Nano Materials: Applications and Properties

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Research Area of Interest

- Defect Studies in Annealed and Nano-annealed, ion-irradiated ZnO material
- Density functional theory (DFT) in B and N doped Single Wall Carbon Nanotubes (SWCNT), Graphene, Silicene, Germanene
- Non-equilibrium Statistical Mechanics (Surface Growth Problem)
- Diamagnetism : Finite Temperature Field Theory
- DC and AC Conductivity in Amorphous System (CMR and Manganite)
- Photo-Catalytic Activity towards degradation of different dyes

- Dr. Dirtha Sanyal (VECC, Kolkata)
- Dr. N. S. Mondal (Haldia Govt. College)
- Dr. A. Ghosh (Bose Institute)
- Dr. Sumona Paul (PDF/RA, IITGuwahati)
- Dr. U.N. Nandi (Scottisch Church College, Kolkata)
- Dr. Anindya Sarkar (Bangabasi Morning College, Kolkata)
- Prof. Mohi Uddin (CUET, Bangladesh)
- Dr. Saptarshi Pal (Asst. Prof, GLA Univ.)
- Dr. Suman Chowdhury (RA, PDF at Shiv Nadar University)

- Sujoy Kumar Mondal (SRF)
- Arka Bandyopadhyay (PDF at IISc)
- Debdas Karmakar (SRF)
- Apu Mondal (SRF/ Asst. Professor)
- Susmita Jana (SRF)
- Supriya Ghoshal (SRF)
- Mainak Ghosh (SRF)
- Debaprem Bhattacharya (SRF/Asst. Professor)
- Deep Mondal (JRF)
- Krishnanshu Basak (JRF)
- Dr. Sumona Sinha (DS Kothari Fellow)
- Dr. Subhadip Nath (Krishnagar College)

Abstract

In this pedagogical talk we would like to discuss the basic science behind nanoscience and nanotechnology suitable for the yound mind. Several examples from nature as well as from basic science will be illustrated. The role of basic quantum mechanics will be highlighted. In the second part, we would like discuss the intriguing physics of two dimensional (2D) materials. Dirac materials are a class of complex and functional nanomaterials offering great potential in the development of new electronic components. A tight binding (TB) model along with density functional theory (DFT) will be used to unravel the characteristic features of Dirac points in these systems.

Plan of The Talk

1. A brief history of Nano Science
2. Quantum Mechanics and its application to Nano Scence
3. DFT Calculations of some 2D structures
4. Conclusions

Why are there no small animals in the polar regions?

- Heat Loss $\propto$ Surface Area (L^2)

- Mass $\propto$ Volume (L^3)

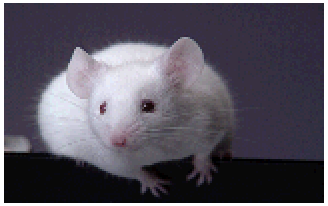
- Heat Loss/Mass $\propto$ Area/Volume

$$= L^2/L^3$$
$$= L^{-1}$$

Heat Loss/Mass $\propto$ Area/Volume

$= L^2/L^3$

$= L^{-1}$



Mouse (L = 5 cm)

$1/L = 1/(0.05\ m)$

$= 20\ m^{-1}$

Polar Bear (L = 2 m)

$1/L = 1/(2\ m)$

$= 0.5\ m^{-1}$

20 : 0.5 or 40 : 1

"'Quantum mechanics' is the description of the behavior of matter and light in all its details and, in particular, of the happenings on an atomic scale. Things on a very small scale behave like nothing that you have any direct experience about. They do not behave like waves, they do not behave like particles, they do not behave like clouds, or billiard balls, or weights on springs, or like anything that you have ever seen."

--Richard P. Feynman

Why do we have quantum mechanics?

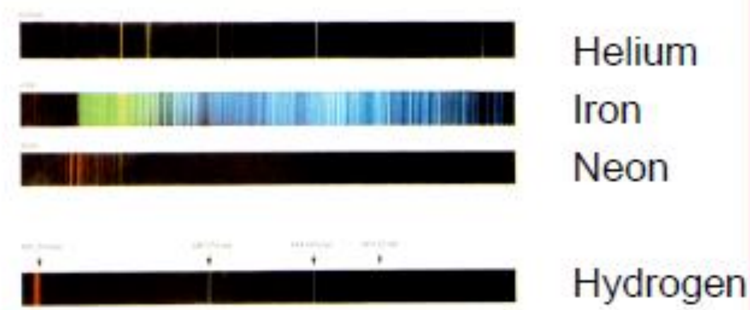
Particles sometimes behave like waves and vice-versa. This duality is something that is contrary to conventional classical mechanics. Quite often, physical phenomena cannot be explained by “classical mechanics”, e.g.

1. The existence of spectral lines
2. Photoelectric effect
3. Particle-wave duality
4. Double-slit experiment
5. Solid-state Physics & the failure of the classical (Drude) model

Spectral lines

sun

Spectra showing wavelengths which are present



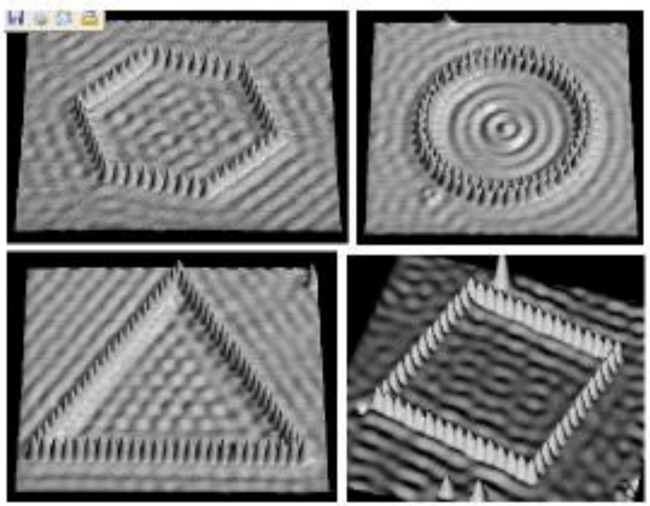
Balmer came up with a simple formula describing the Hydrogen spectrum:
$\lambda = 364.5n^2/(n^2-4)$..........$n = 3,4,5,6$

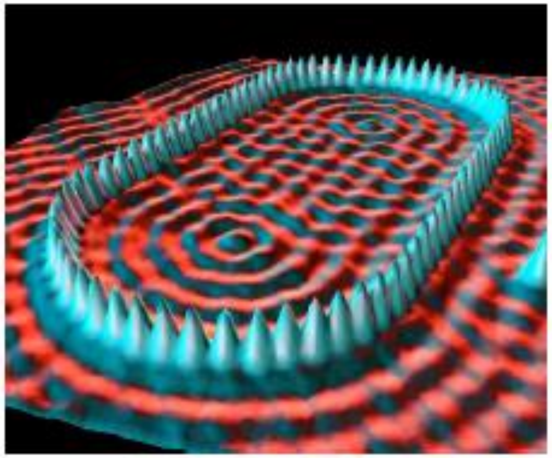
what is an electron?

I.e. particle or wave, both, or neither?

Answer – we don't know for sure, but if we assume it is a wave (actually a wave-packet), we will *always* predict the correct behavior.
If we assume it is a particle, we will sometimes be right, but most of the time we will be wrong……

Examples: Scanning tunneling microscope images of Iron atoms on a copper Surface. These structures are containing electron waves on the surface.





N.B. These are real images, not simulations!

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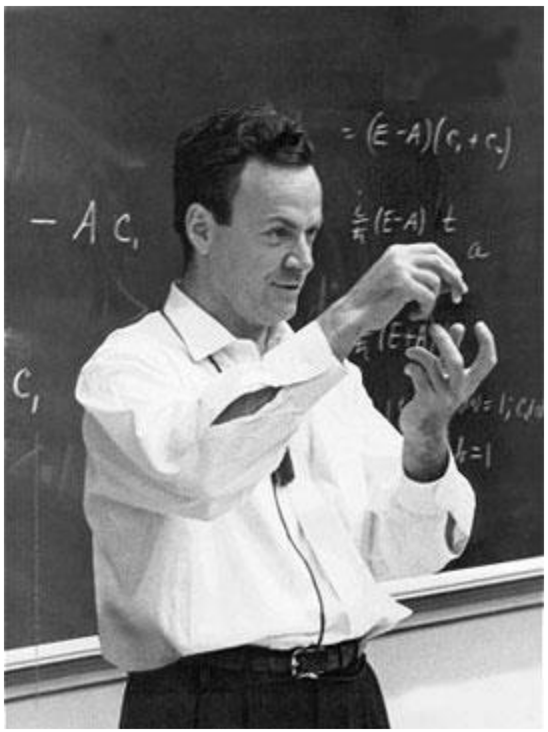
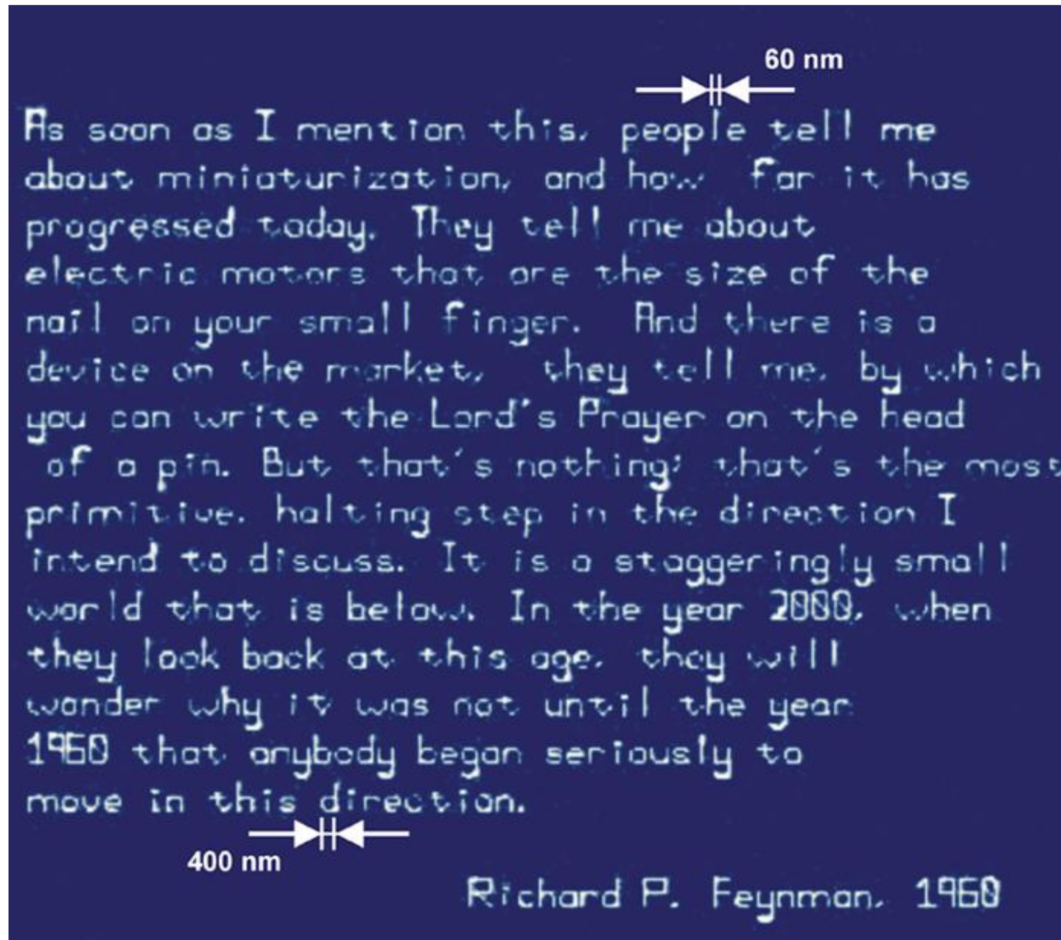
There's Plenty of Room at the Bottom

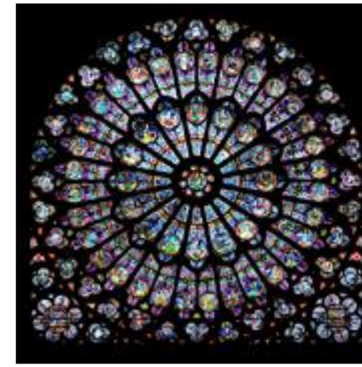
Richard P. Feynman

Talk given to the American Physical Society, 1959





The Very Beginnings…



- 500 – 1400 – Stained Glass
- 800 - 1600 – Nanoparticles in pottery
- 1200 - 1700 – Damascus Steel swords

- ~1910 – Particle sizes described in "nanometers"
- 1959 – Feynman's speech:
- *"The principles of physics, as far as I can see, do not speak against the possibility of maneuvering things atom by atom"*

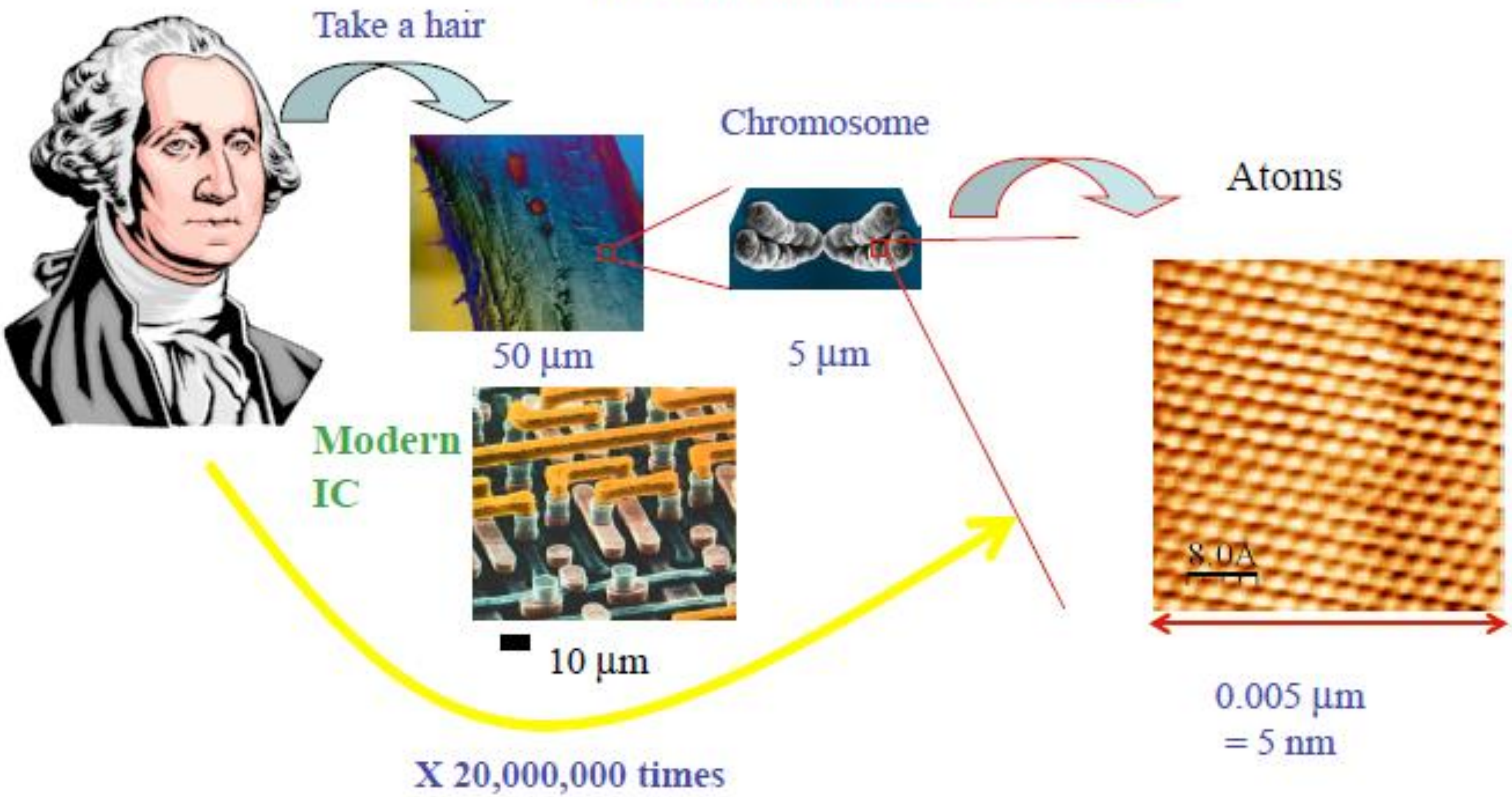
Then…

- 1970 – "Nanotechnology" coined (Taniguchi)
- 1981 – First atoms seen (Binnig and Rohrer, STM)
- 1986 – Engines of Creation, the Coming Age of Nanotechnology by Richard Drexler

"Nanotechnology is the principle of atom manipulation atom by atom, through control of the structure of matter at the molecular level. It entails the ability to build molecular systems with atom-by-atom precision, yielding a variety of nanomachines"

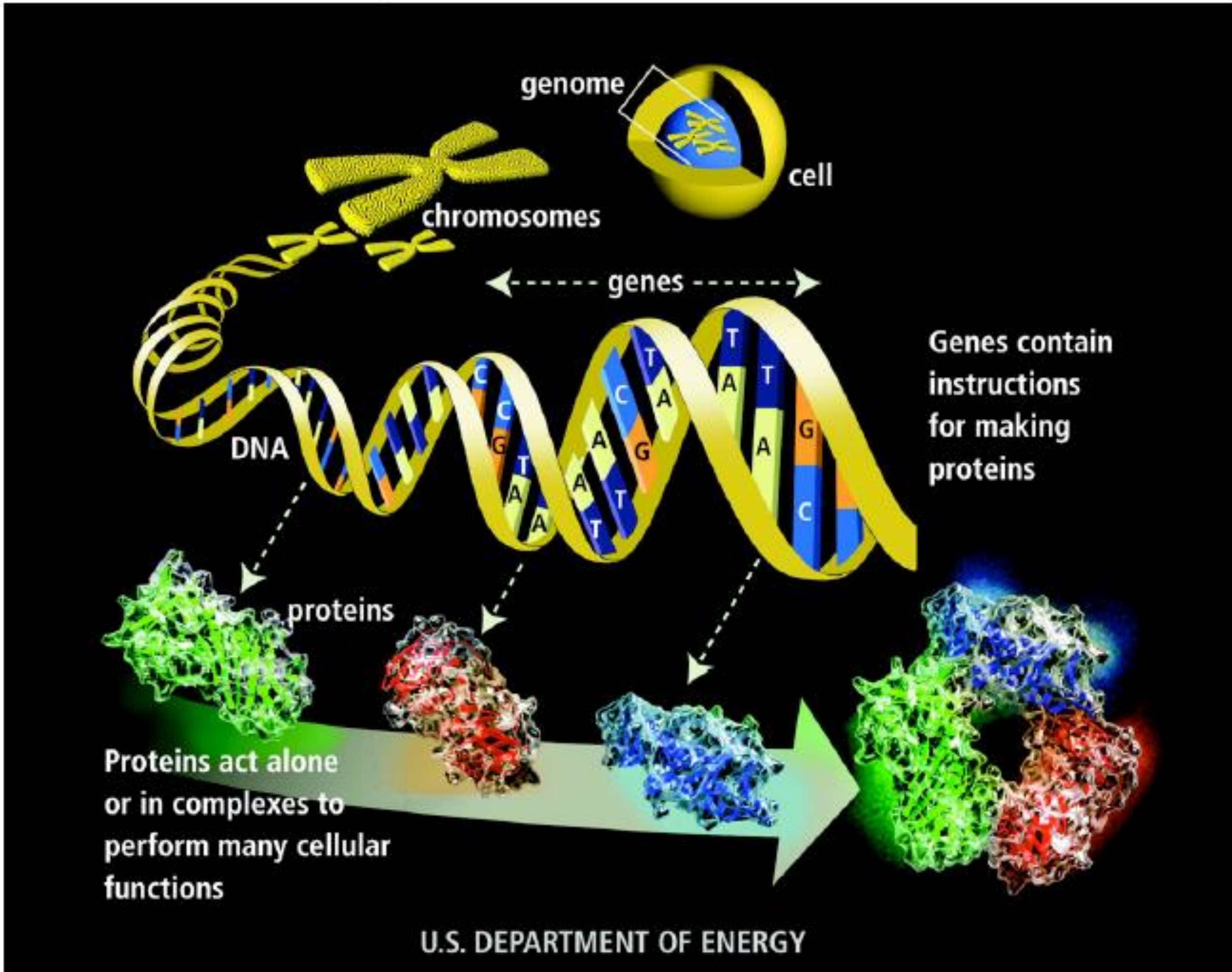
How big is a nanometer?

