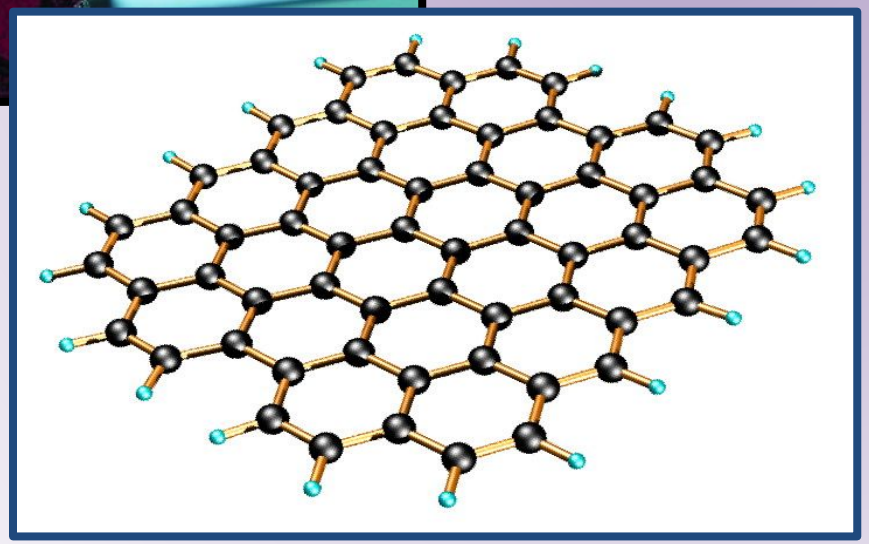
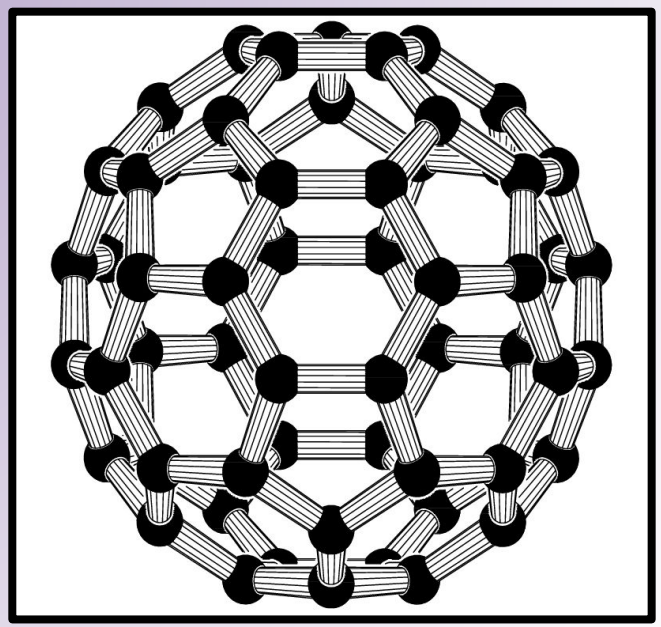
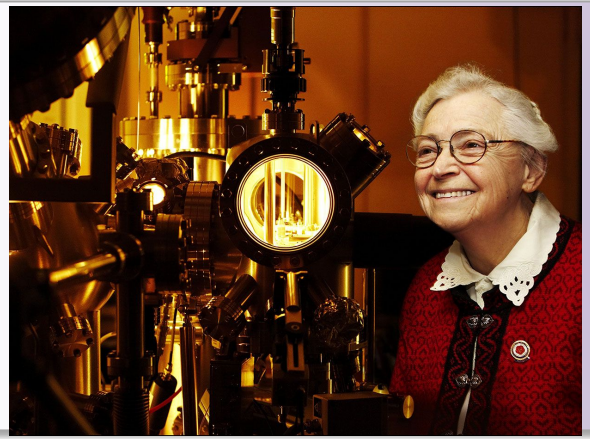


Mildred Dresselhaus was a **nanotechnologist** who made integral contributions to the understanding of many forms of carbon, particularly **graphene**, **fullerenes**, and **carbon nanotubes**.







