Introduction to Fullerene

PHY 891
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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 Å
  - On pentagon 1.46 Å
  - On hexagon 1.40 Å
- Diameter 7.10 Å
  - Outer diameter 10.34 Å
- Binding energy 7.4 eV/atom
  - Less than BE of carbon in graphite and graphene
- Cohesive energy 1.4 eV/atom
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, \textit{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 $C_{60} \sim 1.5$ eV
  - Charge contour
Electrical conductivity

- Stoichiometry dependence
  - Alkali metal-doped $C_{60}$
- Temperature dependence
  - Alkali metal-dope $M_x C_{60}$
Specific heat

- Temperature dependence
  - Low temperature
  - Intermediate temperature
  - Very high temperature
Widely studied theoretically and experimentally

Interesting behavior in physical properties

Various application