micro.magnet.fsu.edu/.webloc



How do we see this?: Electron microscope & Scanning-probe microscope

The most famous nanostructure.......DNA



History of Nanomaterials

The Lycurgus Cup- A Roman Nanotechnology
4th Century AD

In reflection In transmission

Au/Ag nanocrystals (70 nm)

Au nanoparticles

- *Damascus blades used in the famous sword of Tipu Sultan*
- *Painting in the Ajanta caves have found existence of carbon nanoparticles.*
- *In Ayurvedic medicine, gold nanoparticles used in medicine.*

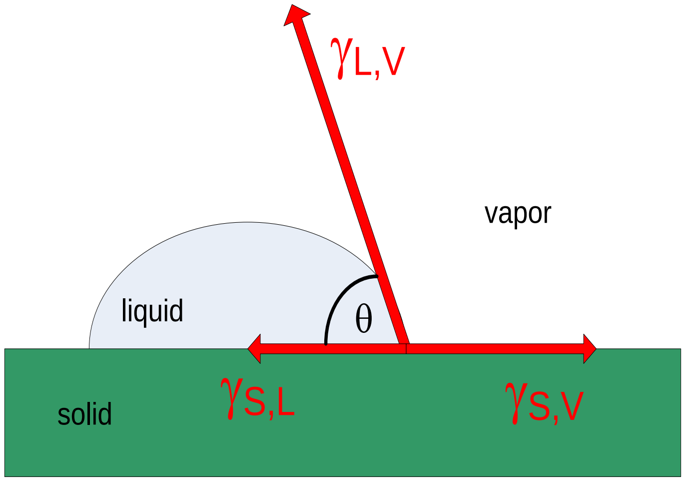
Interesting statement in Vedas
"Anoraniyam Mahatmayam"-----

This statement truly conceptualizes nanoscience.

Universe or the universal consciousness, is just one, which is the smallest of the smallest, and biggest of the biggest.

"Nanotechnology is not really new; it's been there….."

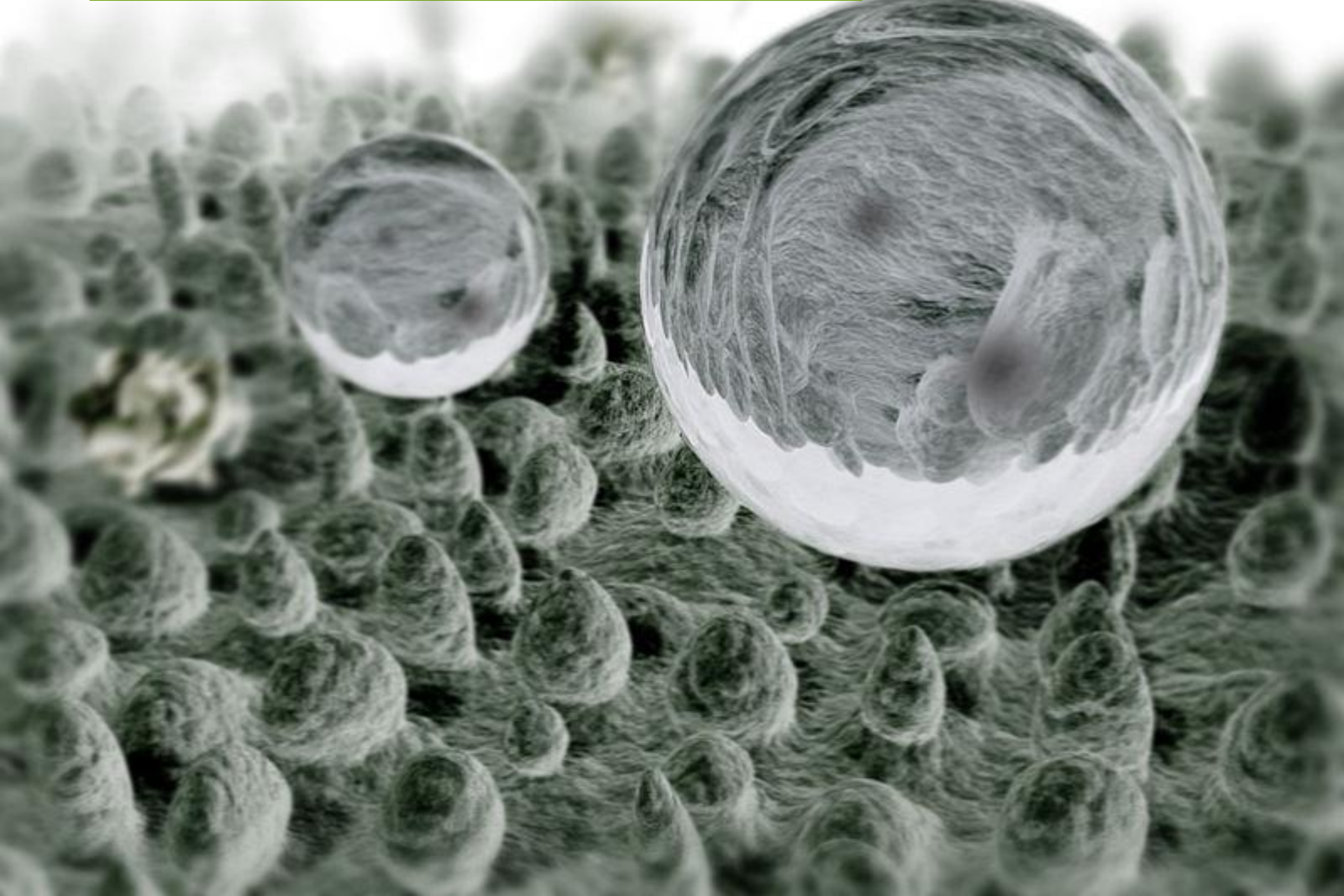
Water on the surface of a lotus leaf

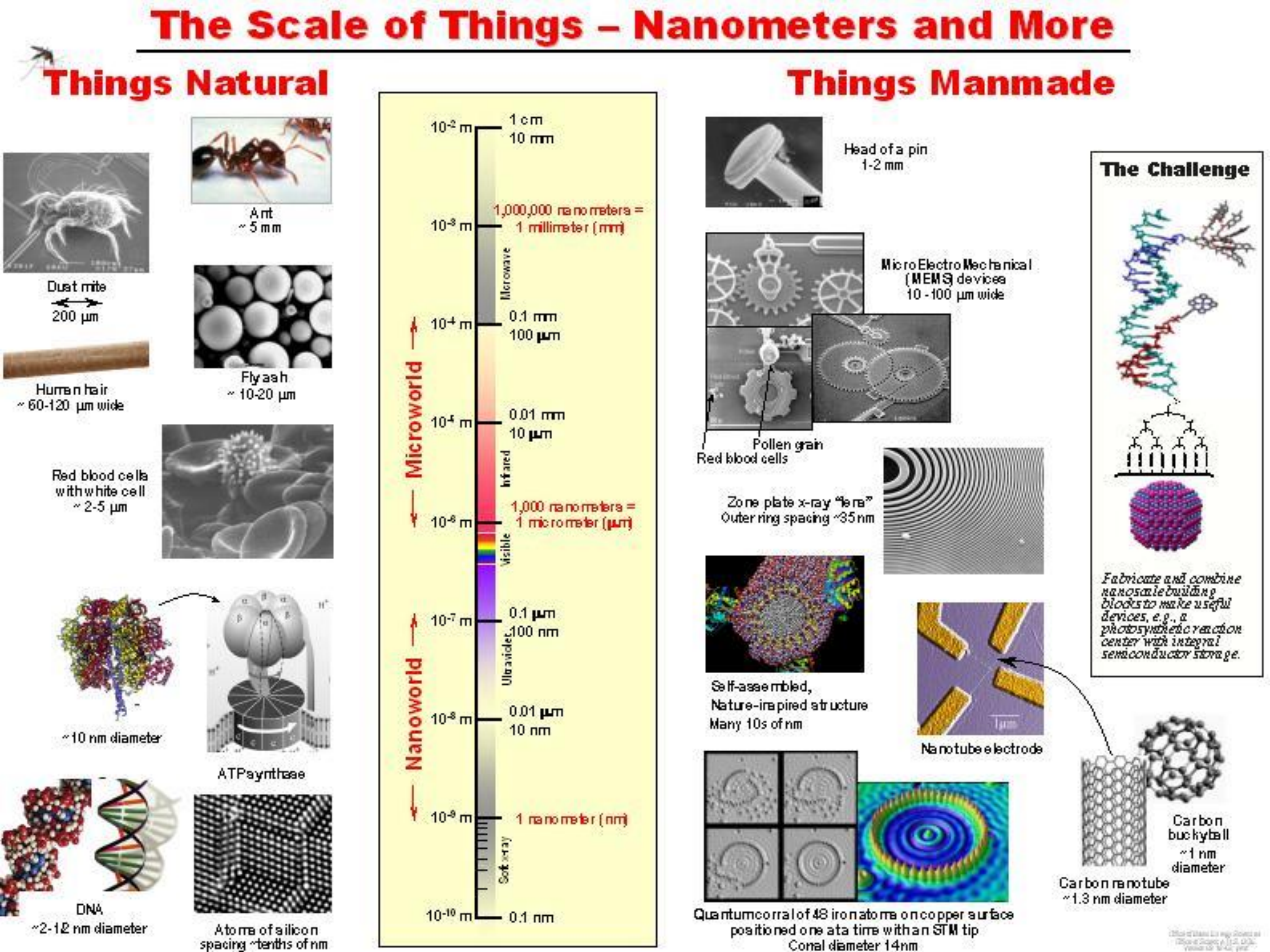


The **lotus effect** in material science is the observed self-cleaning property found with lotus plants. Although lotuses prefer to grow in muddy rivers and lakes, the leaves and flowers remain clean.
Their microscopic structure and surface chemistry mean that the leaves never get wet. Rather, water droplets roll off a leaf's surface like mercury, taking mud, tiny insects, and contaminants with them. This is known as the **lotus effect**.

Some nanotechnologists are developing methods to make paints, roof tiles, fabrics and other surfaces that can stay dry and clean themselves in the same way as the lotus leaf. This can usually be achieved by treatment of the surface with a fluorochemical or silicone treatment

Computer graphics of lotus leaf surface



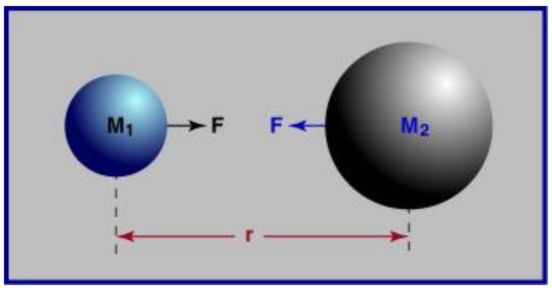

The Scale of Things – Nanometers and More
Things Natural
Things Manmade
Dust mite
200 µm
Ant
~ 5 mm
Fly ash
~ 10-20 µm
Human hair
~ 60-120 µm wide
Red blood cells
with white cell
~ 2-5 µm
~10 nm diameter
ATP synthase
DNA
~2-1/2 nm diameter
Atoms of silicon
spacing ~tenths of nm
10⁻² m
1 cm
10 mm
10⁻³ m
1,000,000 nanometers =
1 millimeter (mm)
Microwave
10⁻⁴ m
0.1 mm
100 µm
Microworld
10⁻⁵ m
0.01 mm
10 µm
Infrared
10⁻⁶ m
1,000 nanometers =
1 micrometer (µm)
Visible
10⁻⁷ m
0.1 µm
100 nm
Ultraviolet
Nanoworld
10⁻⁸ m
0.01 µm
10 nm
10⁻⁹ m
1 nanometer (nm)
Soft x-ray
10⁻¹⁰ m
0.1 nm
Head of a pin
1-2 mm
MicroElectroMechanical
(MEMS) devices
10 -100 µm wide
Pollen grain
Red blood cells
Zone plate x-ray "lens"
Outer ring spacing ~35 nm
Self-assembled,
Nature-inspired structure
Many 10s of nm
Nanotube electrode
Carbon nanotube
~1.3 nm diameter
Carbon
buckyball
~1 nm
diameter
Quantum corral of 48 iron atoms on copper surface
positioned one at a time with an STM tip
Corral diameter 14nm
The Challenge
Fabricate and combine
nanoscale building
blocks to make useful
devices, e.g., a
photosynthetic reaction
center with integral
semiconductor storage.

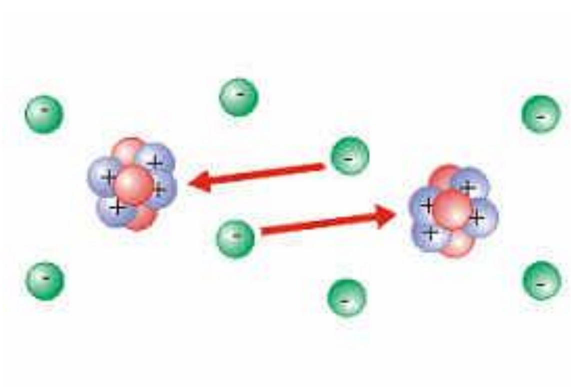
Scale Changes Everything

- Four important ways in which nanoscale materials may differ from macroscale materials
  - Gravitational forces become negligible and electromagnetic forces dominate
  - Quantum mechanics is the model used to describe motion and energy instead of the classical mechanics model
  - Greater surface area to volume ratios
  - Random molecular motion becomes more important

Dominance of Electromagnetic Forces

- **Because the mass of nanoscale objects is so small, gravity becomes negligible**





- **Gravitational force is a function of mass and distance and is weak between (low-mass) nanosized particles**
- **Electromagnetic force being a function of charge and distance - is not affected by mass, so it can be very strong even when we have nanosized particles**
- **The electromagnetic force between two protons is 10^{36} times stronger than the gravitational force!**

Nanoscience is where atomic physics converges with the physics and chemistry of complex systems.

Quantum Mechanics

Statistical Mechanics

Quantum Mechanics dominates the world of atoms, but typical nanosystems may contain from hundreds to tens of thousands atoms.

Emergent behavior

How much a system is quantum mechanical?

The properties of materials can be different at the Nanoscale for two main reasons:

First, Nanomaterials have a relatively **larger surface area** when compared to the same mass of material produced in a larger form.

Nano particles can make materials more **chemically reactive** and affect their strength or electrical properties.

Second, quantum effects can begin to dominate the behaviour of matter at the Nanoscale

Nanoscale materials are divided into three category,

1. **Zero dimension** – length , breadth and heights are confined at single point. (for example, Nano dots)
2. One dimension – It has only one parameter either length (or) breadth (or) height (example:very thin surface coatings)
3. **Two dimensions-** it has only length and breadth (for example, nanowires and nanotubes)
4. **Three dimensions** -it has all parameter of length, breadth and height. (for example, Nano Particles).

Color

- In a classical sense, color is caused by the partial absorption of light by electrons in matter, resulting in the visibility of the complementary part of the light
- On a smooth metal surface, light is totally reflected by the high density of electrons ⟹ no color, just a mirror-like appearance.
- Small particles absorb, leading to some color. This is a size dependent property.
  Example: Gold, which readily forms nanoparticles but not easily oxidized, exhibits different colors depending on particle size.
    - Gold colloids have been used since early days of glass making to color glasses. Ruby-glass contains finely dispersed gold-colloids.
    - Silver and copper also give attractive colors

What is a color of gold?

Size-dependent color of gold

Absorption peak broadens and shifts to longer wavelengths.
Reflection, leading to scattering, is weak at small sizes and increases when > 50 nm.

100 nm gold particles
$\lambda abs = 575$ nm
Color = purple-pink

20 nm gold particles
$\lambda abs = 521$ nm
Color = red

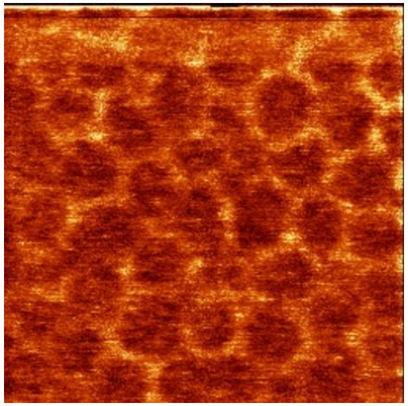
1 nm gold particles
$\lambda abs = 420$ nm
Color = brown-yellow

Optical Properties Example: Gold

- Bulk gold appears yellow in color
- Nanosized gold appears red in color
  - The particles are so small that electrons are not free to move about as in bulk gold
  - Because this movement is restricted, the particles react differently with light

Optical properties are connected with electronic structure, a change in zone structure leads to a change in absorption and luminescence spectra.

"Bulk" gold looks yellow



12 nanometer gold particles look red

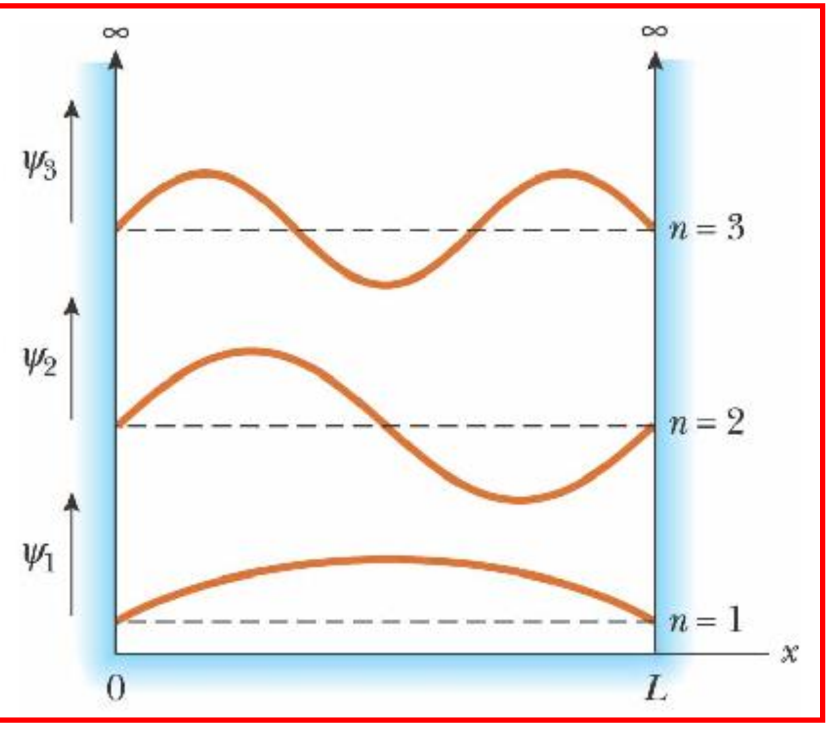
Particle in the Infinite Potential Well

$$\psi_n = \sqrt{\frac{2}{L}}\sin\left(\frac{\pi x}{L}n\right)$$

n defines states, we take $n > 0$

Energy for the n^{th} state is

$$E_n = \frac{\pi^2\hbar^2}{2mL^2}n^2$$



Why are Cherries Red and Blueberries blue ?