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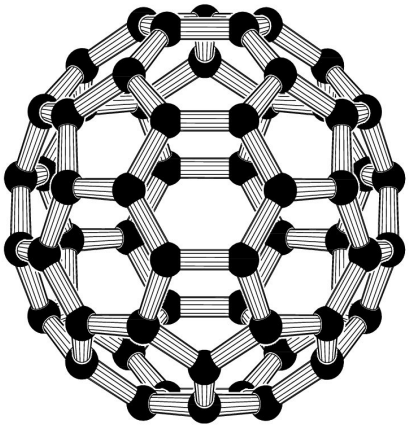
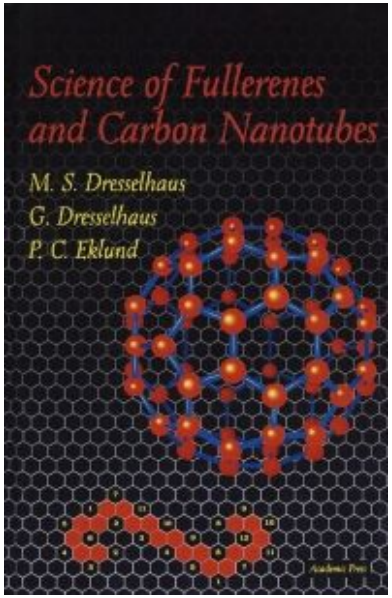
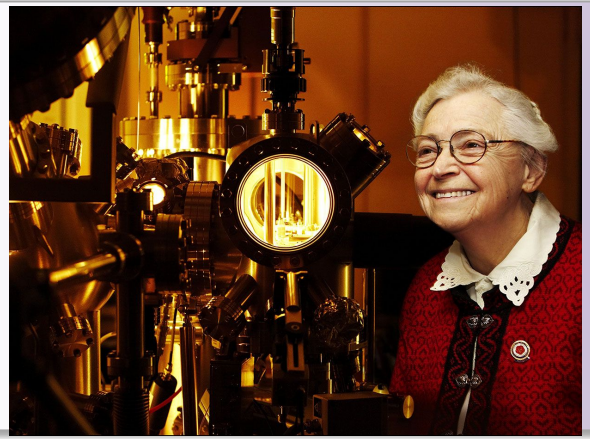
Dresselhaus's theoretical and experimental work studying carbon laid the foundation for the discovery of **buckminsterfullerenes**, also known as "**buckyballs**".





These are a type of **fullerene**: molecules made of carbon atoms arranged in a "**truncated icosahedron**" structure.

In 1996, Mildred Dresselhaus, Gene Dresselhaus, and Peter C. Eklund published "Science of fullerenes and carbon nanotubes": the first book that provides a comprehensive resource on fullerenes and discusses their applications.



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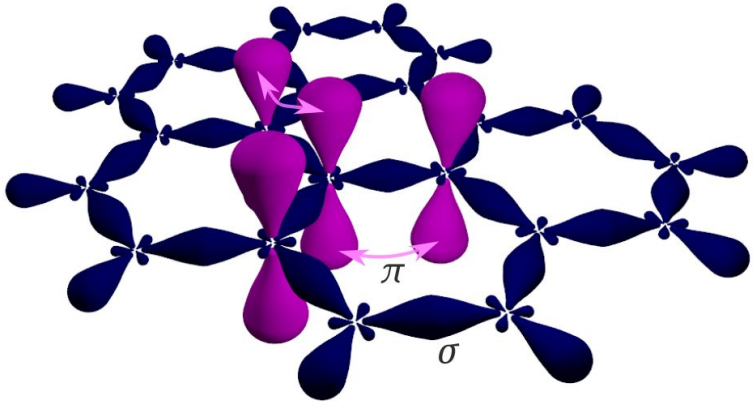
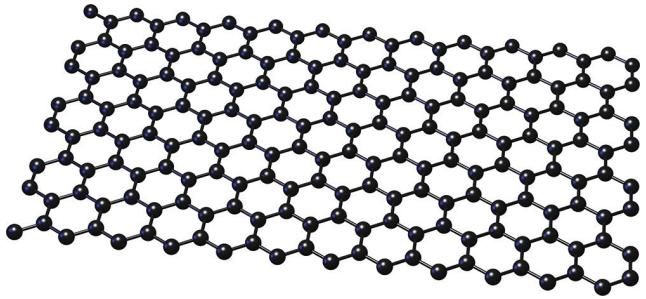
Mildred Dresselhaus laid the foundation of graphene research which led to the 2010 Nobel Prize in Physics, awarded to André Geim and Konstantin Novoselov for isolating and demonstrating the properties of graphene.

Graphene is a **two-dimensional** crystal of carbon atoms arranged in a **honeycomb lattice**.

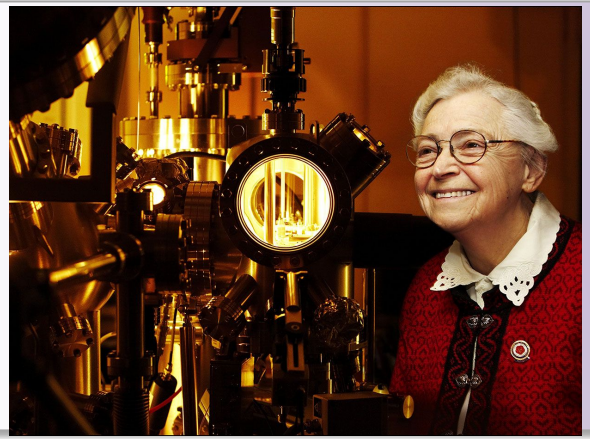


Each carbon atom has 4 **valence electrons**:

- Three are connected to three nearest neighbors by **sigma bonds**
- One is a **free pi electron**



The free pi electrons behave like **massless Dirac fermions** which move at relativistic speeds along graphene's plane.



