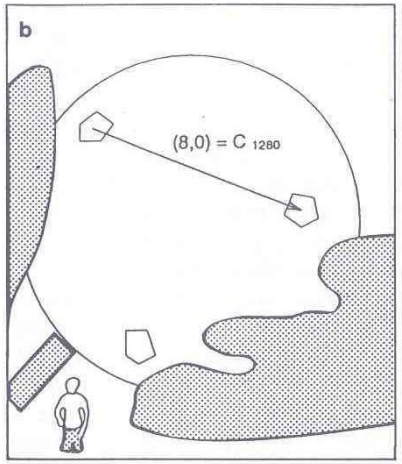
- Early history
- Astronomical observation
- Architectural analogs
- Biological and geological examples





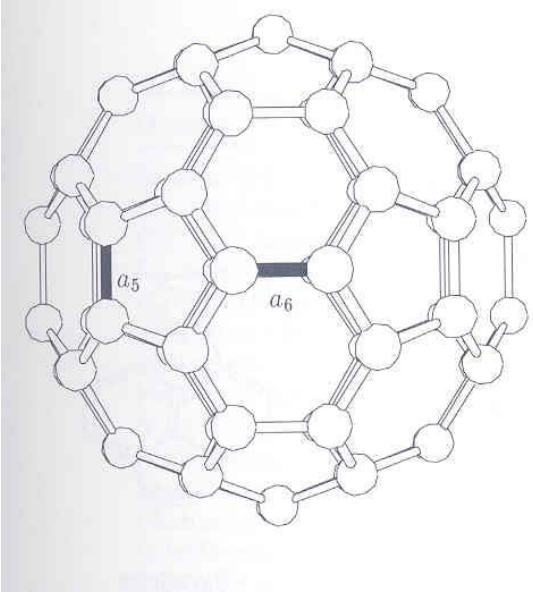






Fullerene structure

- Average bond length 1.44 A
  - On pentagon 1.46 A
  - On hexagon 1.40 A
- Diameter 7.10 A
  - Outer diameter 10.34 A
- Binding energy 7.4 eV/atom
  - Less than BE of carbon in graphite and ghaphene
- Cohesive energy 1.4 eV/atom



Fullerence structure

- Euler's theorem (for polyhedra)

$$f + v = e + 2$$

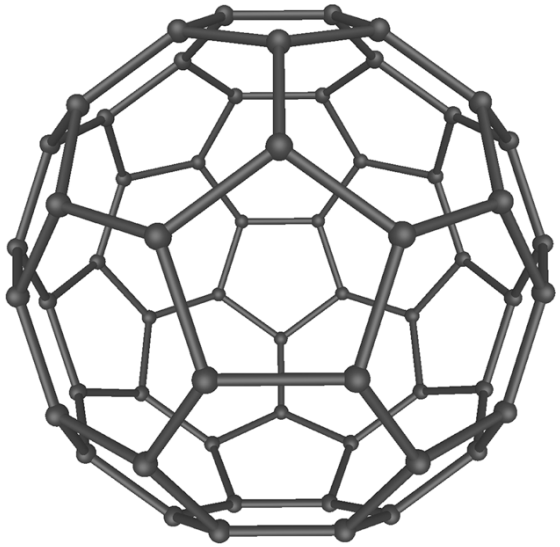
where $f, v,$ and e are respectively the numbers of faces, vertices, and edges of the polyhedra.