The Colour of Fruit

Let's put in numbers. $h = 6.6 \times 10^{-34}$ J-s. The electron mass, $m_e = 9.1 \times 10^{-31}$ kg. For the length of the box, let's take L to be that of a medium-sized molecule, that is, $L = 0.8 \times 10^{-9}$ m (0.8 nanometers, 0.8 nm). Then,

$$\Delta E = \frac{3(6.6 \times 10^{-34})^2}{8(9.1 \times 10^{-31})(0.8 \times 10^{-9})^2} = 2.8 \times 10^{-19} \text{J}.$$

This energy corresponds to

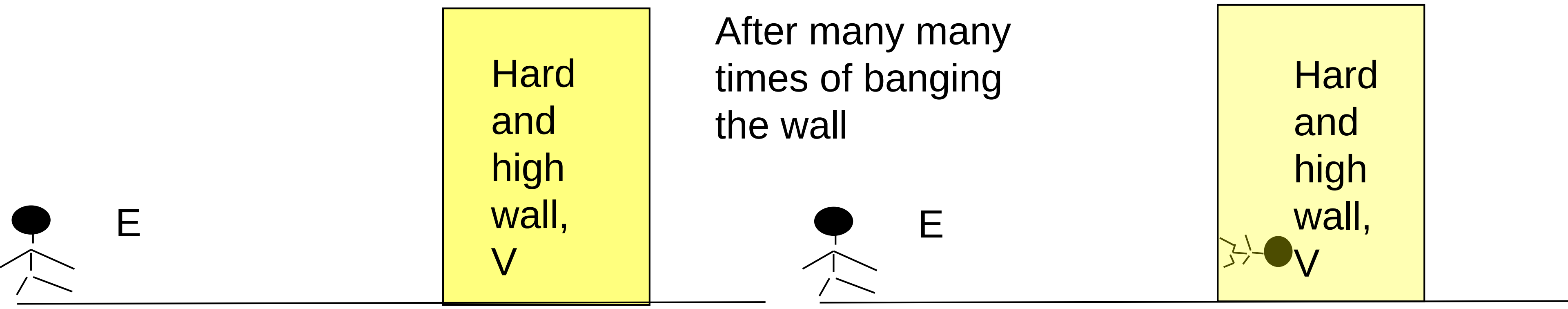
$\lambda = 7.06 \times 10^{-7}$ m = 706 nm ⟹ **Deep Red Colour**

If L=0.7 nm, λ=540 nm → **Green Colour**

If L=0.6 nm, λ=397 nm → **Blue Colour**

Quantum tunneling effect

The quantum tunnelling effect allows a confined particle within a finite potential well to penetrate through the classically impenetrable potential wall

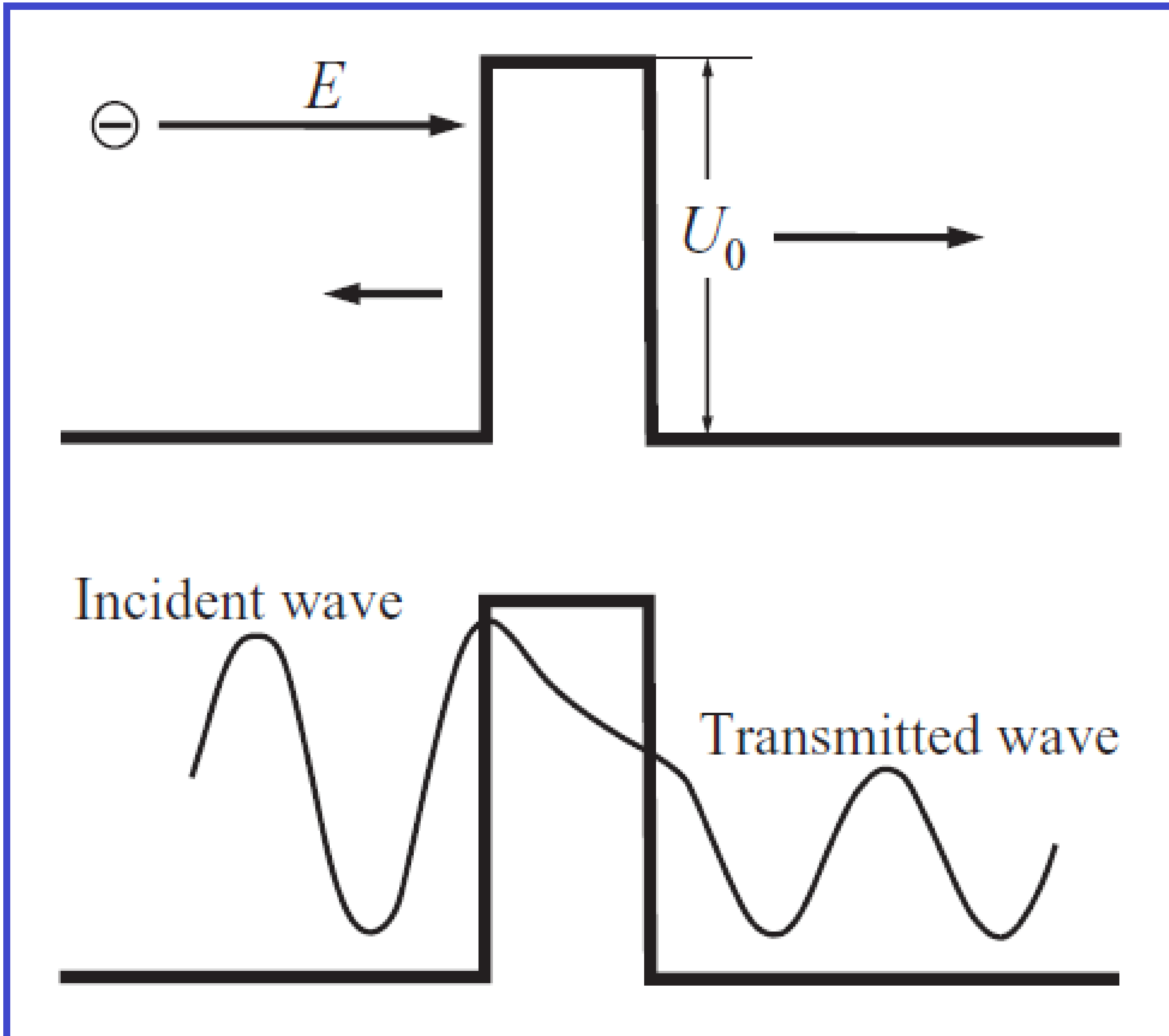


Why tunneling phenomena can happen

- It's due to the continuity requirement of the wave function at the boundaries when solving the T.I.S.E
- The wave function cannot just "die off" suddenly at the boundaries of a finite potential well
- The wave function can only diminishes in an exponential manner which then allow the wave function to extent slightly beyond the boundaries

$$\psi(x) = \begin{cases} A_+ \exp(Cx) \neq 0, & x \leq 0 \\ A_- \exp(-Cx) \neq 0, & x \geq L \end{cases}$$

- The quantum tunneling effect is a manifestation of the wave nature of particle, which is in turns governed by the T.I.S.E.
- In classical physics, particles are just particles, hence never display such tunneling effect


E
U_0
Incident wave
Transmitted wave

Real example of tunneling phenomena: Atomic force microscope

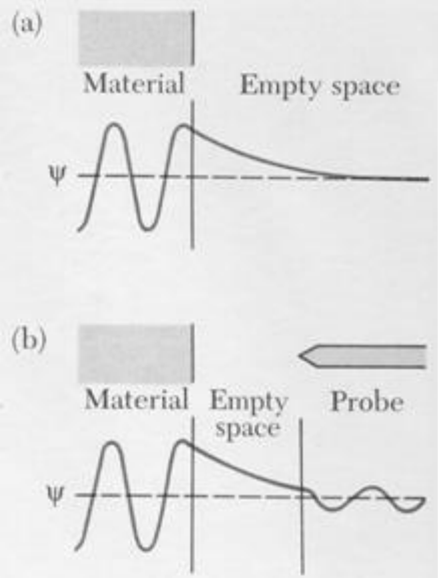


Figure 3 (a) The wavefunction of an electron in the surface of the material to be studied. The wavefunction extends beyond the surface into the empty region. (b) The sharp tip of a conducting probe is brought close to the surface. The wavefunction of a surface electron penetrates into the tip, so that the electron can "tunnel" from surface to tip.

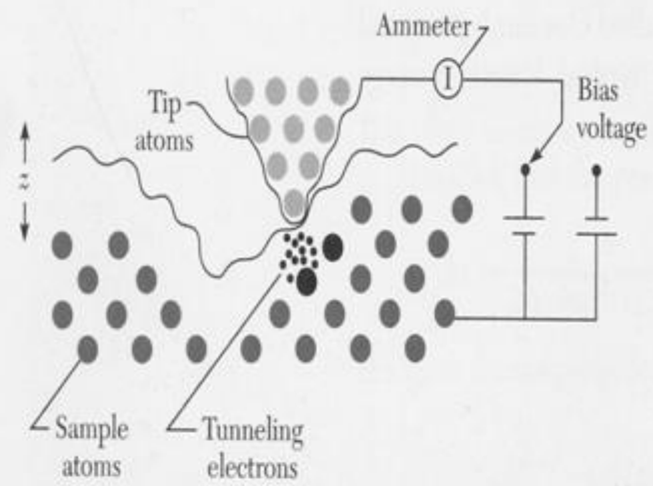


FIGURE A Highly schematic diagram of the scanning tunneling microscope process. Electrons, represented in the figure as small dots, tunnel across the gap between the atoms of the tip and sample. A feedback system that keeps the tunneling current constant causes the tip to move up and down tracing out the contours of the sample atoms.

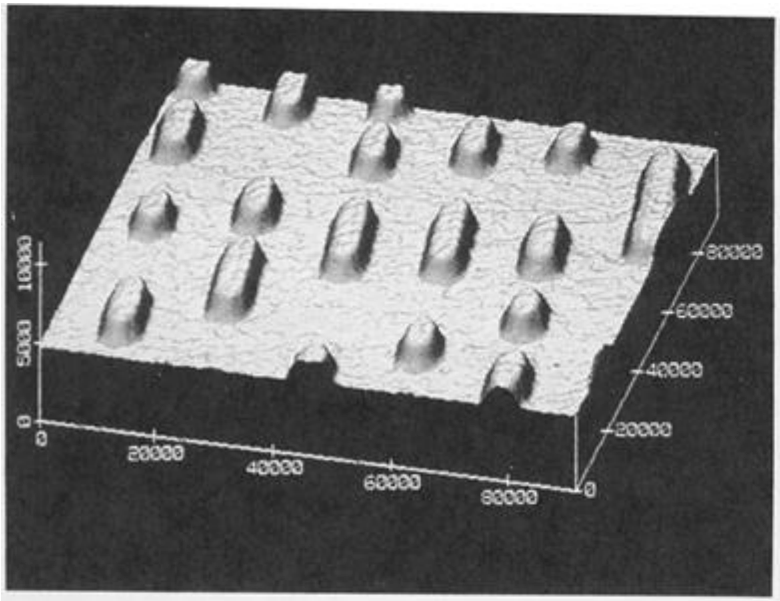
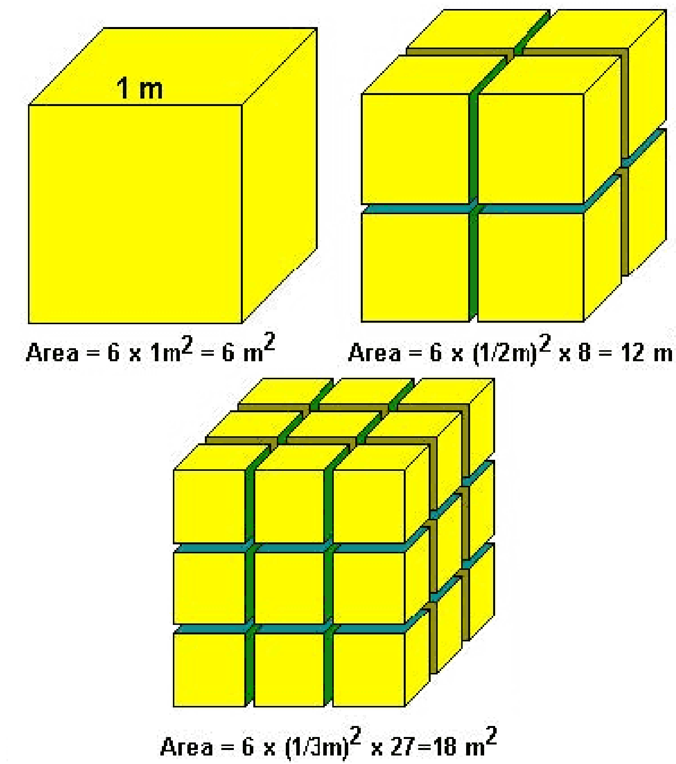
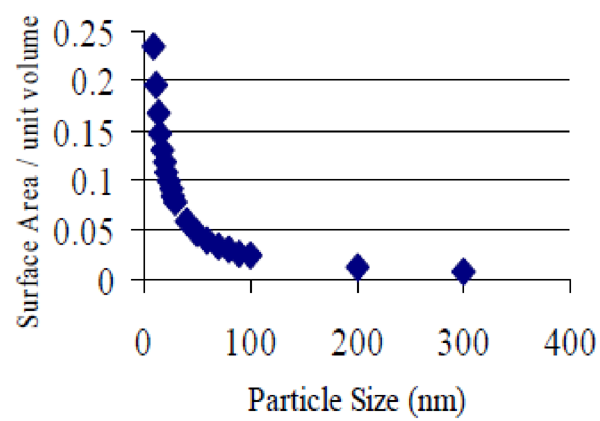


FIGURE D An atomic force microscope scan of a stamper used to mold compact disks. The numbers given are in nm. The bumps on this metallic mold stamp out 60 nm-deep holes in tracks that are 1.6 μm apart in the optical disks. *Photo courtesy of Digital Instruments.*

Surface Area to Volume Ratio Increases

- As surface area to volume ratio increases
  - A greater amount of a substance comes in contact with surrounding material
  - This results in better catalysts, since a greater proportion of the material is exposed for potential reaction





What are Quantum Dots?

- Quantum dots are semi-conductors that are on the nanometer scale.
- Obey quantum mechanical principle of quantum confinement.
- Exhibit energy band gap that determines required wavelength of radiation absorption and emission spectra.
- Requisite absorption and resultant emission wavelengths dependent on dot size.

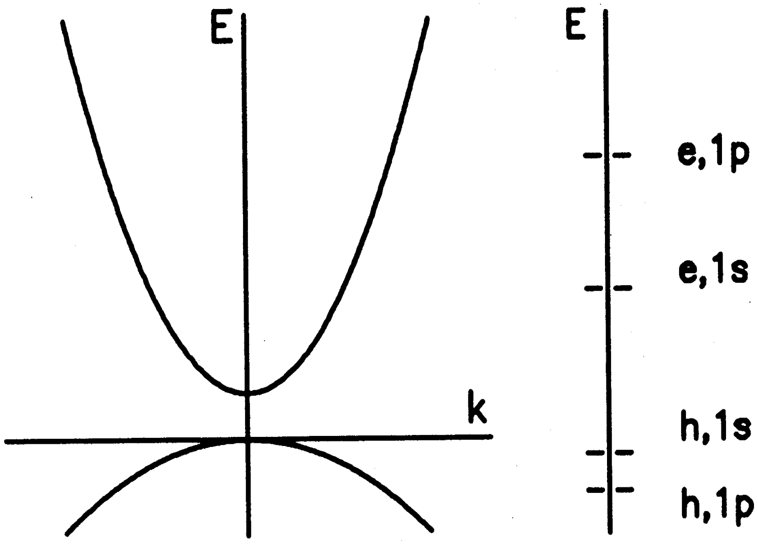
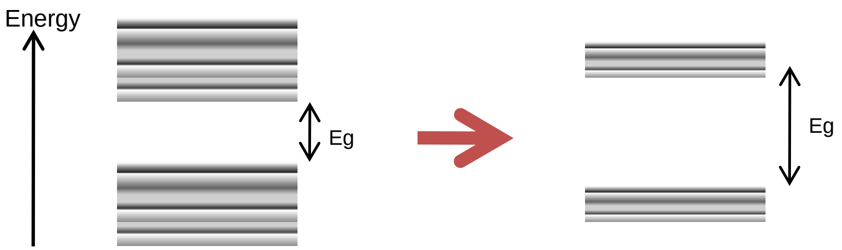


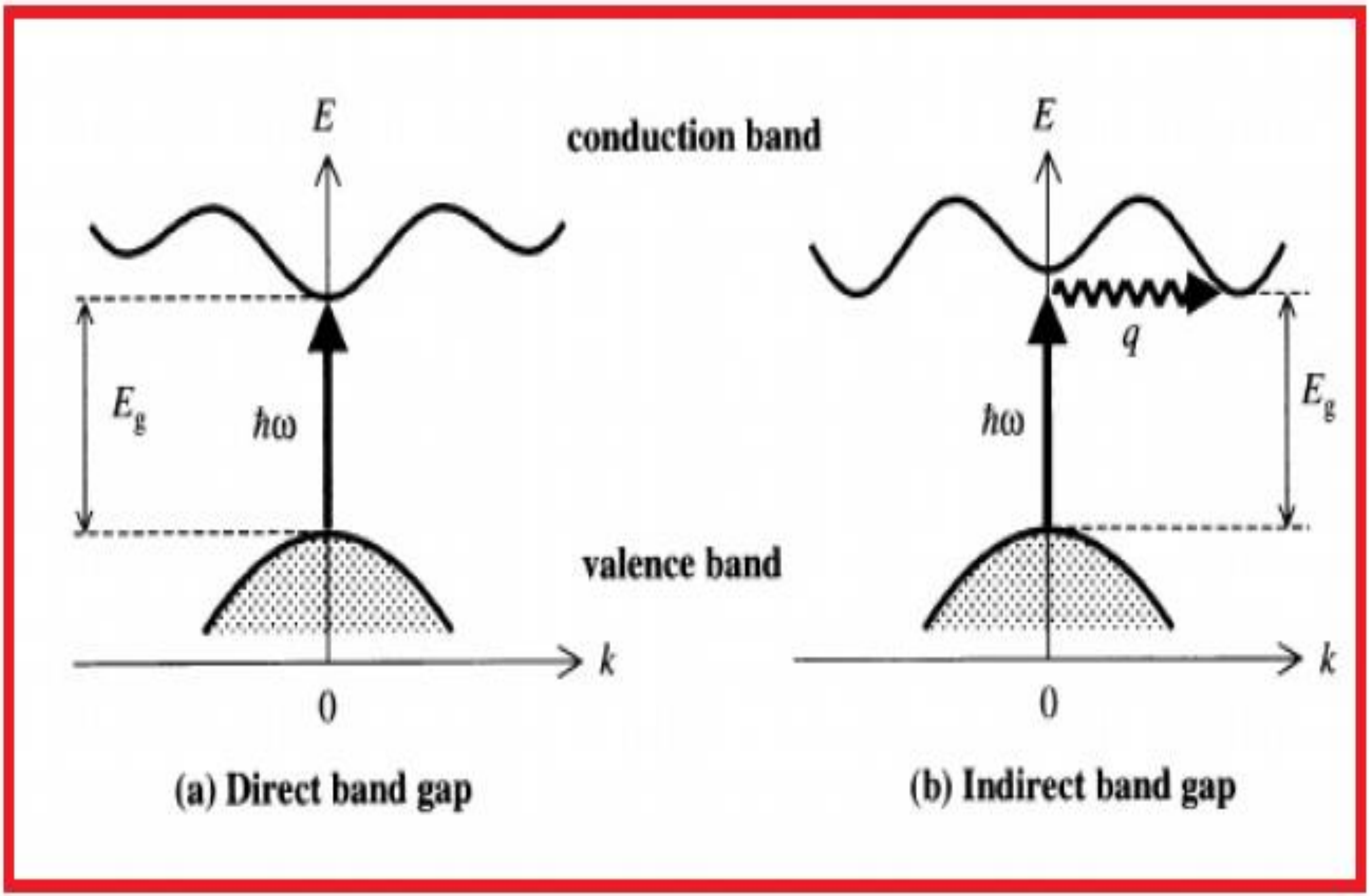
Fig. 1. Schematic plot of the single particle energy band gap. The upper parabolic band is the conduction band, the lower the valence.