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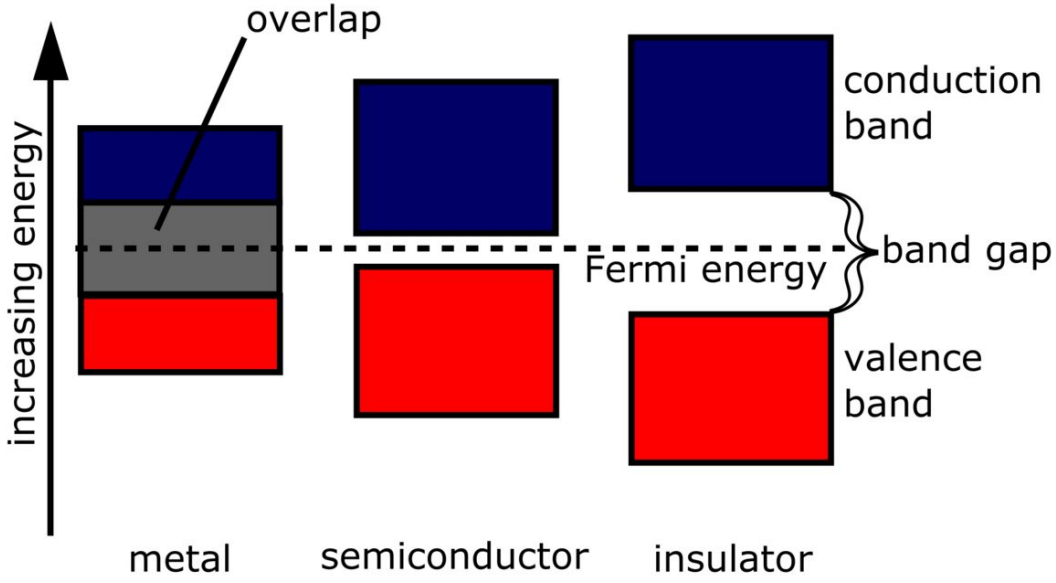
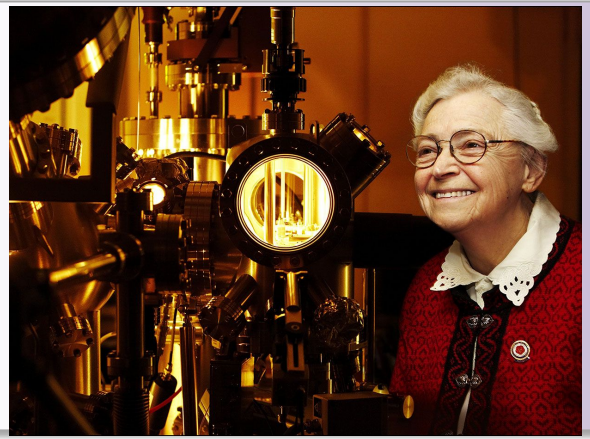


Band structure describes the energy levels of electrons in solids. It dictates whether the outermost electrons will be able to flow through the solid with or without added energy.

Metals are good electrical conductors and **insulators** are poor electrical conductors.

Graphene is both a metal and a **semiconductor**.



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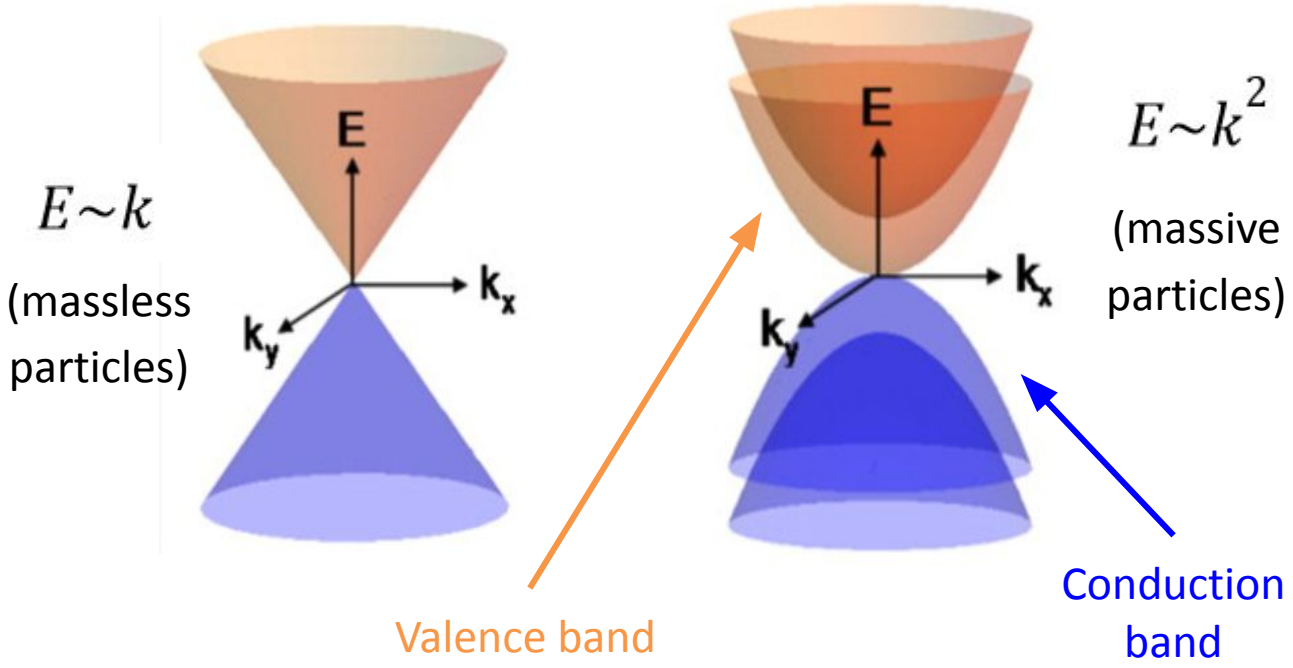
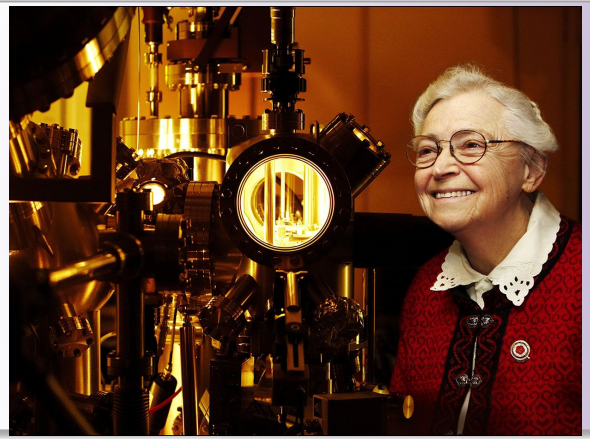
The **free valence electrons** in graphene behave either like **massless** or **massive particles**, depending on their momenta (or wavevectors).





