Engineering Physics

(PHY1701)

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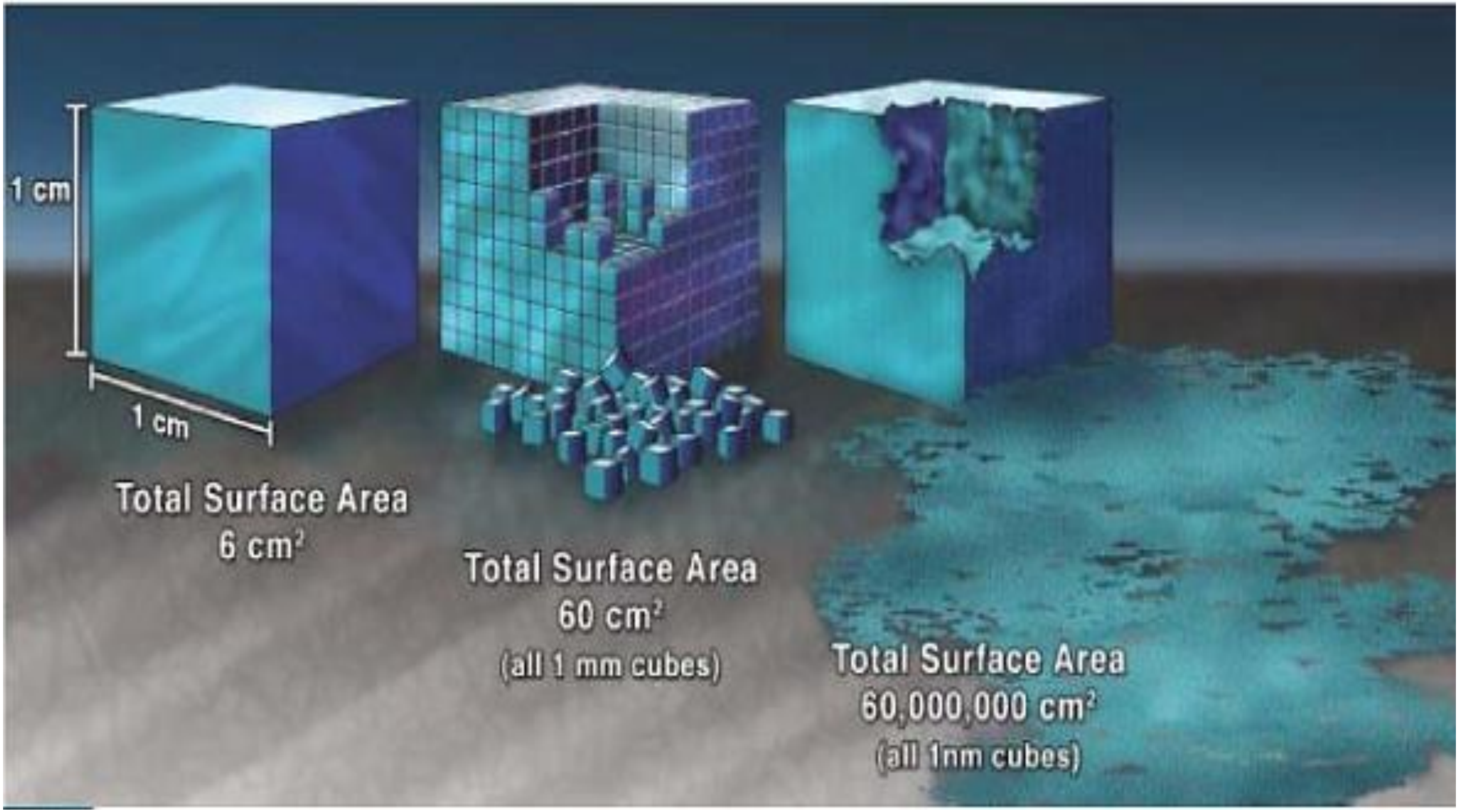
Contents

❖ Introduction to Nano Technology, Charles P Poole Jr., Frank J Owens, Willey Publication. (CF)