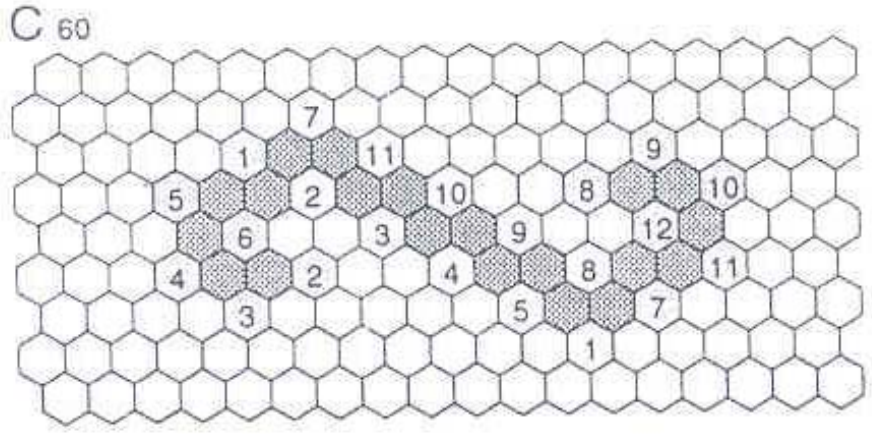
$$f = p + h$$

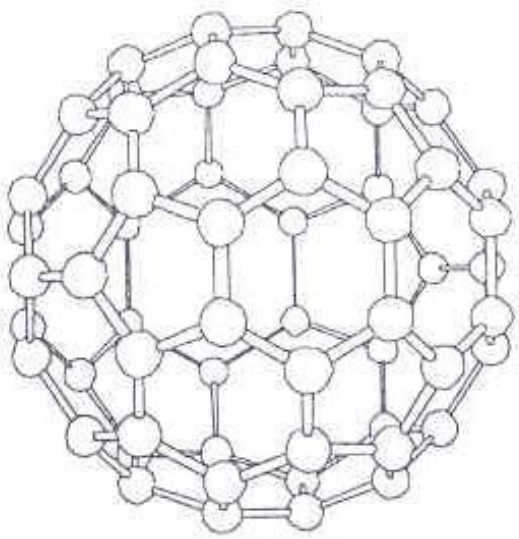
$$2e = 5p + 6h$$

$$3v = 5p + 6h$$

- >>> $6(f + v - e) = p = 12$



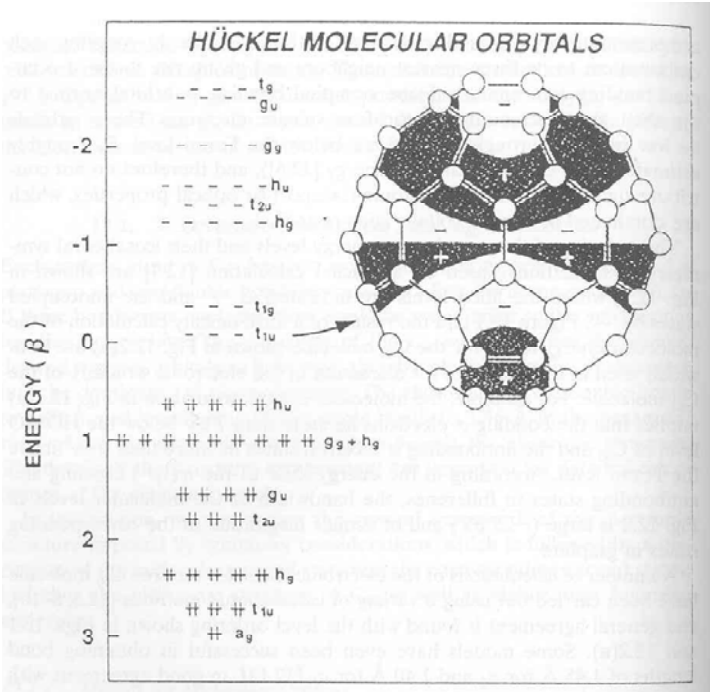




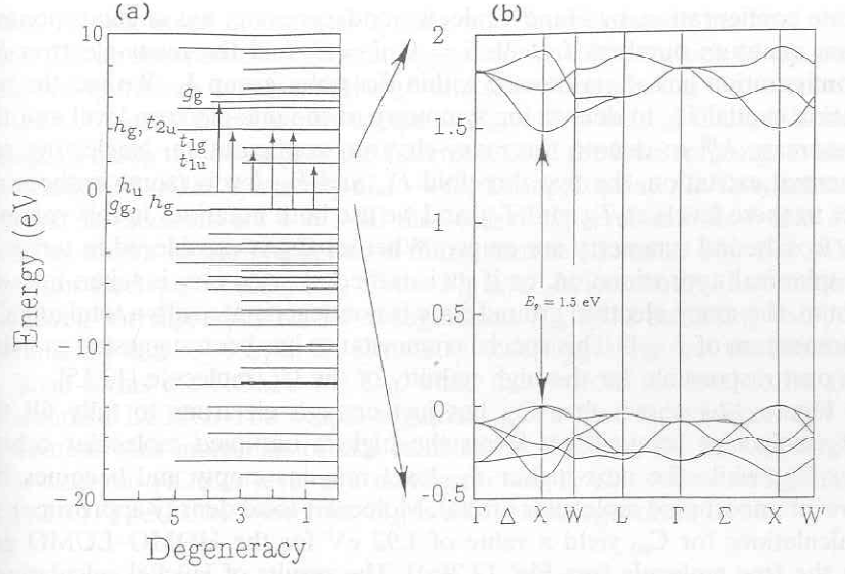
Fullerene folding from graphene

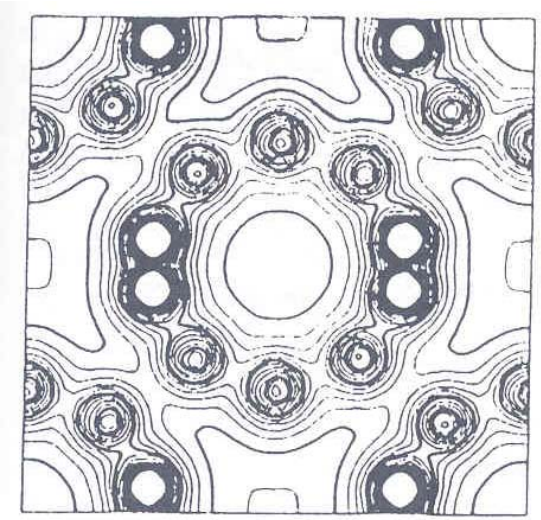
Electronic structure

- Electronic levels for free C_{60} molecules
  - Models for molecular orbital
    - Huckel model–physical discussion, tight-binding, *ab* initio
    - Every atom is equivalent