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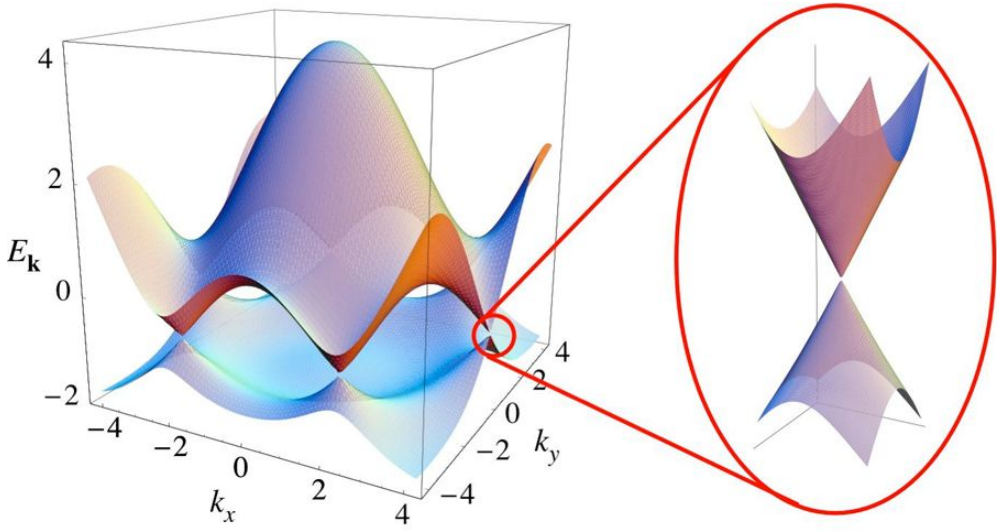
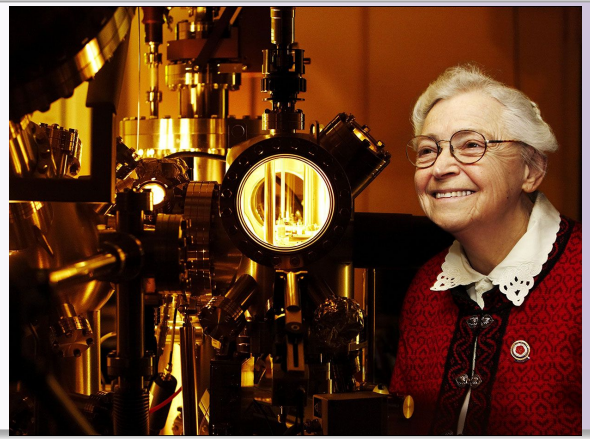


$$E(\mathbf{k}) = \pm\gamma_0\sqrt{1 + 4\cos^2\frac{1}{2}ak_x + 4\cos\frac{1}{2}ak_x \cdot \cos\frac{\sqrt{3}}{2}ak_y}$$

The **band structure** reveals two properties of graphene:

1. It can be **metallic**: current flows freely at the **Dirac points** (where energy E=0).
2. It can be a **semiconductor**: external energy is needed for current to flow at the **band gaps**.