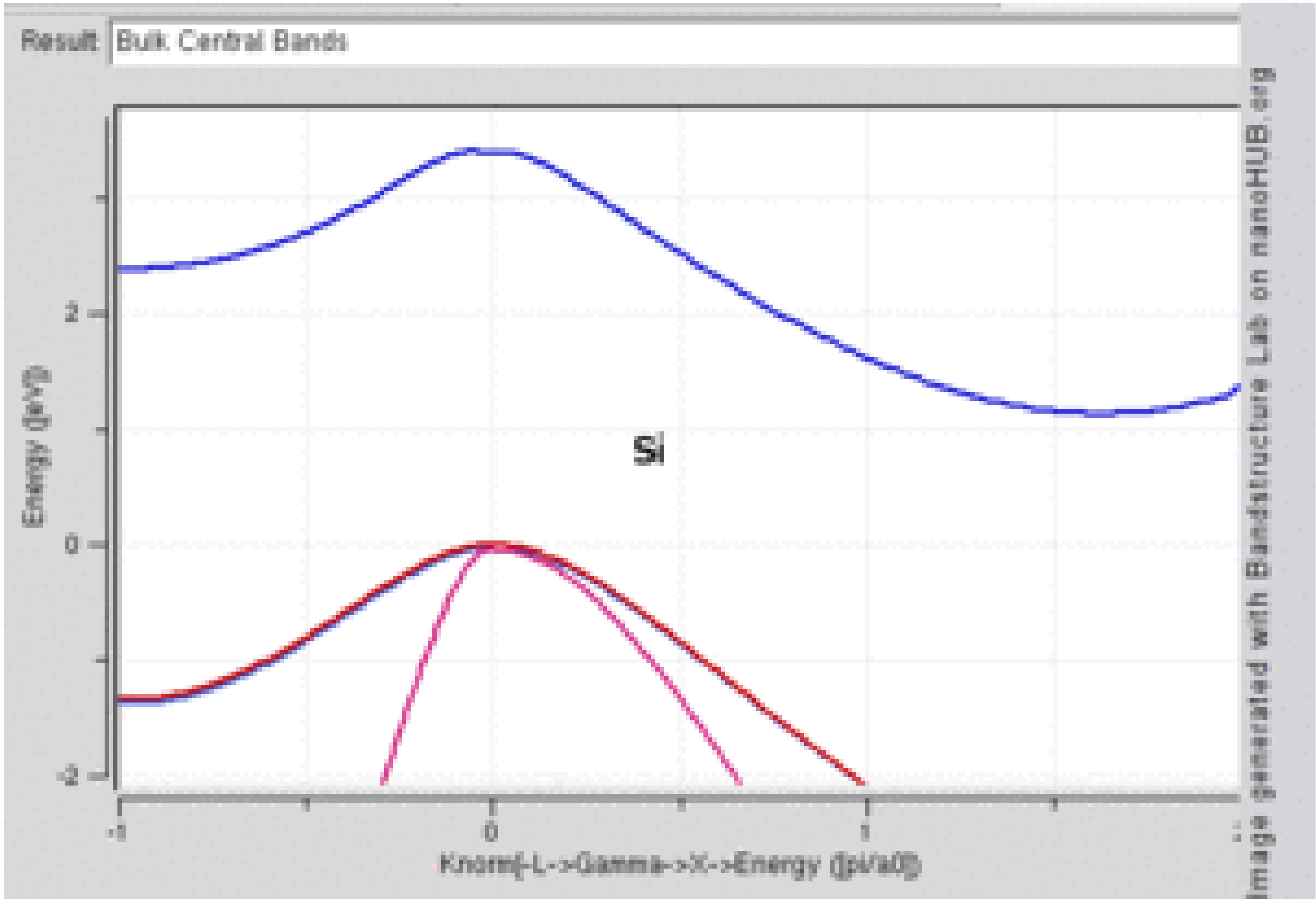
Quantum Confinement

- **The reduction in the number of atoms in a material results in the confinement of normally delocalized energy states.**
- **Electron-hole pairs become spatially confined when the diameter of a particle approaches the de Broglie wavelength of electrons in the conduction band.**
- **As a result the energy difference between energy bands is increased with decreasing particle size.**



Direct vs Indirect Band Gap



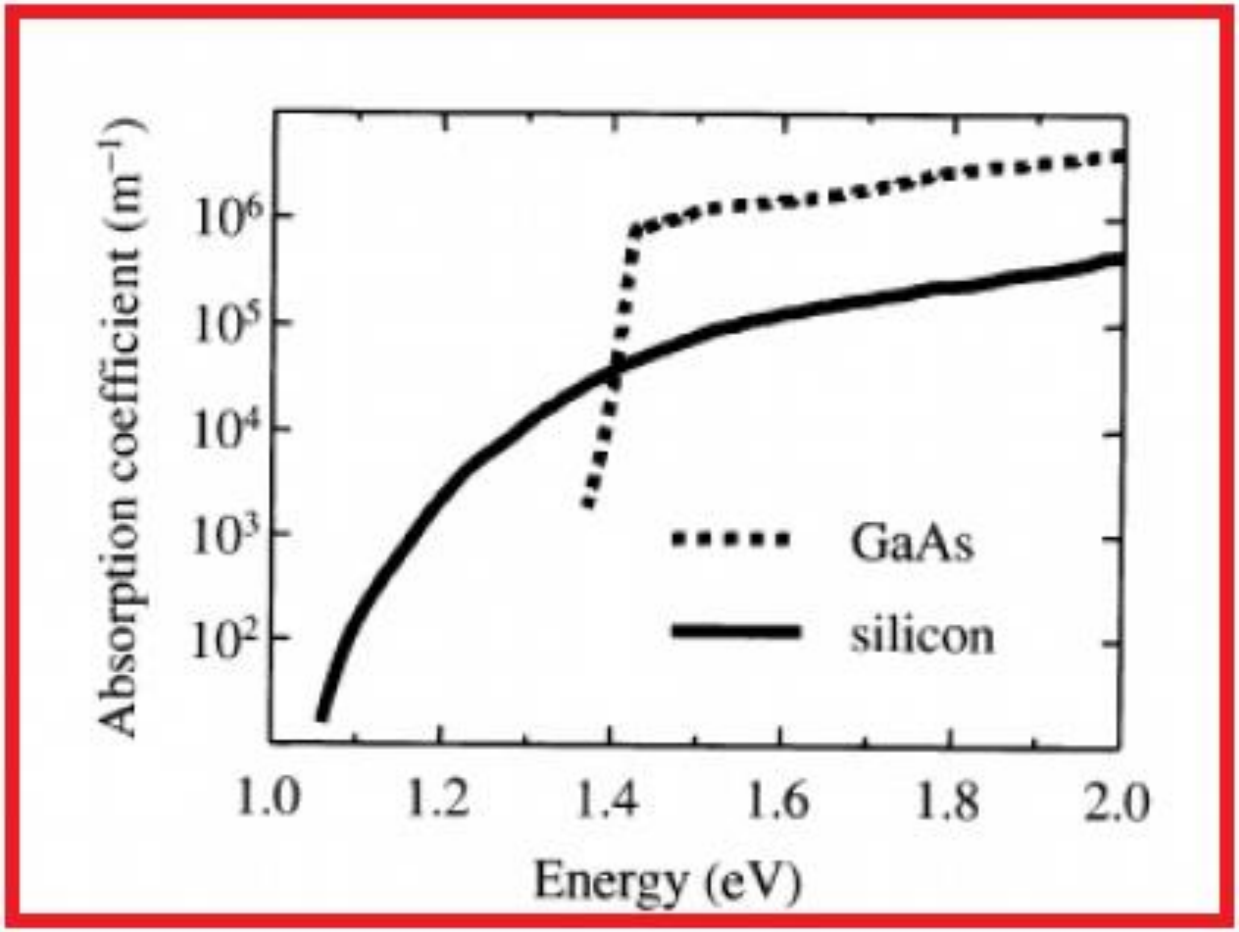


Si (1.17 eV, 1.14 eV) and Ge (0.74, 0.67 eV) are indirect band gap semiconductor with minima at X and L point

GaAs (1.52 eV, 1.43 eV) and InAs (0.43 eV, 0.36 eV) are direct bandgap semiconductors

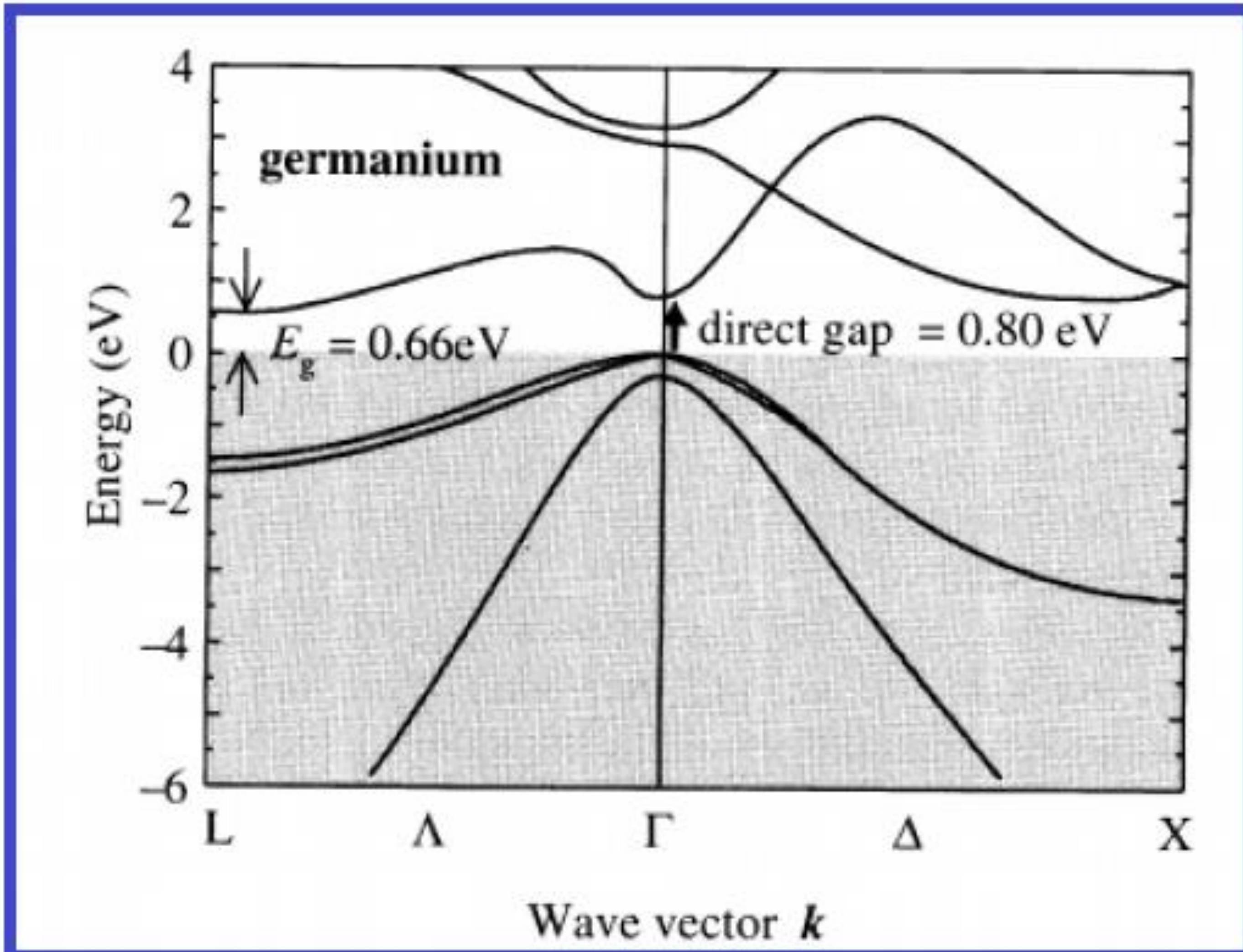
It might seem strange then that Si is the most widely used semiconductor solar cell. The main reasons behind this are the following:

1. Its band gap is the perfect size to capture the photon distribution that comprise the solar spectrum.
2. It is abundant in earth (i. e. its availability in large quantities).
3. It is environmentally benign.
4. Most importantly, there is the availability of very good technological assistance for Si-processing (i.e. its ease of process to produce electronic grade material with high purity).
5. It can accept both p and n-type dopants easily.
6. Finally, it is quite easy in producing large wafers in different orientations.



Comparison of the absorption coefficient of GaAs and silicon near their band edges. GaAs has a direct band gap at 1.42 eV, while silicon has an indirect gap at 1.12 eV. Note that the vertical axis is logarithmic.

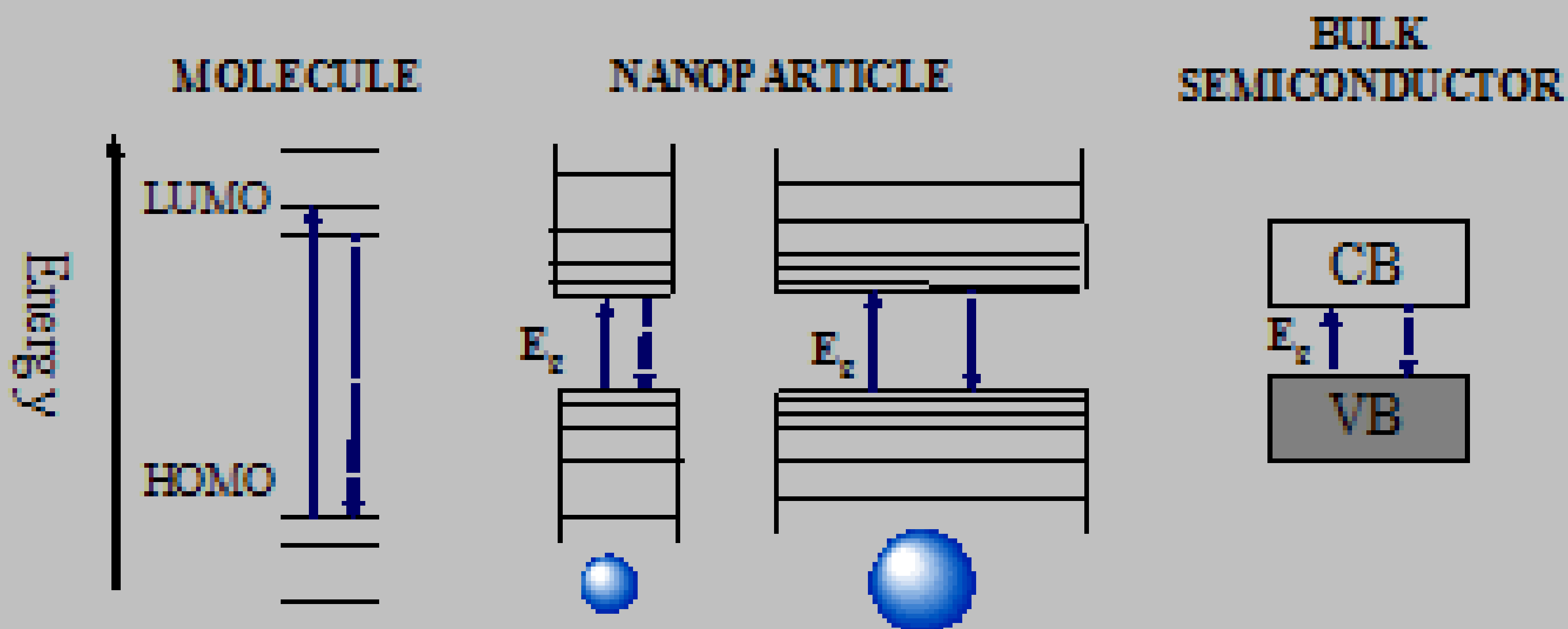
$$\alpha^{\text{indirect}}(\hbar\omega) \propto (\hbar\omega - E_{\text{g}} \mp \hbar\Omega)^2$$



$\alpha^{\text{indirect}}(\hbar\omega) \propto (\hbar\omega - E_g \mp \hbar\Omega)^2$

$\alpha^2 \propto (\hbar\omega - E_g^{dir})$, where $E_g^{dir} = 0.80$ eV

Energy Level Diagram: Quantum Size Effects



$$E = E_g + \frac{\hbar^2 \pi^2}{2R^2}\left(1/m_e + 1/m_h\right) - \frac{1.8e^2}{\epsilon R}$$

Variation of band gap with crystallite size

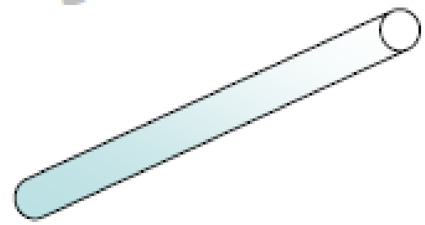
The first term is the energy expression for quantum localization (justified from uncertainty principle) and scales as D^{-2} for electron as well as hole. The second term is the Coulomb attractive interaction, which increases as D^{-1}. Third term is the salvation energy loss. In large gap polycrystalline materials having crystallites diameter 30–60 Å, it is seen that the third term is very negligible compared to the first and second one. Hence, with reasonably good approximation, the change in band gap energy ΔE_g is written as

$$\Delta E_g = \frac{\hbar^2 \pi^2}{2\mu D^2} - \frac{1.8e^2}{\tilde{\varepsilon}_2 D}$$