    - Successful in calculation of ionization potential and electron affinity



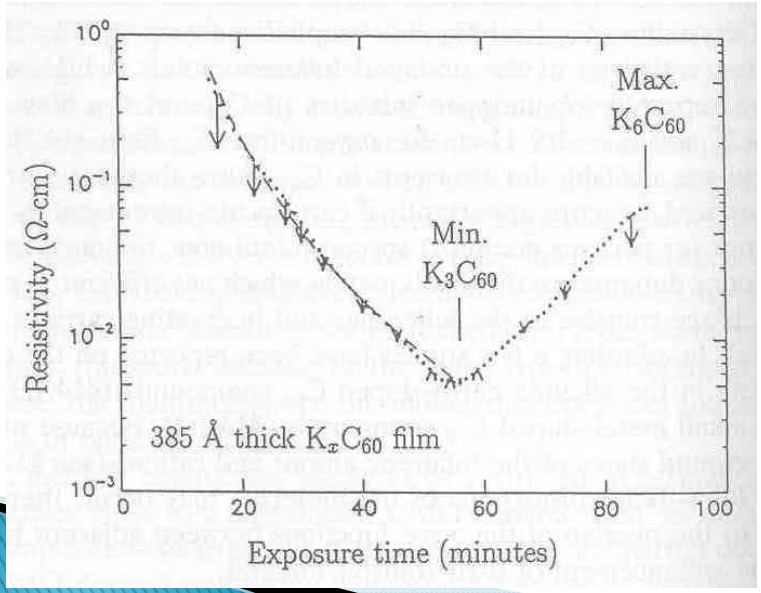
- Electronic structure of Fullerenes in the solid state
  - Overview of the electronic structure in the solid state
    - One-electron band calculation approach
    - Intramolecular interactions approach
    - Both provide determinations of HOMO-LUMO gap
  - Band calculations for solid C_{60}
    - LDA in density functional calculation
    - Band gap of C_{60} ~ 1.5 eV
    - Charge contour