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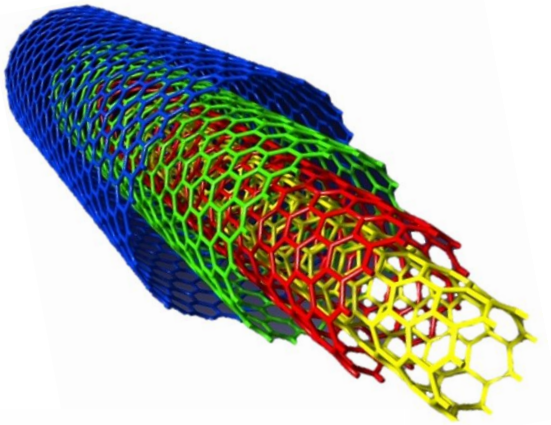
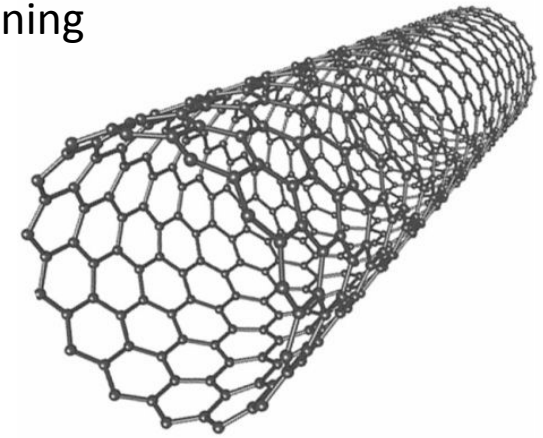
In 1992, Dresselhaus and others published a paper giving the first theoretical predictions of the electron properties of single-walled carbon nanotubes.

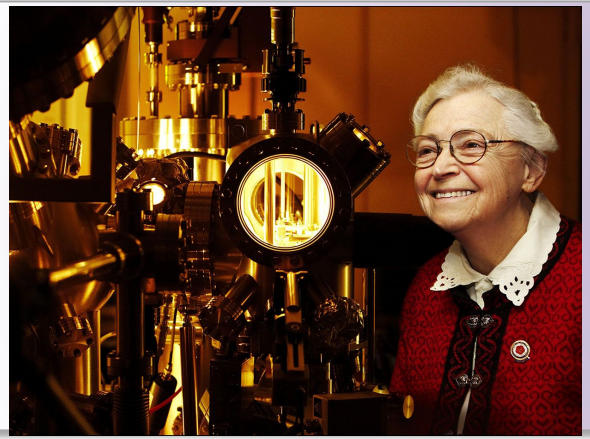


An ideal **single-walled carbon nanotube** (SWCNT) can be thought of as a sheet of graphene rolled into an infinitely long cylinder.

SWCNT's cross-sections are constrained to around 1 nm, meaning electrons can only propagate along the tubular axis - making the carbon nanotube a **one-dimensional conductor**.



Two or three SWCNTs can be nested together to form **multi-wall carbon nanotubes** (MWCNTs).



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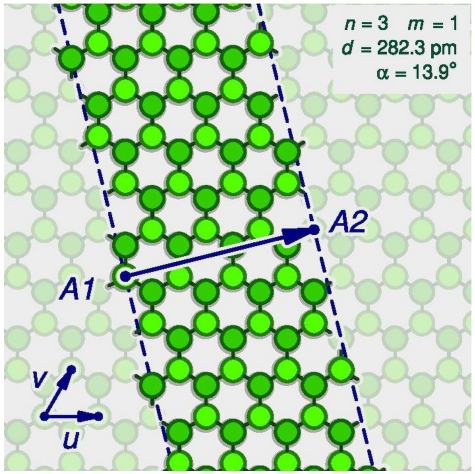
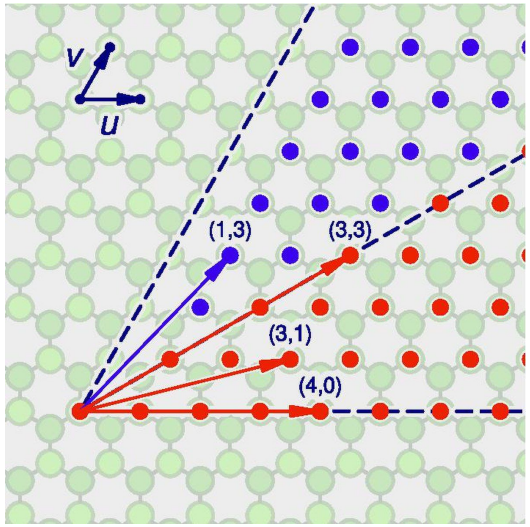


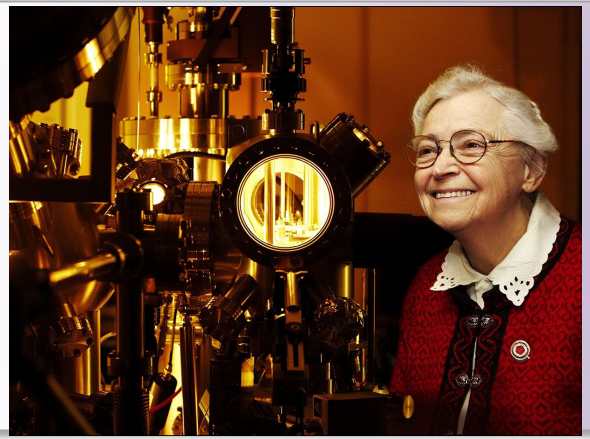


The configuration of a nanotube is given by its **(n,m) notation**.