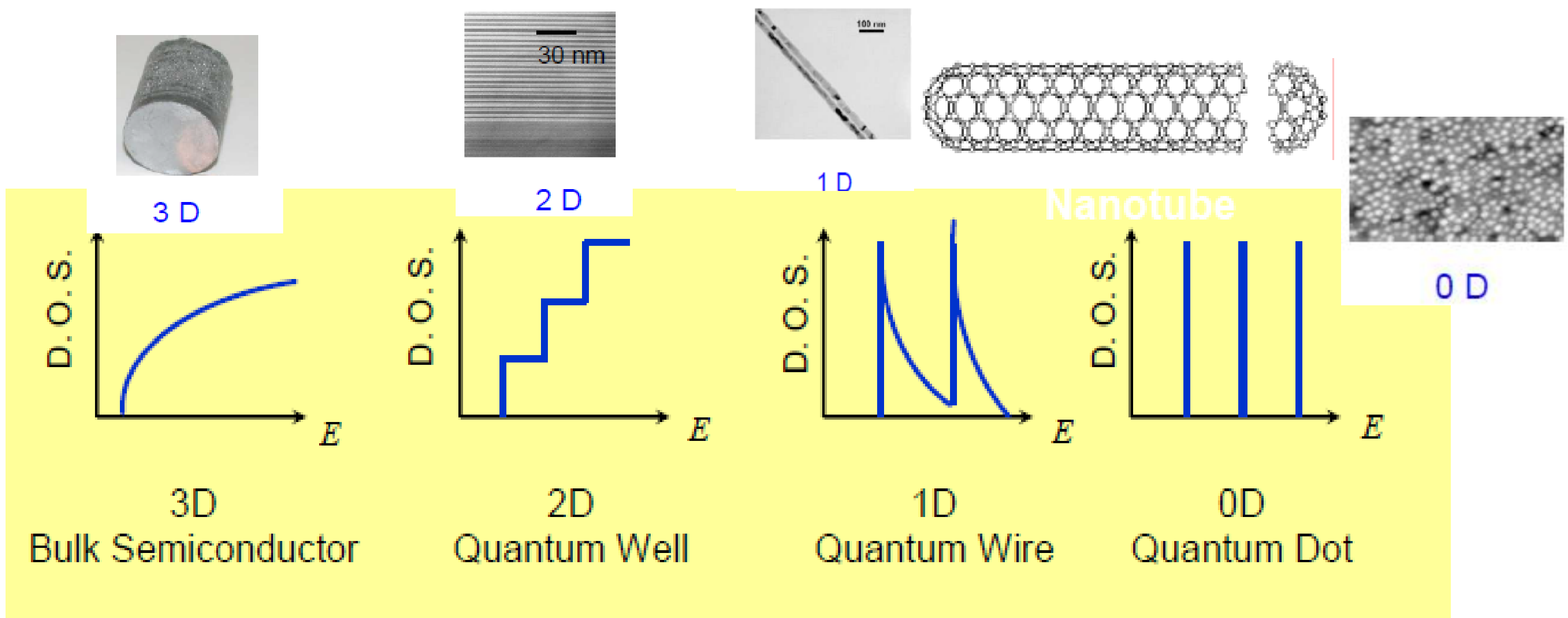
It is to be noted that the above relation is strictly valid only for 3d direct gap materials.

This renders the shift to blue region of bulk band gap for nanocrystalline samples

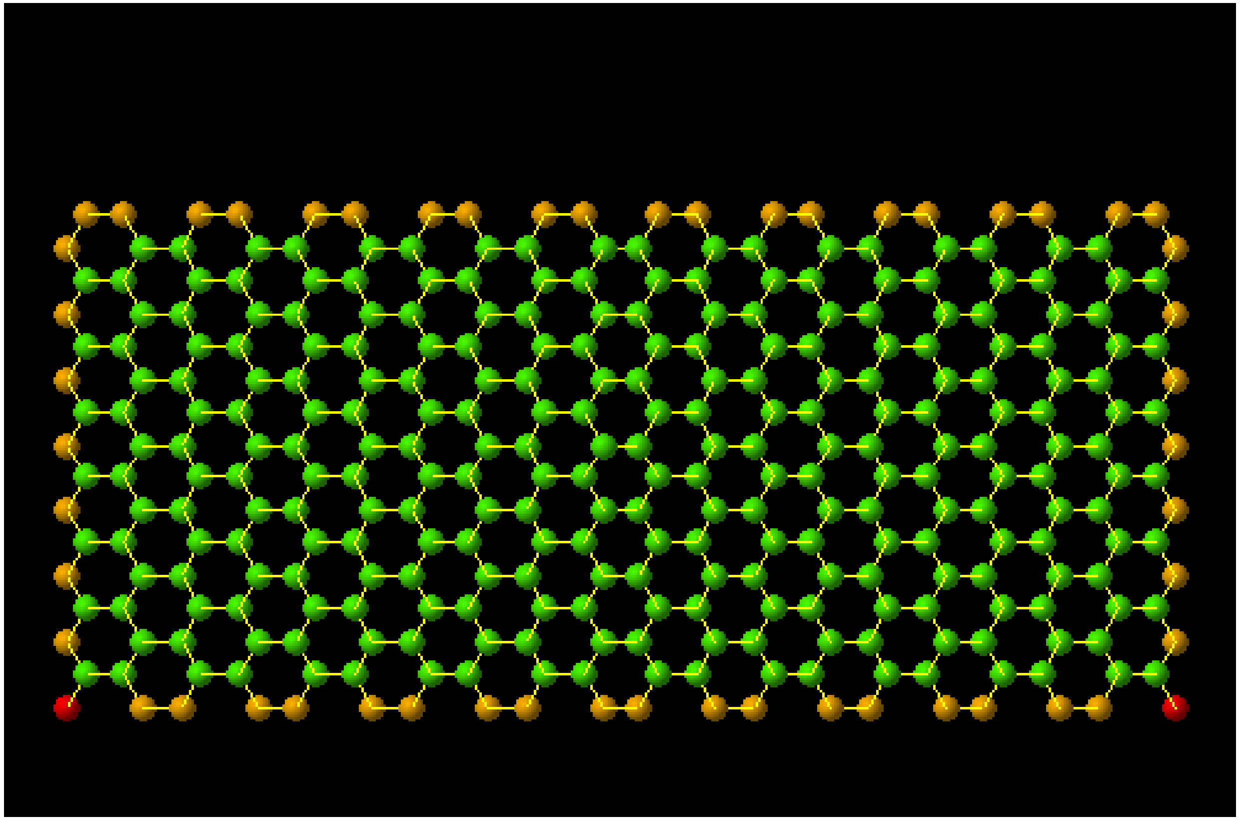
One Dimensional Systems:



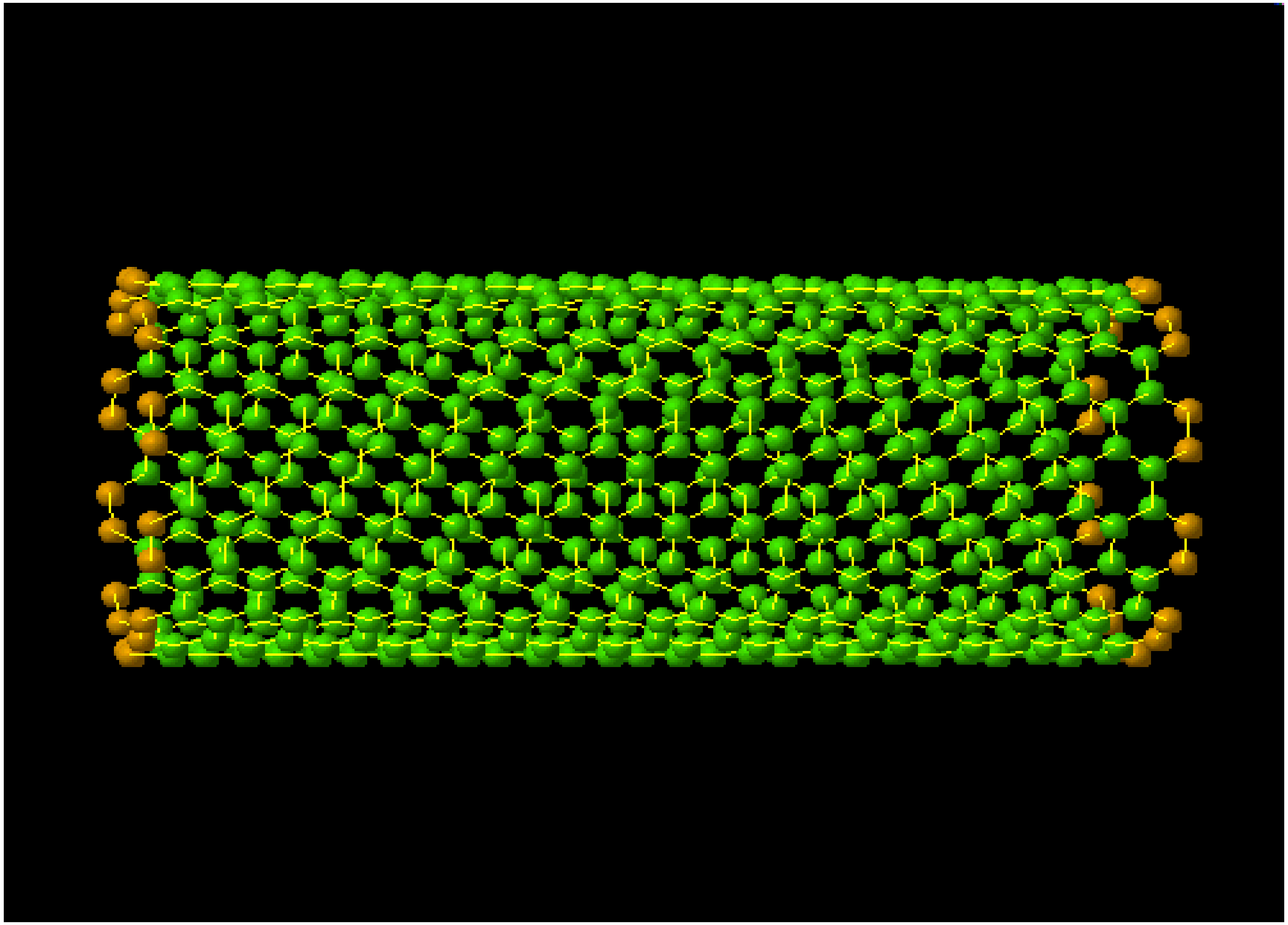
- High aspect ratio
- Enhanced density of states
- Single wall carbon nanotubes SWNT: Chirality and diameter-dependent properties



(10,10) Nanotube

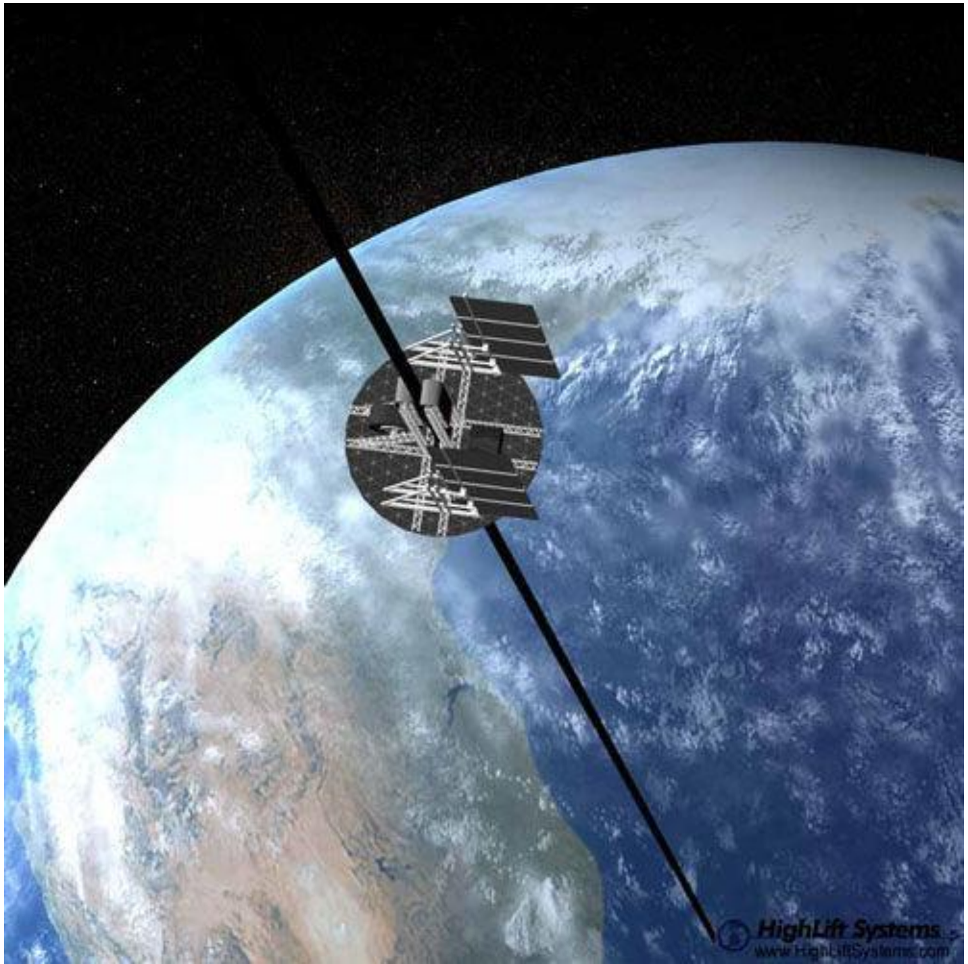


Rotation



Nanotubes’ excellent strength to weight ratio

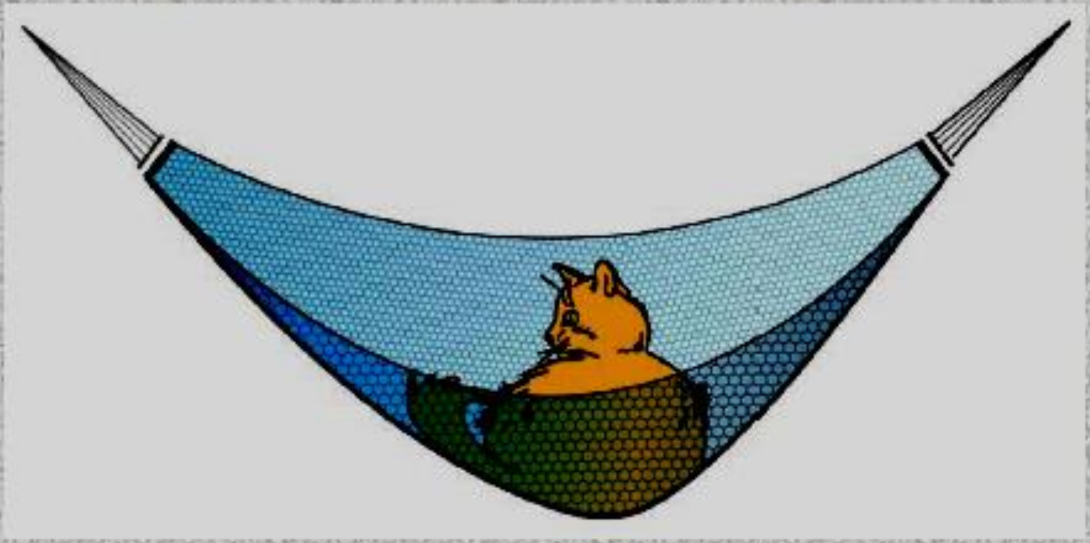
creates the potential to build an elevator to space.



Graphene vs (scaled down) steel film of the same thickness

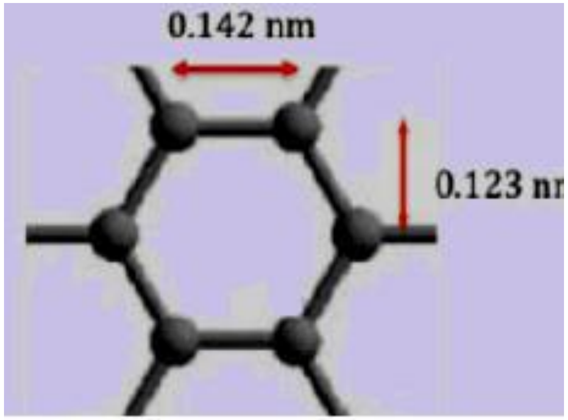
Take-home message 5

=> Graphene is more than 100 times stronger than the strongest steel!



[Can put a 4Kg mass (e.g. a cat) on a 1 m^2 graphene (if one can make it). Cartoon taken from Nobel Prize announcement]

Computation of Young's Modulus of CNT



Name of Elements	Li	Be	B	C(Dia)	C(Graph
Atomic Number	3	4	5	6	6
Y(GPa)	11.5	289	440	1140	8.3
Melting Point (^{0}C)	181	1277	2030	3550	3550
Density (10^3 Kg/m^3)	0.531	1.85	2.34	2.25	2.25

Table 1: Comparison of Various physical parameters with diamond and graphite

Computation of Young's Modulus of CNT

$$Y = \frac{kl_0}{A} \quad k = -\left[\frac{d^2U}{dr^2}\right]_{r=R_0} \quad U_1(r) = U_0\left[\left(\frac{R_0}{r}\right)^{12} - 2\left(\frac{R_0}{r}\right)^{6}\right]$$

Microscopic Specimen
of length l_0 and area A
Equilibrium distance R_0

Increase of bond lengths $\frac{R_0 dx}{l_0}$

Tension in each chain
Of Atoms

$$\frac{kR_0 dx}{l_0}.$$

Stress developed $\frac{kdx}{l_0 R_0}$

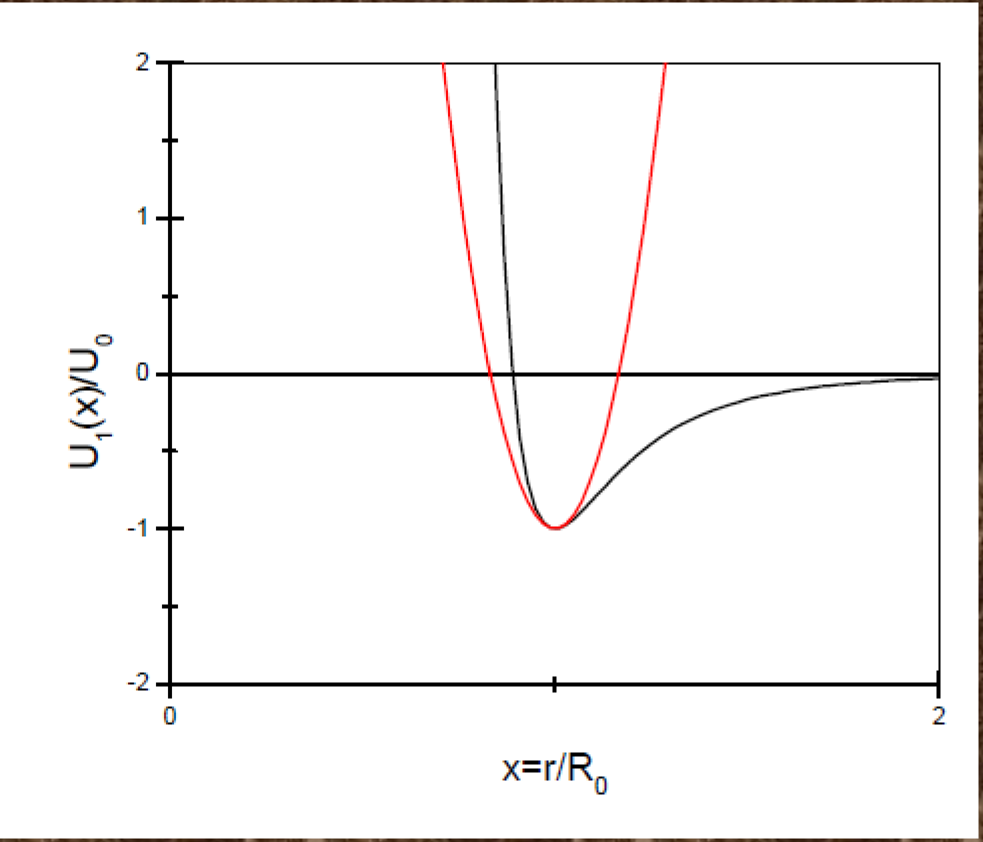
$$Y = \frac{1}{R_0}\left[\frac{d^2U}{dr^2}\right]_{r=r_0}$$

$$F = -\frac{72U_0}{R_0^2}x_0 = -kx_0$$

$$Y = \frac{288U_0}{\pi a d^2}$$

$$Y \propto \frac{U_0}{R_0^3}$$

Computation of Young's Modulus of CNT



	Expt	Morse	U_1	U_2	U_3	U_4
(9,0) SWCNT Y (GPa)	270-950	1000	9533 948(*)	1872	1071	825
(9,0) SWCNT σ_{max} (GPa)	20-130	500	1560.5 158(*)	936	1071	389