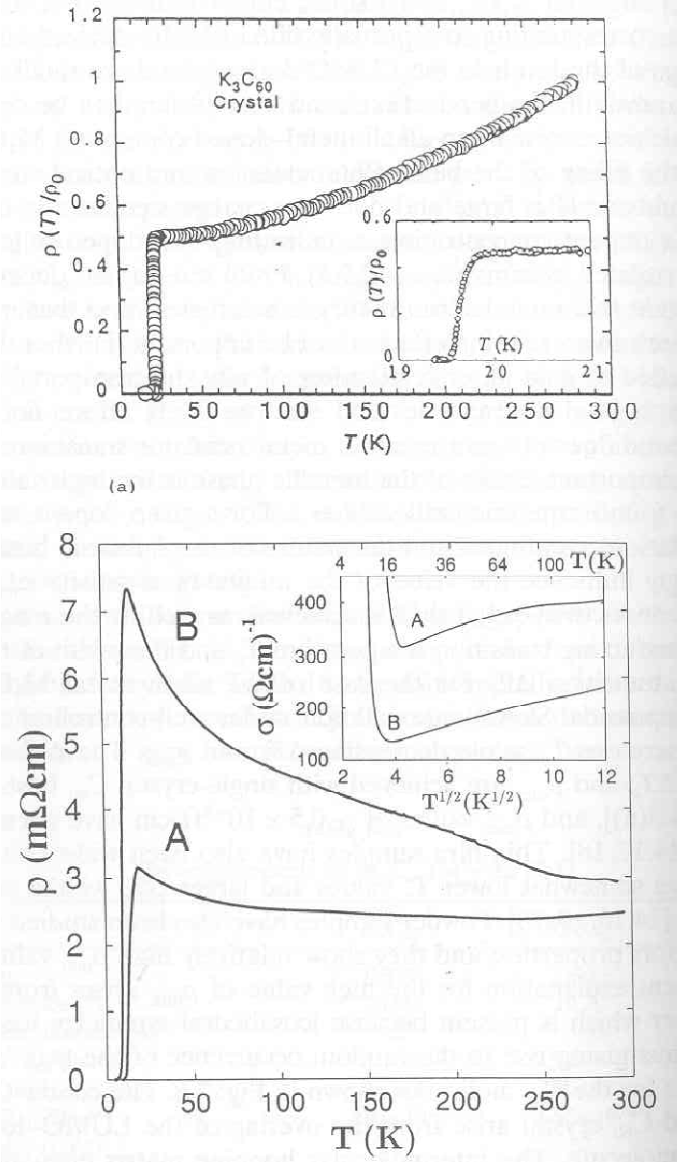




Electrical conductivity

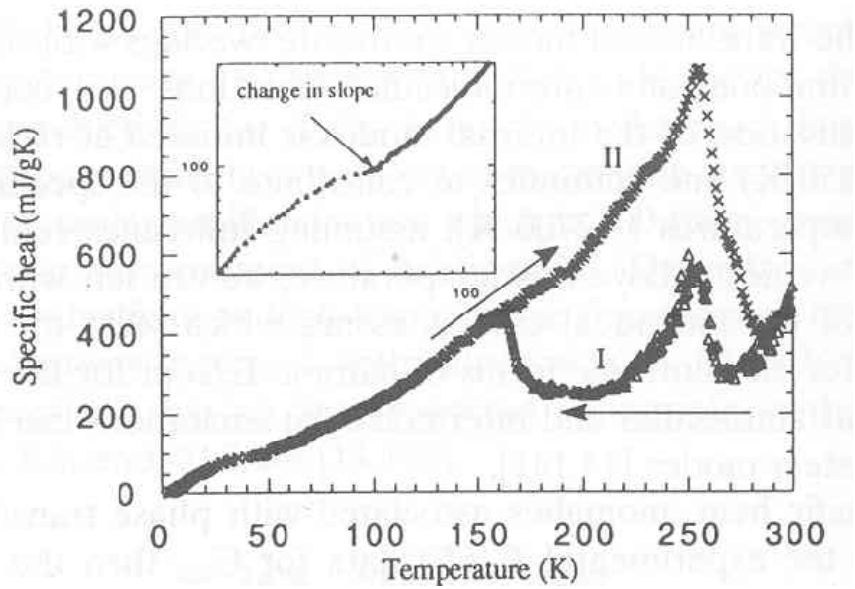
- Stoichiometry dependence
  - Alkali metal–doped C_{60}
- Temperature dependence
  - Alkali metal–dope M_XC_{60}





Specific heat

- Temperature dependence
  - Low temperature
  - Intermediate temperature
  - Very high temperature



Conclusion

- Widely studied theoretically and experimentally
- Interesting behavior in physical properties
- Various application