Imagine the nanotube is unrolled into a sheet of graphene. This splits an atom (A) into two halves (A1 and A2) at either side of the sheet. The "**chiral vector**" pointing from A1 to A2 is:

$$\mathbf{c}_k = n\mathbf{u} + m\mathbf{v}$$

(n,m) notation describes the nanotube's geometry, which will determine its electrical properties



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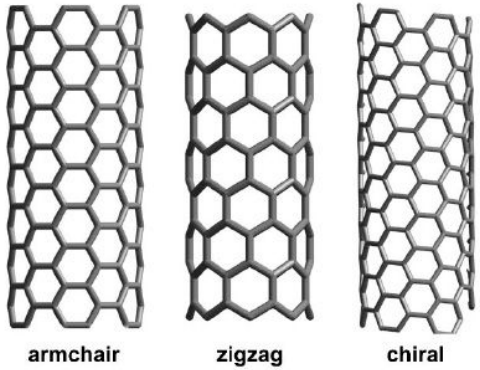
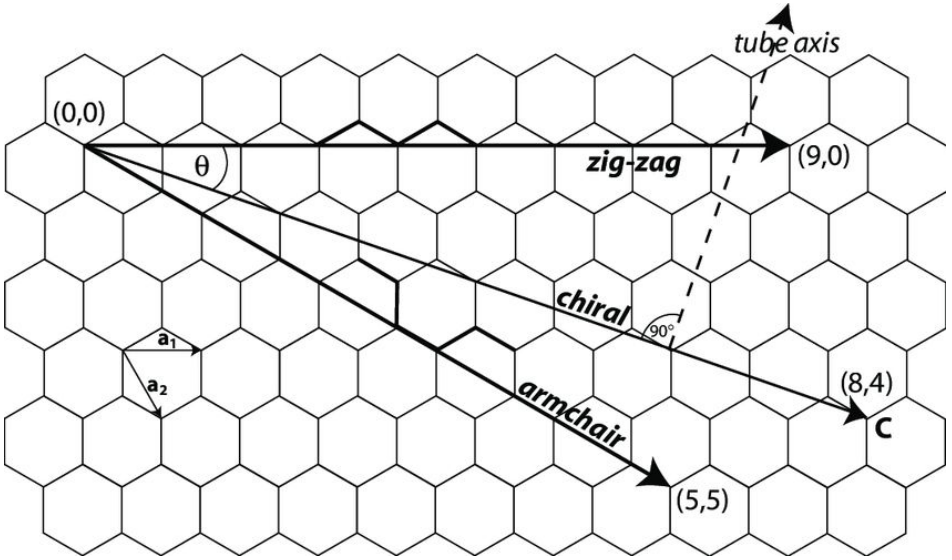
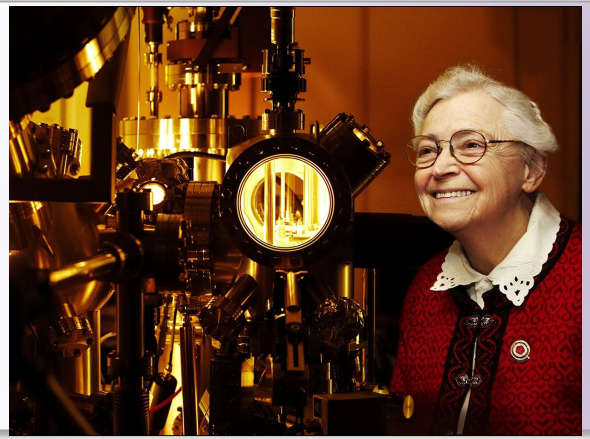


An (n,m) nanotube is **chiral** if m > 0 and m ≠ n. The **achiral** nanotubes are:

1. "**zigzag**" nanotubes have (n,m) = (n,0)
2. "**armchair**"nanotubes have (n,m) = (n,n) with n ≠ 0



If n = m, the nanotube is **metallic**. If n − m is a multiple of 3 and n ≠ m, the nanotube is **quasi-metallic** with a very small band gap.