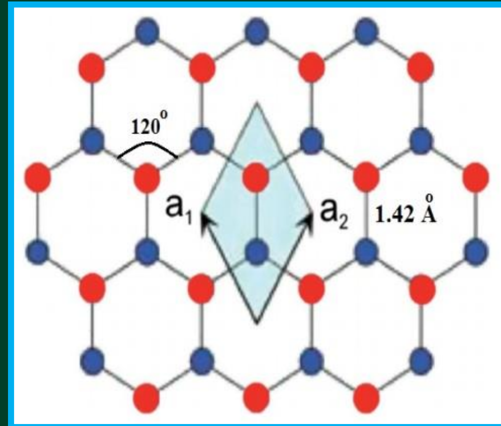
$$Y(T) = \frac{4mnU_0}{\pi a_0(1+\alpha T)d_0^2(1+\alpha T)^2} \approx \frac{4mnU_0}{\pi a_0 d_0^2(1+3\alpha T)}$$

$$Y(T) \approx \frac{Y(0)}{1+3\alpha T}$$

Graphene

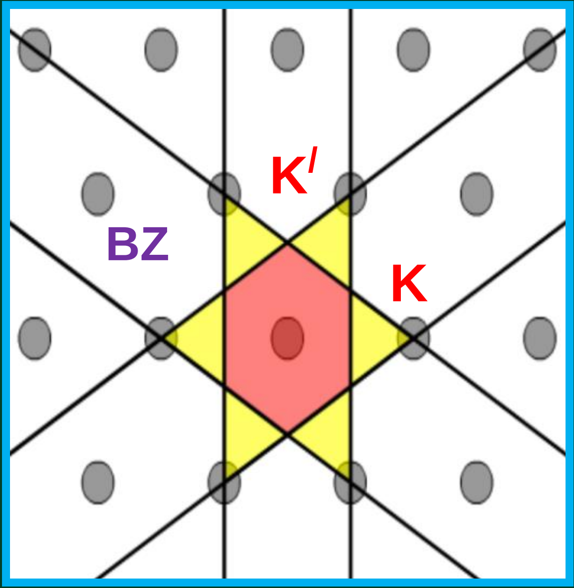
'Carbon has been investigated for more than half a century without exhausting its wonders & challenges.'

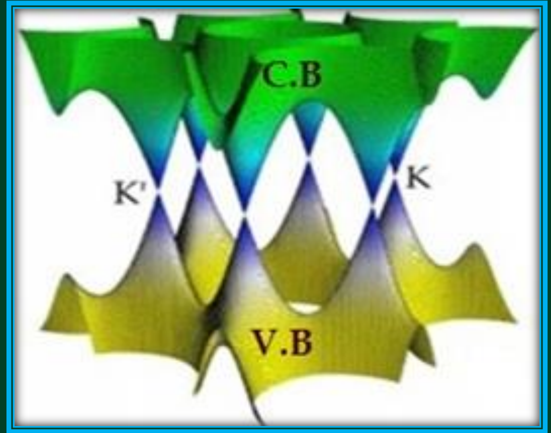
Graphite
Graphene



Geim & Novoselov

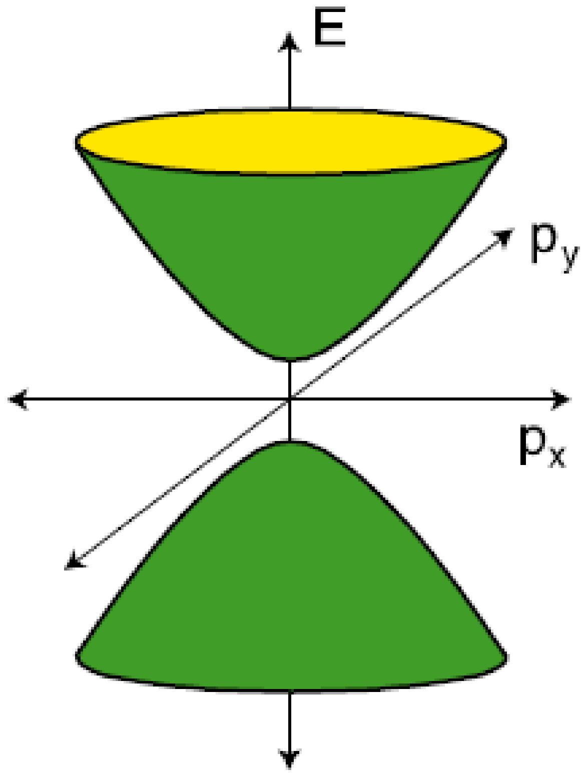
GRAPHENE HAS BEEN CONSIDERED AS A REVOLUTIONARY MATERIAL





Semimetal

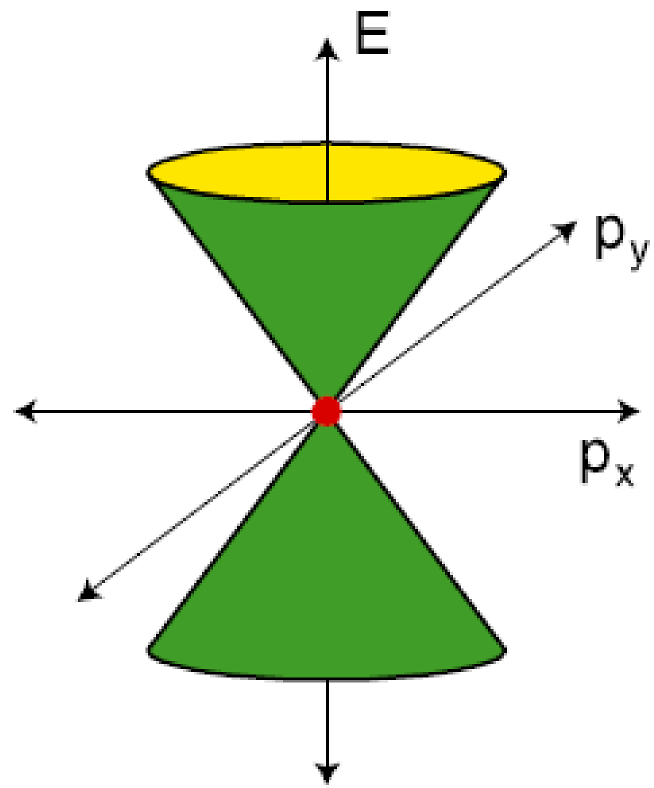
Semiconductor



$$E_c = E_c^0 - \frac{p^2}{2m_c^*}$$

$$E_v = E_v^0 - \frac{p^2}{2m_v^*}$$

Graphene

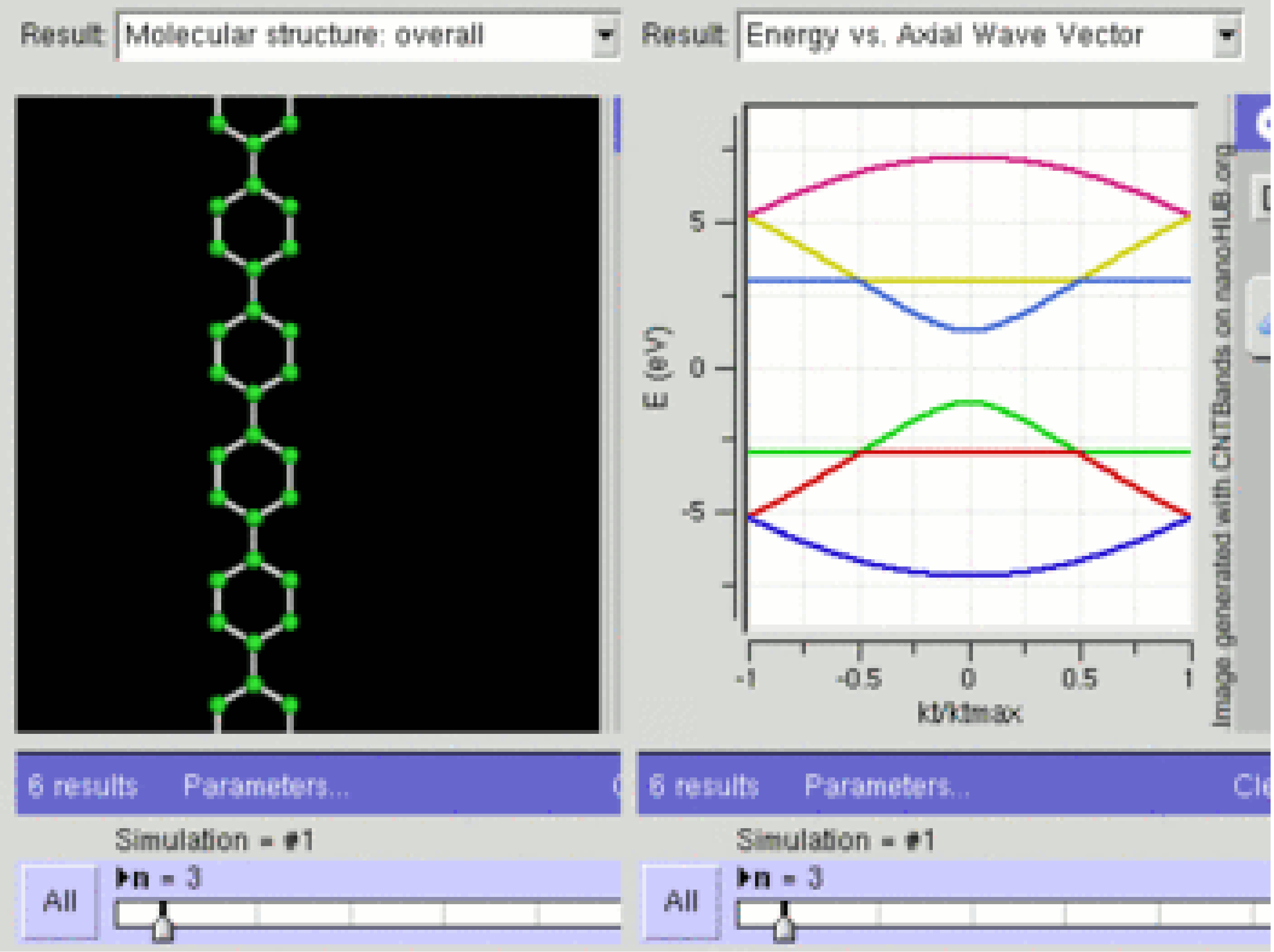


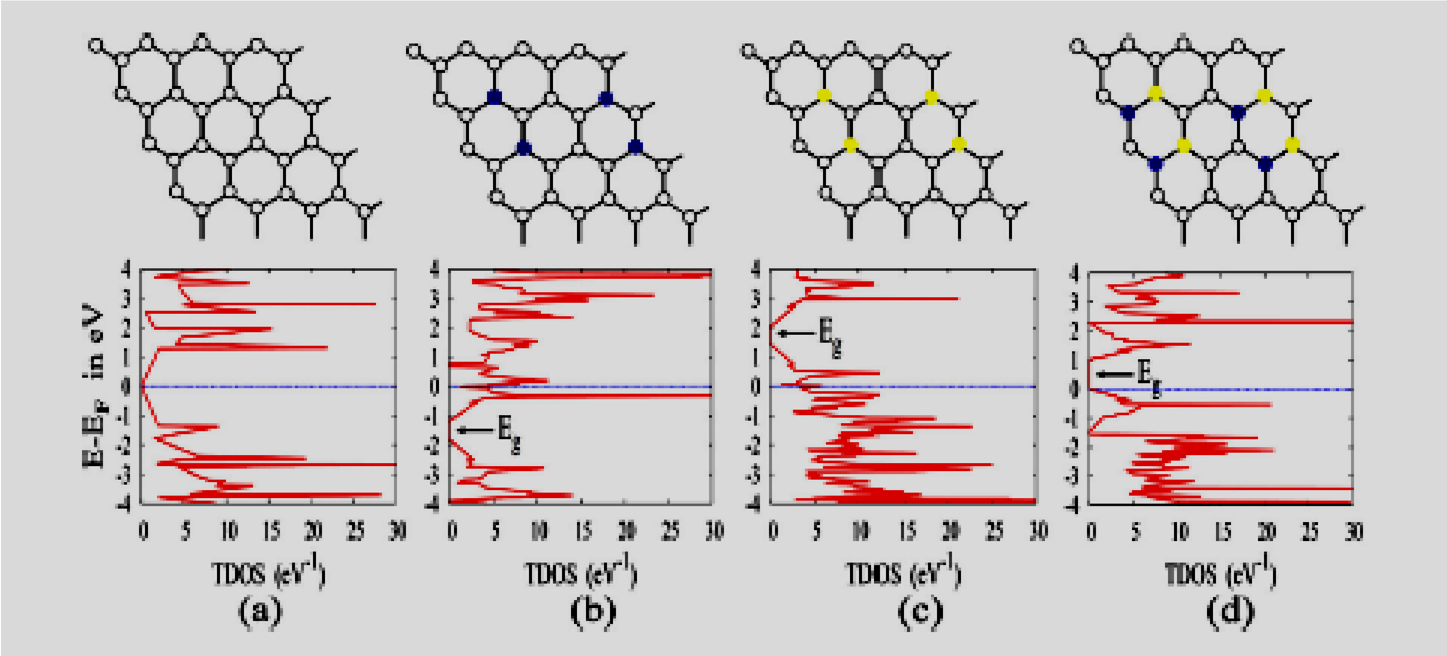
$$E = \pm \mathrm{v}_F \, |\vec{p}\,|$$

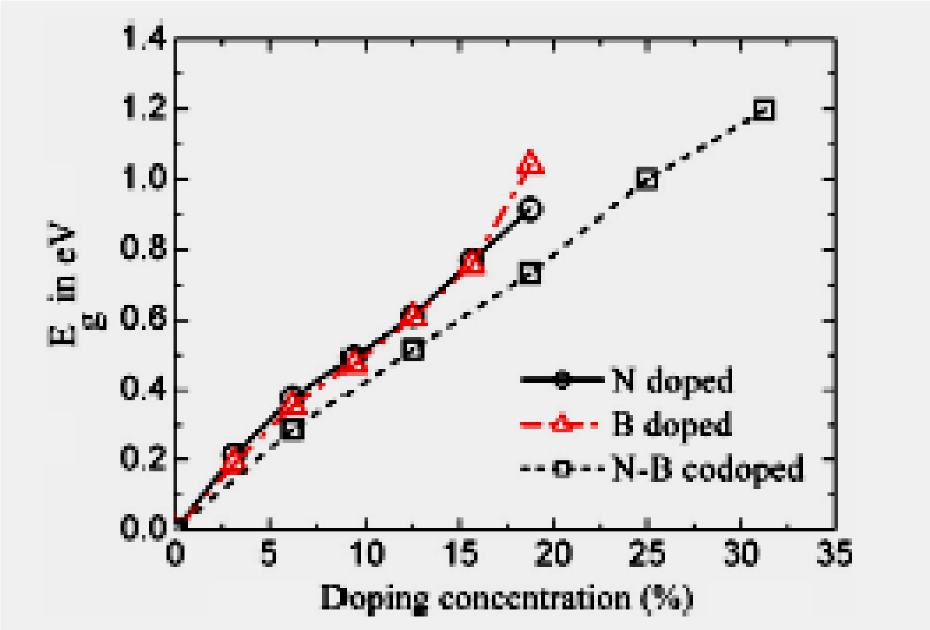
"Fermi velocity"

$$\mathrm{v}_F = 8 \times 10^5 \, m/s$$

Band Structure of Graphene Nanoribbon I







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(2020) 10:2502 | https://doi.org/10.1038/s41598-020-59262-2