Surface to Volume ratio



Surface Effects

- The surface to volume ratio follows an inverse power law
- The fraction of atoms on the surface increases with decreasing the size
- Large surface is favorable for applications such as catalysis.
- As a particle decreases in size, a greater proportion of atoms are found at the surface compared to those inside.
- For example, a particle of
  - Size-30 nm-> 5% of its atoms on its surface
  - Size-10 nm->20% of its atoms on its surface
  - Size-3 nm-> 50% of its atoms on its surface

Nanoparticles are more reactive than large particles (Catalyst)

Surface to Volume ratio

Cubic:

Surface area $S = 6a^2$

Volume $V = a^3$

Surface area to volume ratio

$$\frac{S}{V} = \frac{6a^2}{a^3} = \frac{6}{a}$$

Sphere

Surface area $S = 4\pi R^2$

Volume of sphere $V = \frac{4}{3}\pi R^3$

Surface to volume ratio $$\frac{S}{V} = \frac{4\pi R^2}{\frac{4}{3}\pi R^3} = \frac{3}{a}$$

Increase in surface area

Imagine a sphere of radius R=1cm. How many no. of tiny spheres of radius r=1nm is possible from the material?

$$\frac{4}{3}\pi R^3 = \frac{4}{3}\pi r^3$$

$$\text{i.e. } R^3 = N\, r^3$$

$$N = \frac{R^3}{r^3} = \frac{1cm^3}{1nm^3} = \frac{10^{-6}m^3}{10^{-27}m^3} = 10^{21}$$

10^{21} tiny 1 nm spheres are formed.

Increase in surface area

Total surface area available on these particles:

Surface area of the big sphere

$S = 4\pi R^2 = 4\pi(10^{-2}\ m)^2 = 4\pi(10^{-4})\ m$

Surface area of the tiny sphere

$S = 4\pi r^2 = 4\pi(10^{-9}\ m)^2 = 4\pi(10^{-18})\ m$

There are 10^{21} numbers of tiny spheres,

so their total surface area

$s_t = 10^{21} \times 4\pi(10^{-18})\ m = 4\pi 10^3\ m^2$

So, $\frac{s_t}{S} = \frac{4\pi \times 10^3 m^2}{4\pi \times 10^{-4} m^2} = 1 \times 10^7$

The surface area has increased by a factor of 10 million times.

Increase in surface area

- Nanoparticles exhibit unique properties due to their high surface area to volume ratio.
- A spherical particle has a diameter (D) of 100nm.
  - Calculate the volume (V) and surface area (SA)