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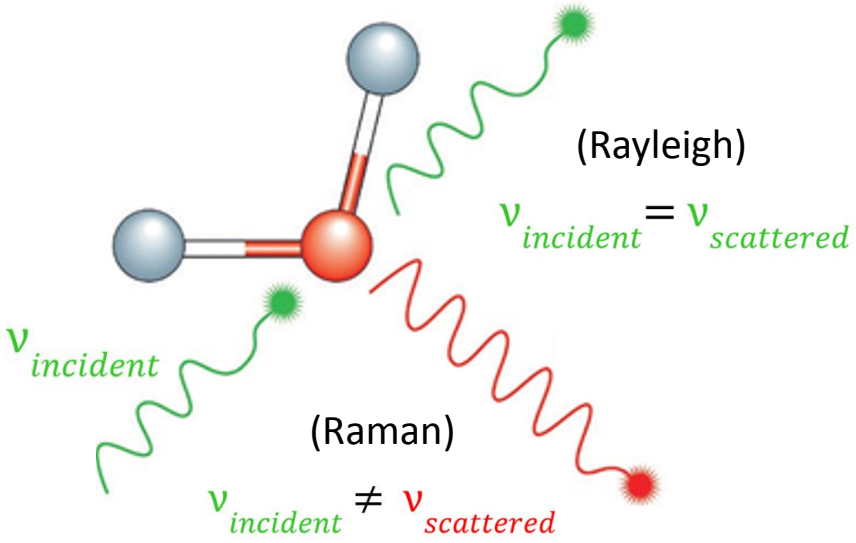
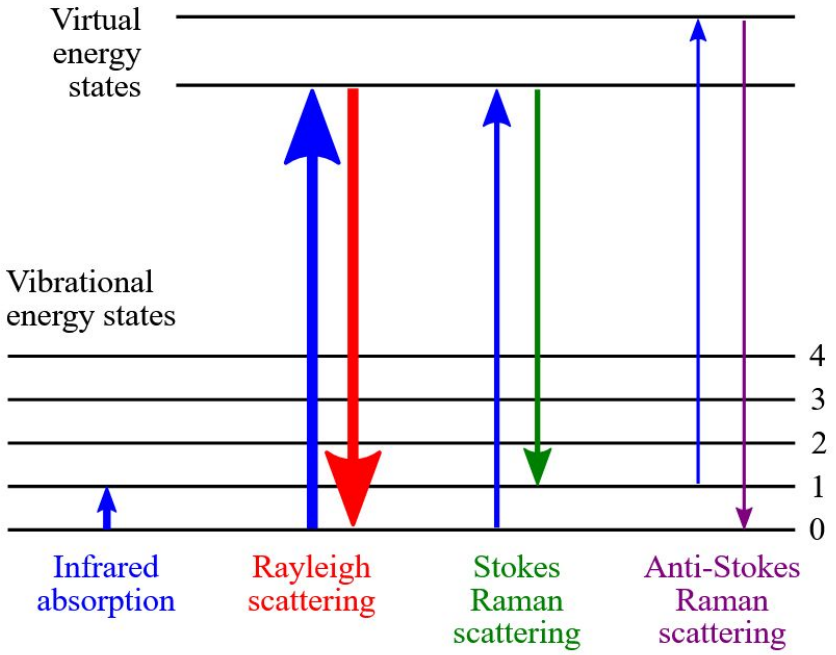
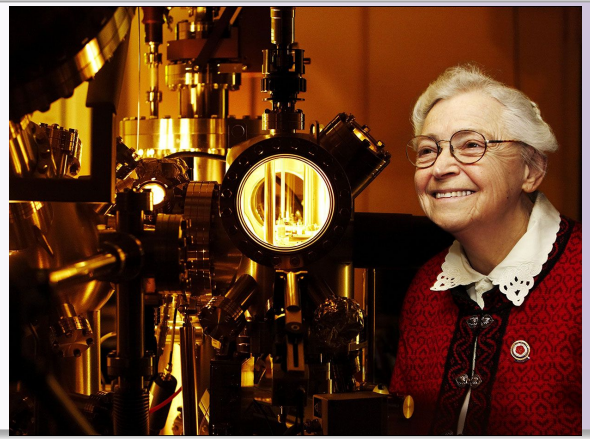
There are two types of scattering of photons by a material:

1. **Raman scattering** = inelastic
2. **Rayleigh scattering** = elastic





In all cases, the final state of the molecule has the same **electronic energy** as the initial state but changes **vibrational energy**.