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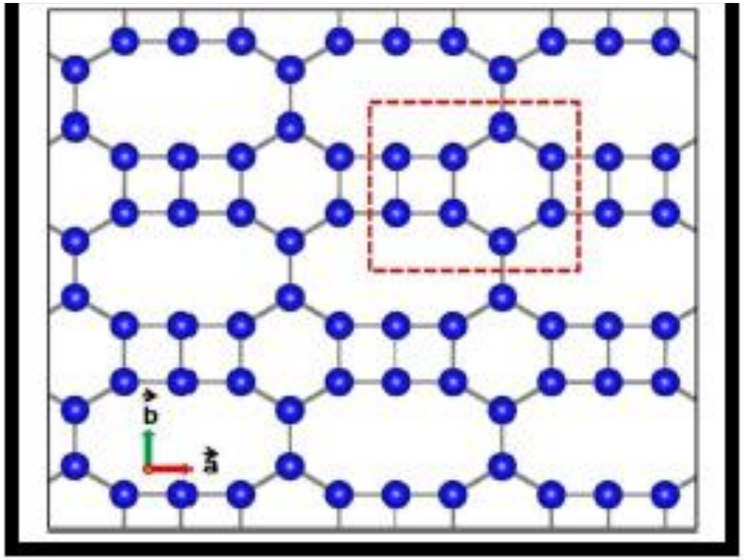
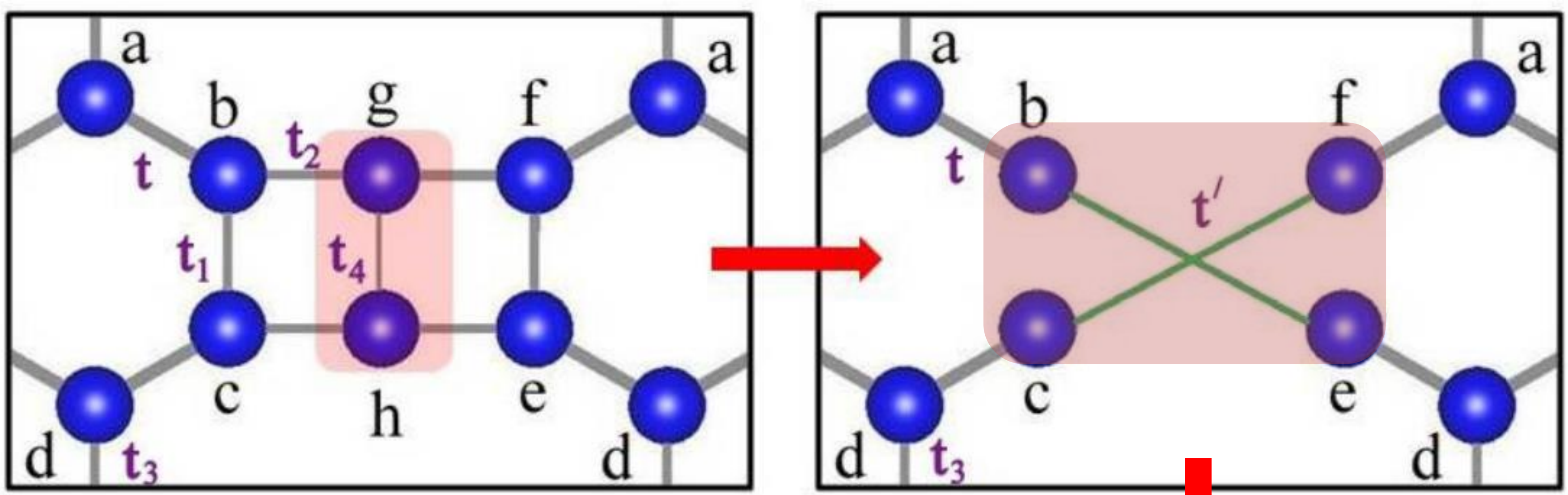
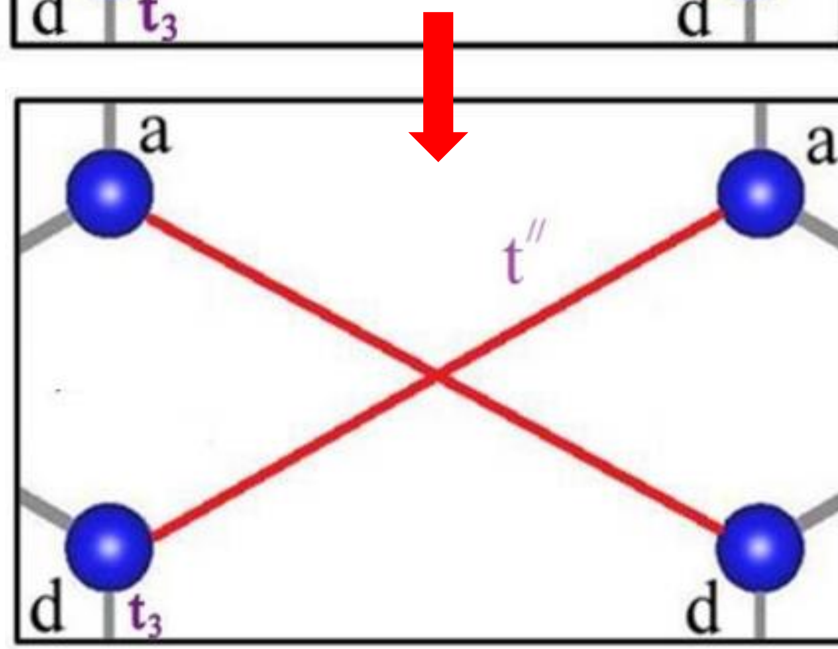
The topology and robustness of two Dirac cones in S-graphene: A tight binding approach

Arka Bandyopadhyay[1], Sujoy Datta[1], Debnarayan Jana[1*], Subhadip Nath[2] & Md. Mohi Uddin[3]



RSRG scheme





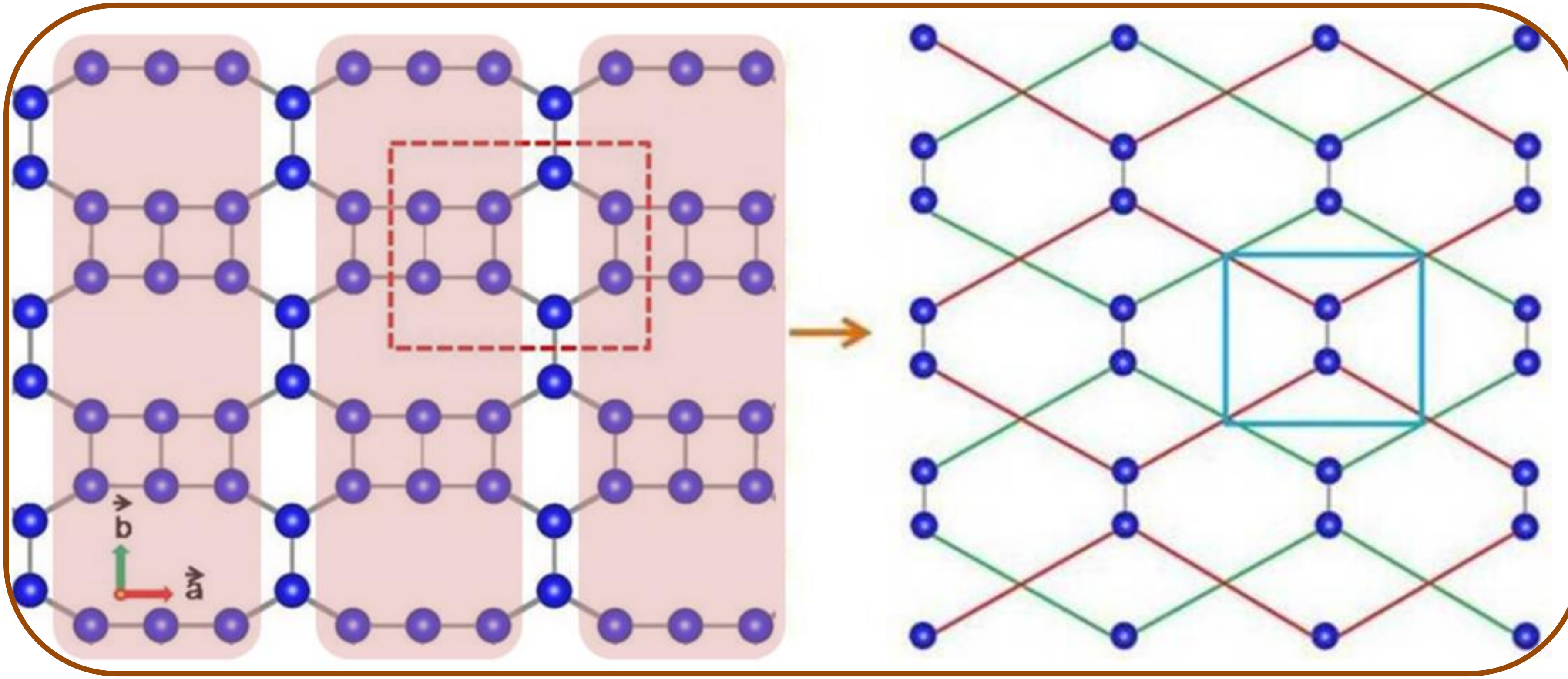
$E \approx \epsilon.$ (Near Fermi level)

$t_2^2 = t_1 t_4$ (Holds good)

$t' = -t_2^2/t_4 = -t_1.$

$t'' = t^2/t_1$

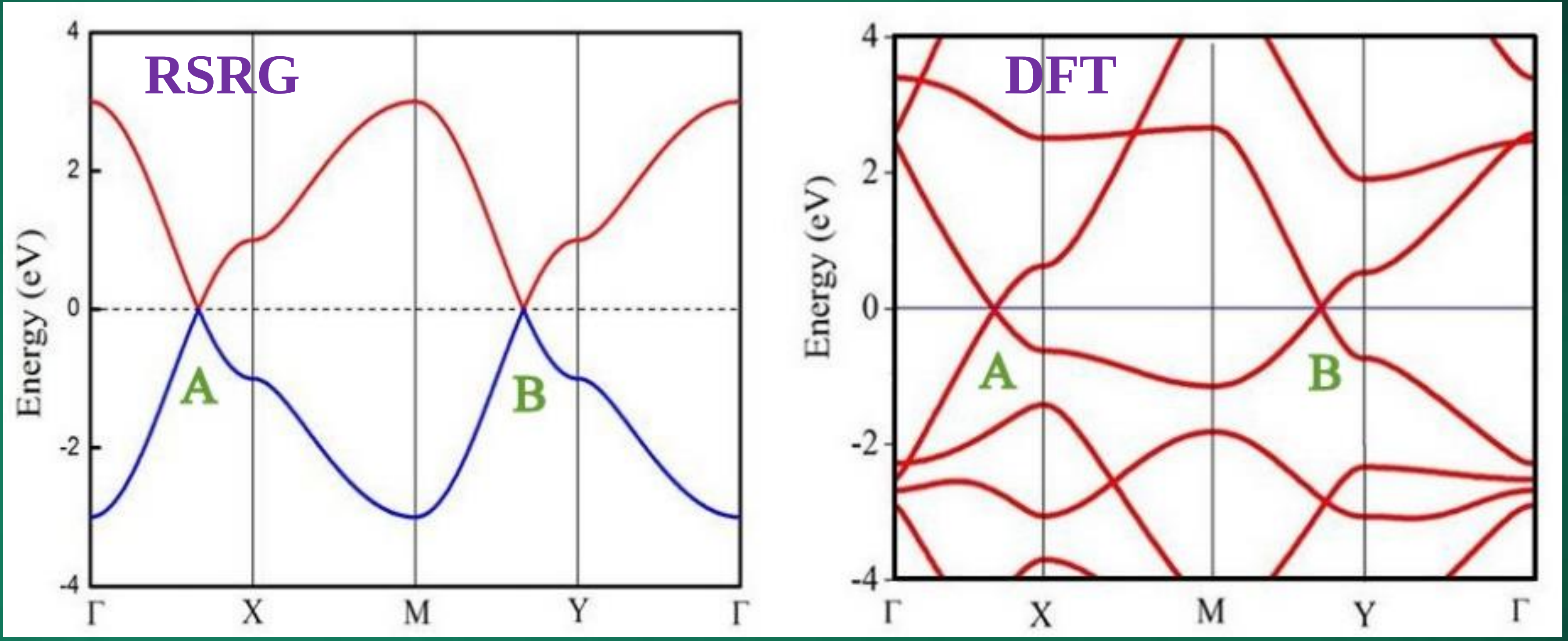
RSRG scheme



• **Renormalized lattice is a two level system.**

• **Uniform hopping in the original lattice leads to uniform hopping in the final system. There values are same.**

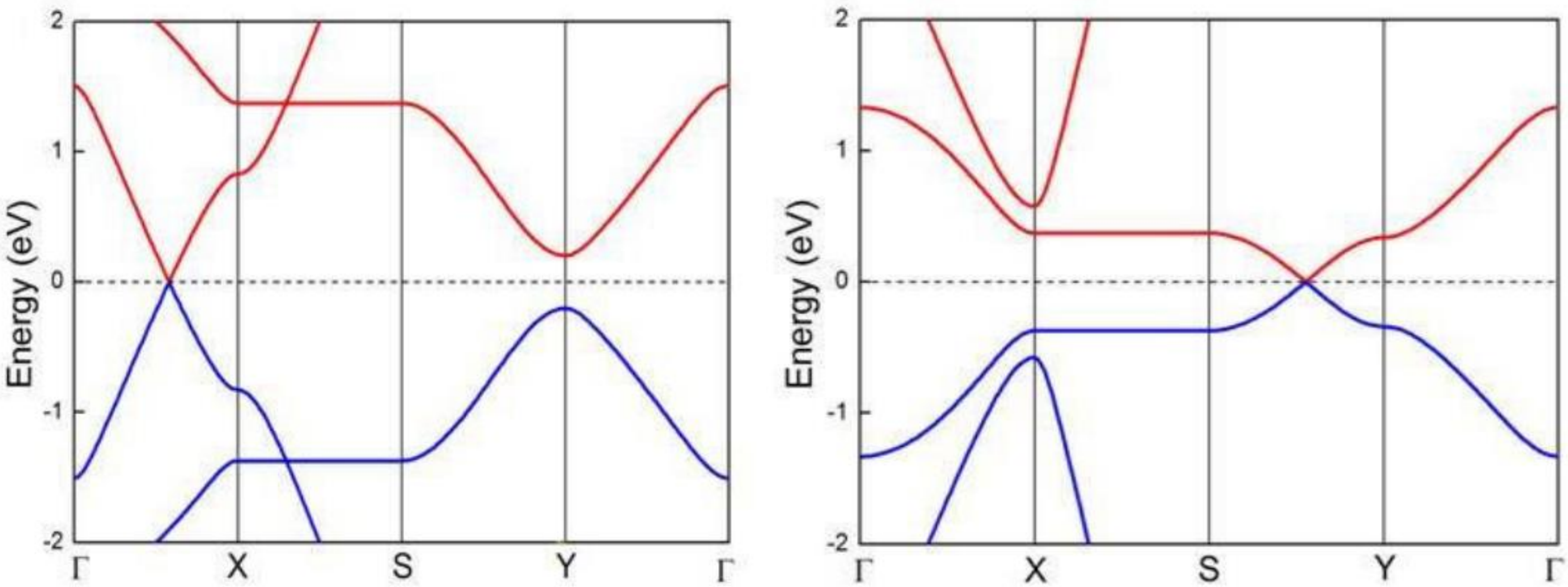
Band structure



$$E_{\pm} = \pm\tau\sqrt{1 + 4\,cos^2(2\pi k_x) + 4\,cos(2\pi k_x)\,cos(2\pi k_y)}.$$

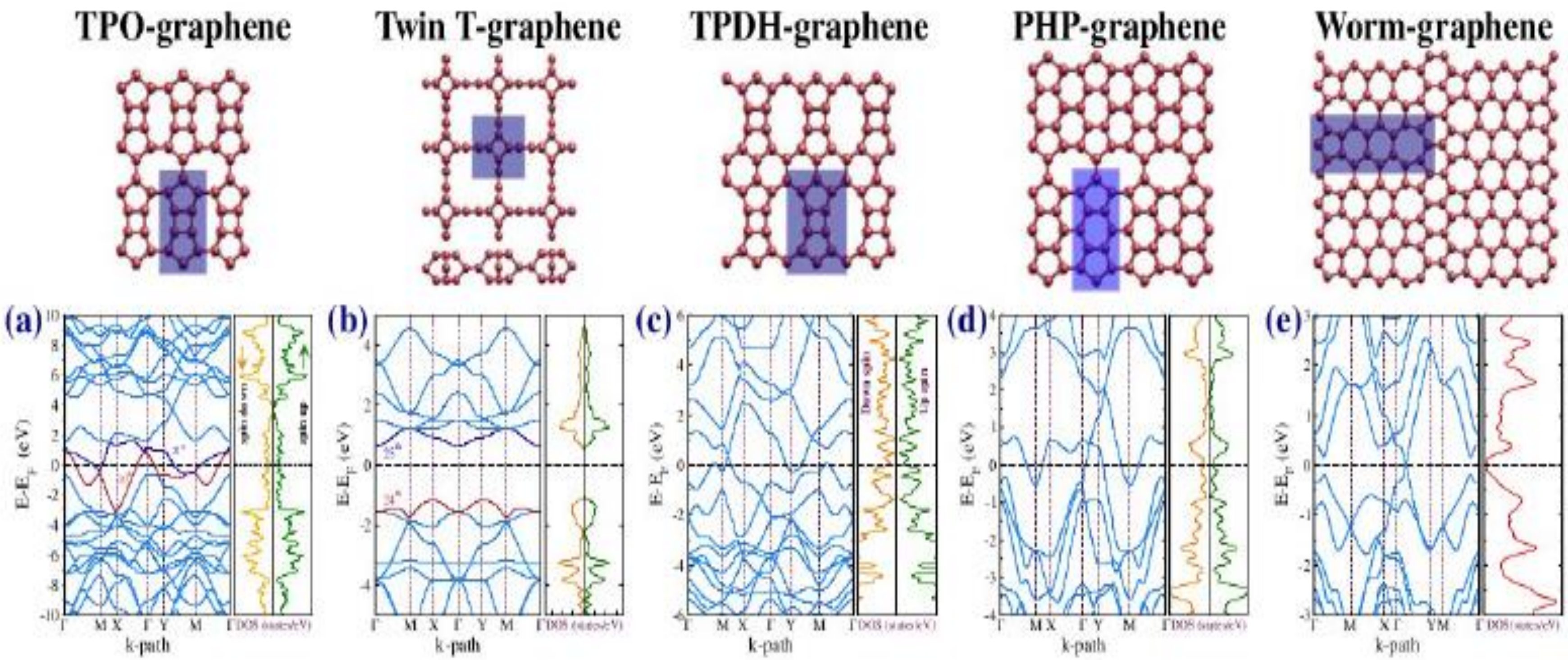
$$q_x = 2\pi k_x/a \text{ and } q_y = 2\pi k_y/b.$$

Individual tuning



Hopping relation	Fate of 'A'	Fate of 'B'
$t_2^2 = t_1 t_4$ and $t_1 t_3 > 2t_2^2$	present	present
$t_2^2 = t_1 t_4$ and $t_1 t_3 < 2t_2^2$	absent	absent
$t_1 > t_2 (= t_4) \leq t$ and $t_3 \leq 2t^2$	absent	present
$\mathrm{t}_4 < 2\tau/3$	present	absent

Five new carbon 2D structures and their electronic property:



TTG indirect bandgap 1.79 eV

Worm-graphene Fermi velocity (max) 6.85 x 10^5 m/s

PHYSICAL REVIEW B **103**, 075137 (2021)

8-16-4 graphyne: Square-lattice two-dimensional nodal line semimetal with a nontrivial topological Zak index

Arka Bandyopadhyay,[1] Arnab Majumdar,[2,*] Suman Chowdhury,[3] Rajeev Ahuja,[2,4,†] and Debnarayan Jana[1,‡]
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[2]*Department of Physics and Astronomy, Box 516, Uppsala University, Uppsala, SE-75120, Sweden*
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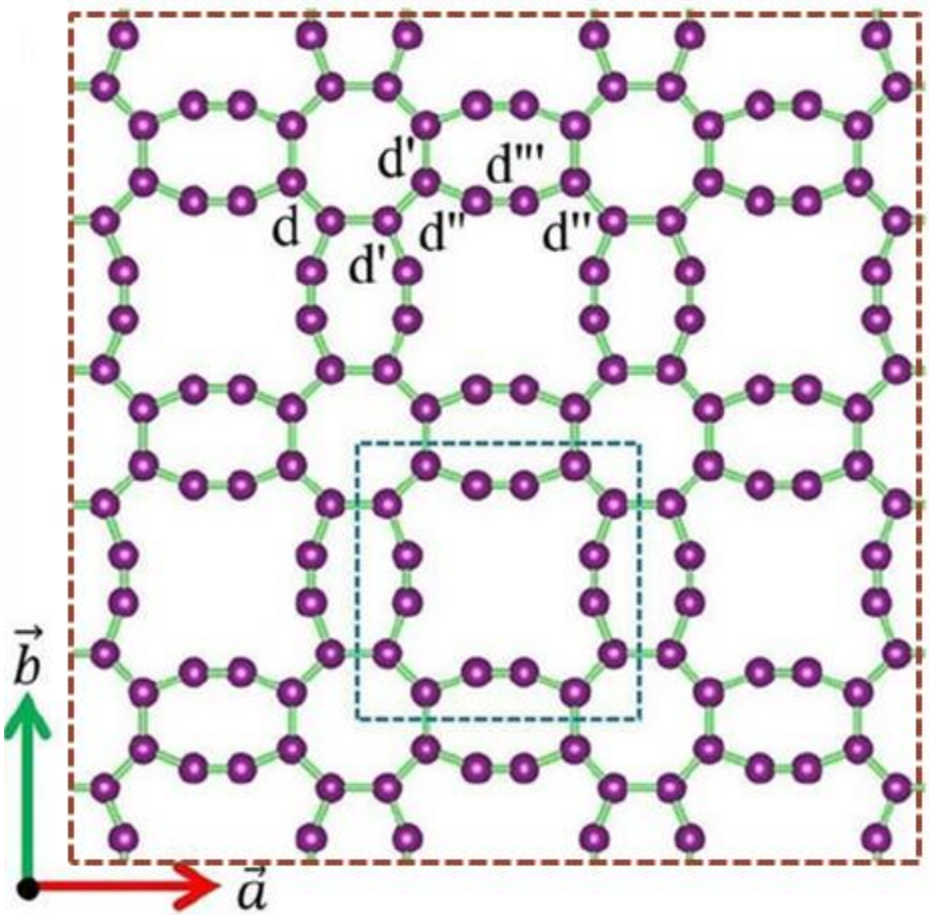
(Received 25 August 2020; revised 2 February 2021; accepted 3 February 2021; published 22 February 2021)

An unprecedented graphyne allotrope with square symmetry and nodal line semimetallic behavior has been proposed in the two-dimensional (2D) realm. The emergence of the Dirac loop around the high-symmetry points in the presence of both the inversion and time-reversal symmetries is a predominant feature of the electronic band structure of this system. Besides, the structural stability in terms of the dynamic, thermal, and mechanical properties has been critically established for the system. Following the *exact analytical* model based on the real-space renormalization group scheme and tight-binding approach, we have inferred that the family of 2D nodal line semimetals with square symmetry can be reduced to a universal four-level system in the low-energy limit. This renormalized lattice indeed explains the underlying mechanism responsible for the fascinating emergence of 2D square nodal line semimetals. Besides, the analytical form of the generic dispersion relation of these systems is well supported by our density-functional theory results. Finally, the nontrivial topological properties have been explored for the predicted system without breaking the inversion and time-reversal symmetry of the lattice. We have obtained that the edge states are protected by the nonvanishing topological index, i.e., Zak phase.