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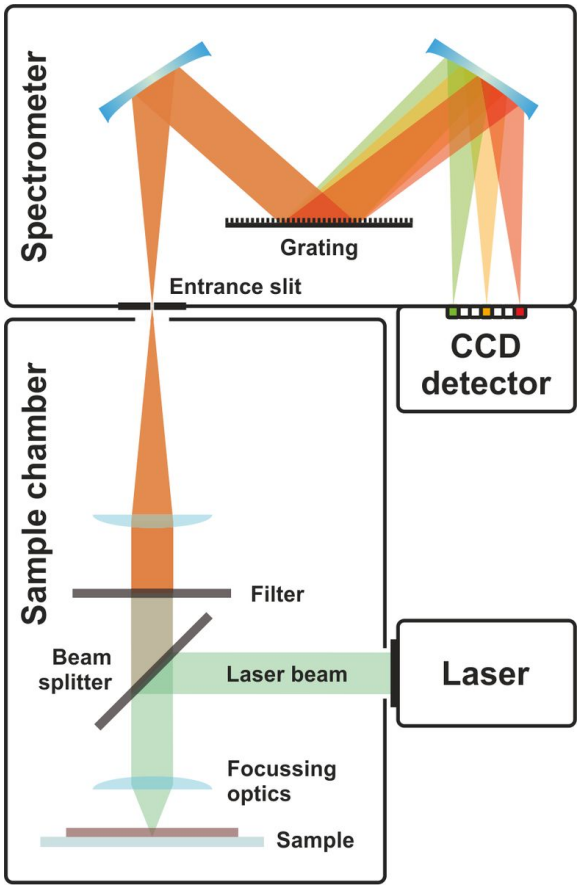
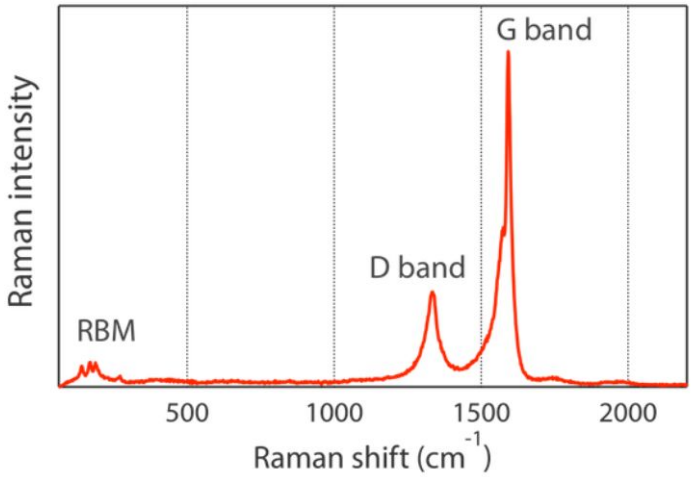
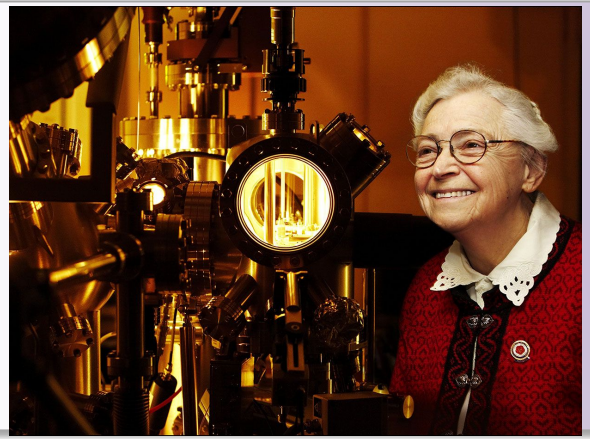


The **Raman spectrum** is the intensity of scattered light as a function of the "**Raman shift**": the frequency difference between the scattered and incident light.

Different molecules will have different Raman spectra because their vibrational modes are unique to their chemical bonds.





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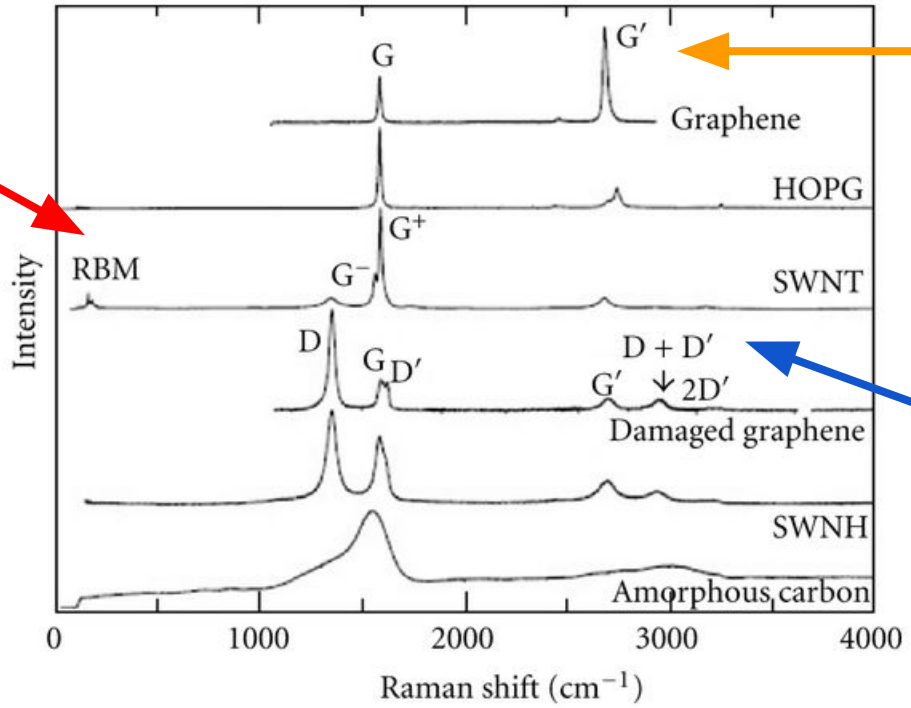
Dresselhaus used **Raman spectroscopy** to show the structure and electronic properties (such as metallicity or semiconductivity) and phonon properties of many **nanocarbons**.

The **radial breathing mode** (RBM) relates the diameter of a carbon nanotube to its optical transition energy



The **G' band** occurs during stretching of the carbon-carbon bonds in the material

The **D band** and the **D' band** are used to identify disorder in the sp2 network of carbon structures