DOI: 10.1103/PhysRevB.103.075137

Interplay between square symmetry and Dirac fermions



The inversion, mirror reflection, and time-reversal symmetries are preserved

The system is dynamically, thermally and mechanically stable.

The plane group is P4mm with lattice constant 7.35 Å.

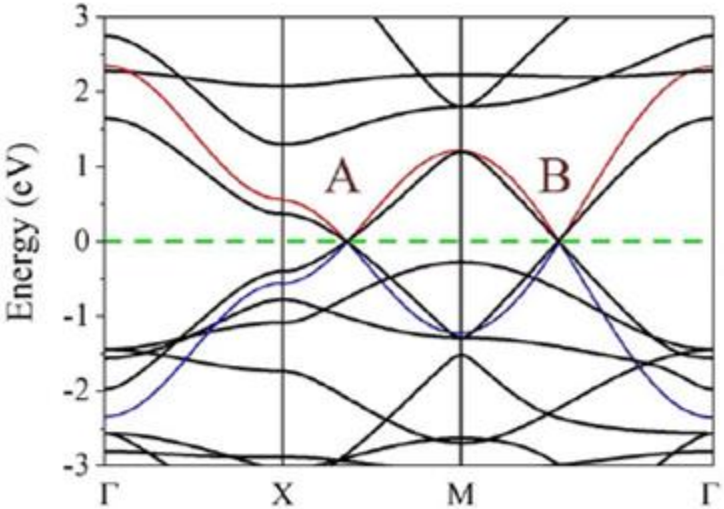
Unit cell consists of 16 carbon atoms with sp and sp^2 hybridizations.

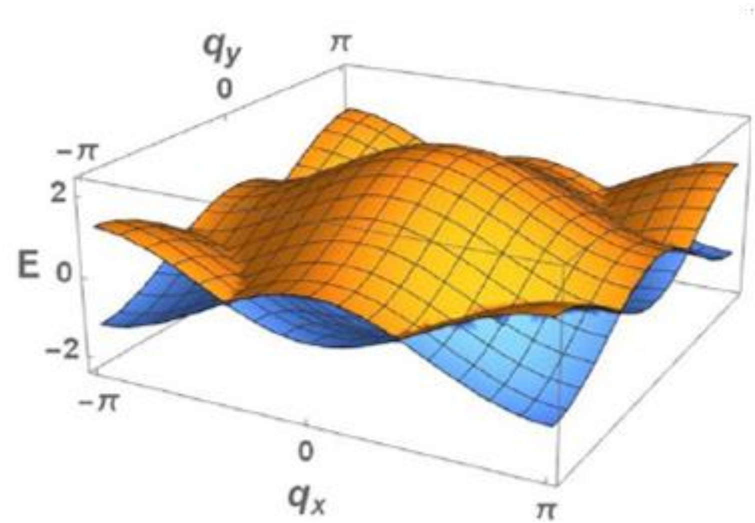
Four distinct bond lengths *d* = 1.42 Å, *d'* = 1.48 Å, *d''* = 1.41 Å, and *d'''* = 1.23 Å.

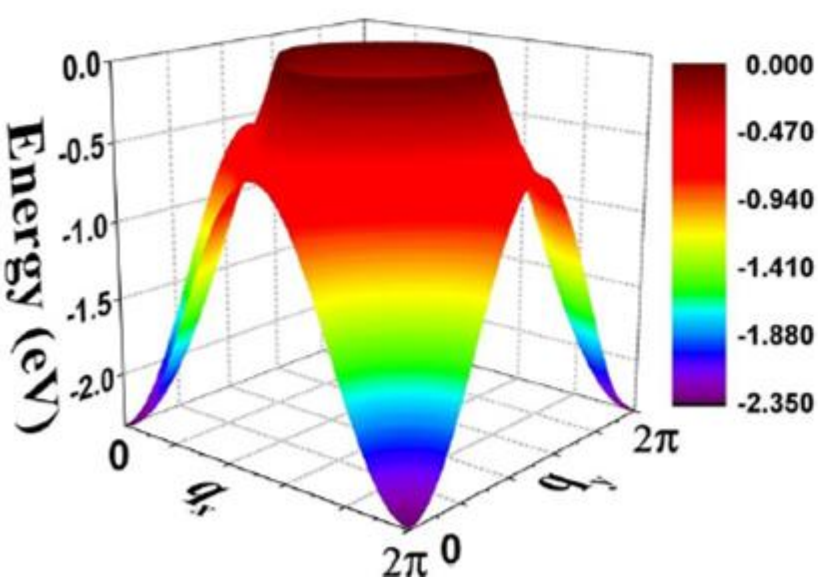
The system is also obtained using the evolutionary algorithm USPEX

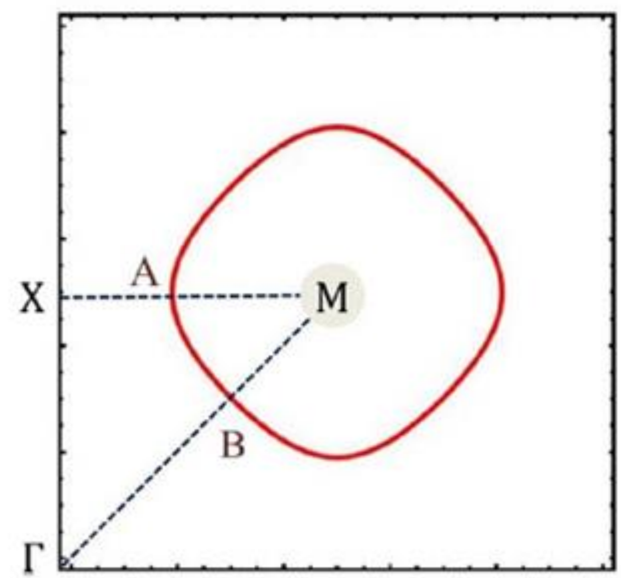
A new square lattice 8-16-4 graphyne and the search for Dirac fermions

Analytical band structure: emergence of nodal ring









Applied Surface Science 563 (2021) 150315

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Full Length Article

Nitrogenated CQD decorated ZnO nanorods towards rapid photodegradation of rhodamine B: A combined experimental and theoretical approach

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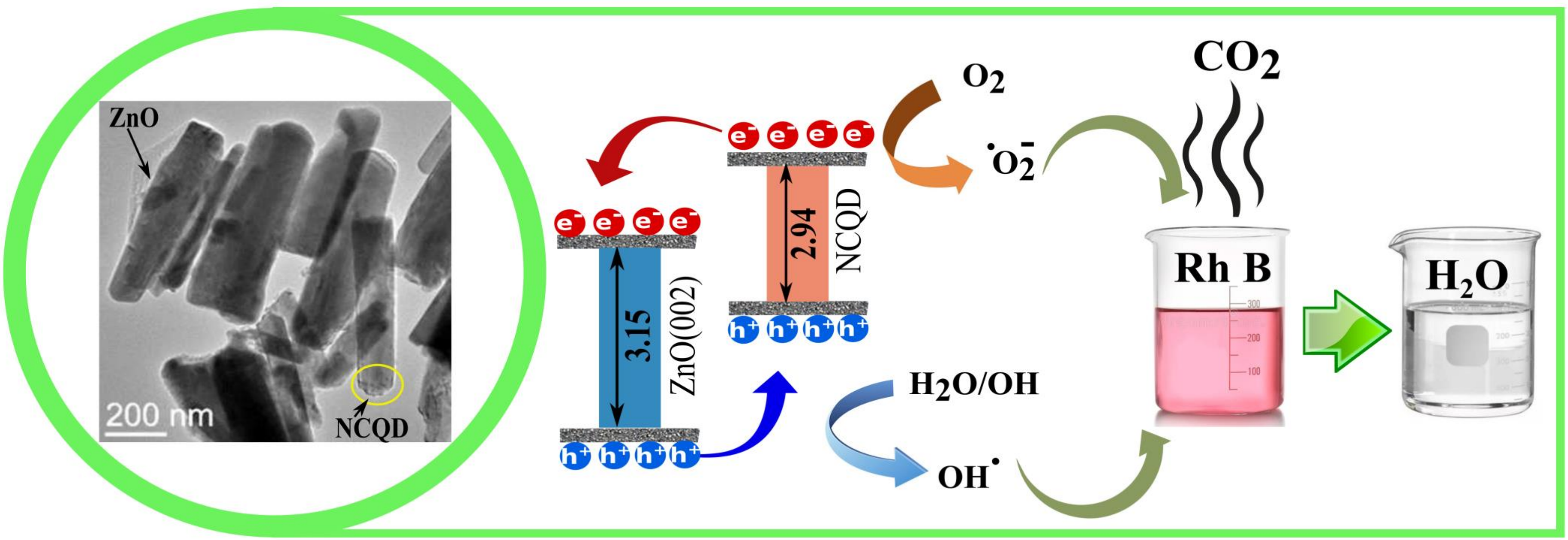

IOP Publishing Journal of Physics: Condensed Matter
J. Phys.: Condens. Matter **34** (2022) 053001 (42pp) https://doi.org/10.1088/1361-648X/ac3075

Topical Review

Emerging properties of carbon based 2D material beyond graphene

Susmita Jana[1], Arka Bandyopadhyay[1], Sujoy Datta[1], Debaprem Bhattacharya[1,2] and Debnarayan Jana[1,*]

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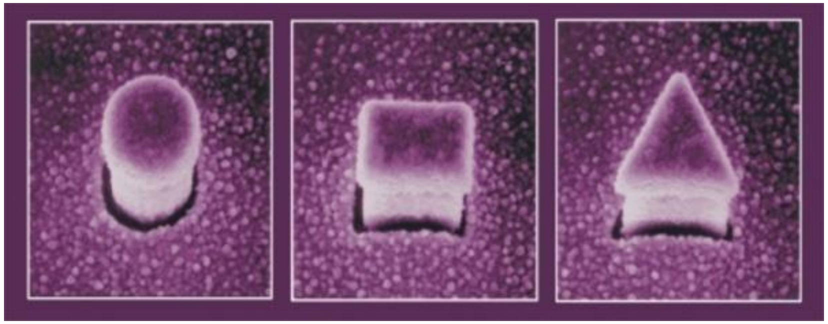
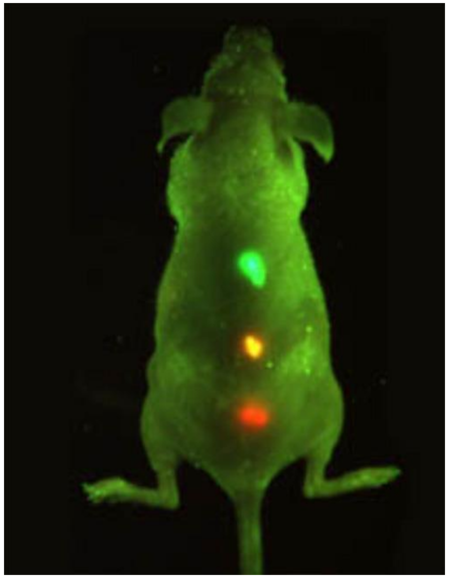
CrossMark

Health Care: Detecting Diseases Earlier

- Quantum dots glow in UV light
  - Injected in mice, collect in tumors
  - Could locate as few as 10 to 100 cancer cells



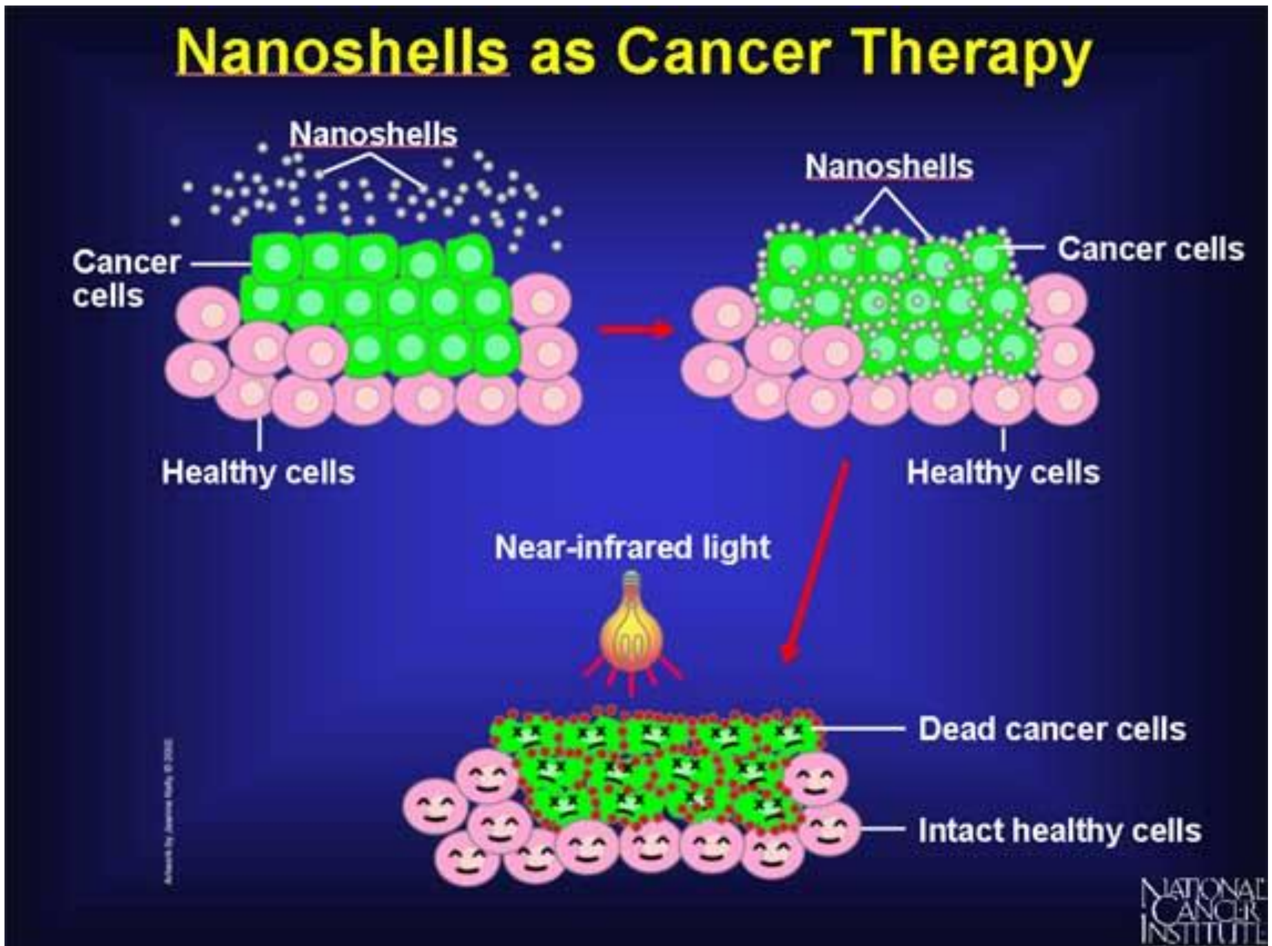
Quantum Dots: Nanometer-sized crystals that contain free electrons and emit photons when submitted to UV light



Early tumor detection, studied in mice

Nano shells as Cancer Therapy

Nano shells are injected into cancer area and they recognize cancer cells. Then by applying near-infrared light, the heat generated by the light-absorbing Nano shells has successfully killed tumor cells while leaving neighboring cells intact.



Nanoshells

Nanoshells kill tumor cells selectively

Conclusions

- Some interesting uncommon analysis of problems have been presented via dimensional analysis.

- Quantum mechanics – particle in a box model and tunneling play an important key role in nano science.

- Surface to volume ratio is the main factor for surface reactivty of nanomaterials.

- Enhancement of bandgap in nanomaterials – prime factor for design of electronic devices

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First we guess it. Then we compute the consequences of the guess to see what would be implied if the law we guess is right. Then we compare the result of the computations to nature, with experiment or experience; compare it directly with observation, to see if it works. If it disagrees with experiment it is wrong. In that simple statement is the key to science. It does not make any difference how beautiful your guess is. It does not make any difference how smart you are, who made the guess or what your name is – if it disagrees with experiment it is wrong. That is all there is to it.

Richard Feynman

My Research Group

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Department of Physics
University of Calcutta

Postdoctoral Fellow

Dr. Sumona Sinha

Thesis Submitted

Apu Mondal

Present Research Fellows

Deep Mondal

Krishnansu Basak

Susmita Jana

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About The Authors

Supriya Ghosal, M.Sc (University of Calcutta), is currently pursuing his doctoral research in the Department of Physics, University of Calcutta. He has qualified in CSIR-NET 2017, JEST 2018 & GATE 2018. His current research focuses on the electronic, optical, thermoelectric as well as photo-catalytic behaviours of various next-generation emerging 2D monolayers and their possible Quantum dots employing Density functional theory.

Dr. Debnarayan Jana, M. Sc (Calcutta) Ph. D (Raman Research Institute, Bengaluru/degree from JNU, New Delhi) is a Professor of Physics in University of Calcutta since 2012. His current research is focused on defect studies in Annealed and Nano-annealed, ion-irradiated ZnO material, Density functional theory (DFT) in 2D materials and Photo-Catalytic Activity towards degradation of different dyes. He was elected as a Fellow of West Bengal Academy of Science and Technology (WAST) in 2015. He has more than 175 papers in national and international peer reviewed journals. Govt. of India has honoured him with prestigious INSA Teachers Award (2020) for his accomplishments as a distinguished teacher over the years.

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