$$V = \frac{4}{3}\pi r^3 = \frac{\pi D^3}{6}$$

$$V = \frac{\pi(100 \times 10^{-9})^3}{6}$$

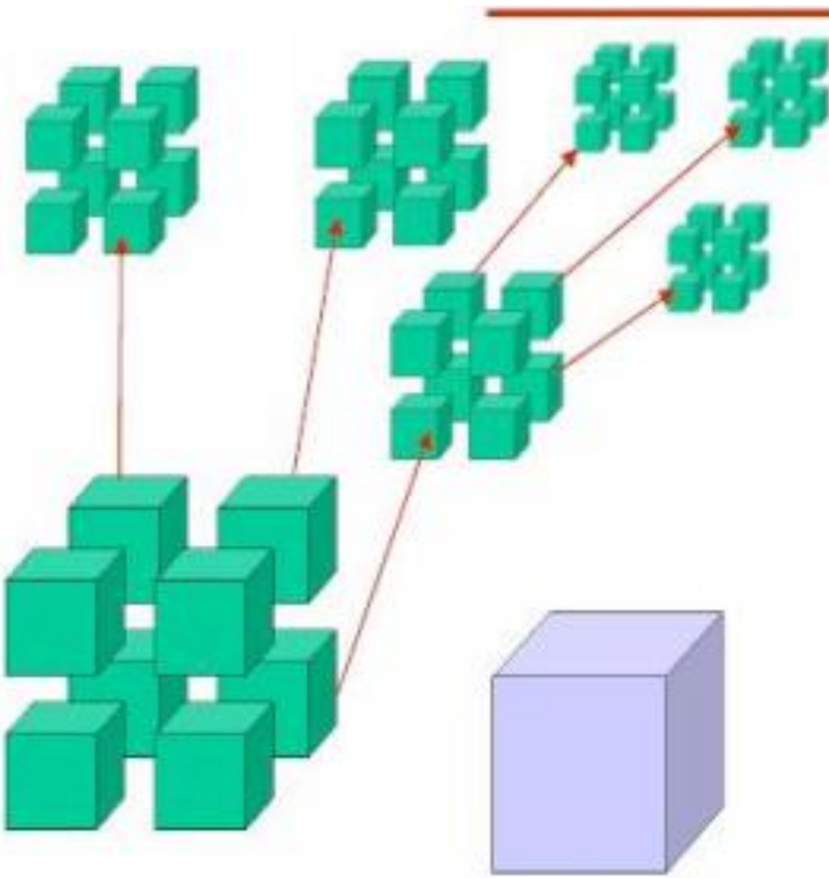
$$V = 5.24 x 10^{-22} m^3$$

$$SA = 4\pi r^2 = \pi D^2$$

$$SA = \pi(100 \times 10^{-9})^2$$

$$SA = 3.141 \times 10^{-14} m^2$$

Increase in surface area



8 Cubes Side L
Each has Surface area $6L^2$
Total Surface Area $48 L^2$

1 Cube
Length of sides 2L
Surface area $24 L^2$

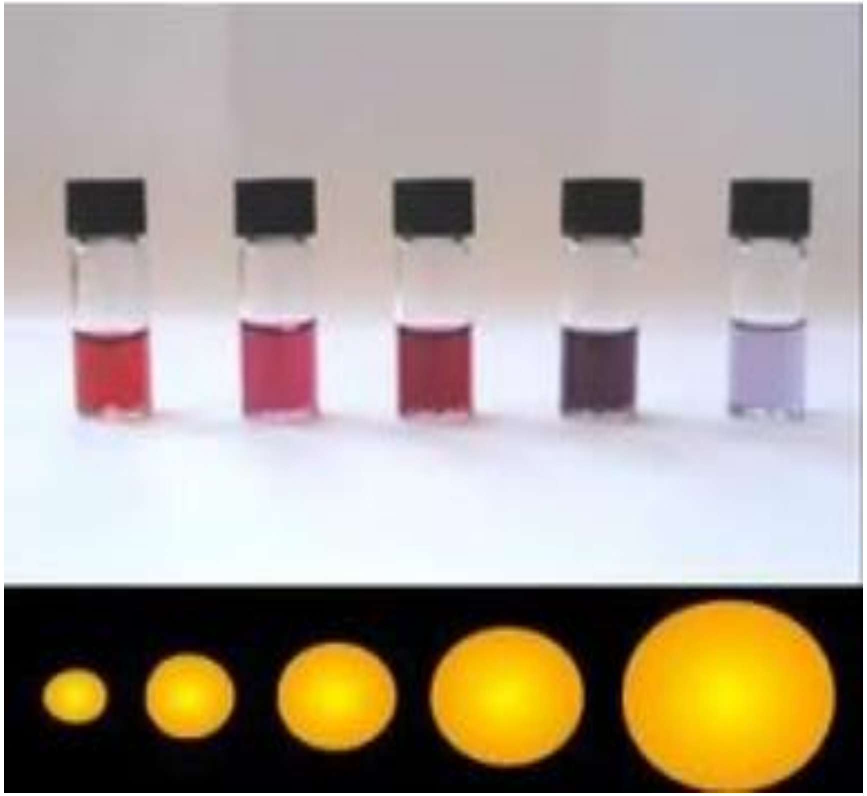
For example, 5 cubic centimeters - about 1.7 cm per side - of material divided 24 times will produce 1 nanometer cubes and spread in a single layer could cover a football field

Quantum confinement

- Quantum effects can begin to dominate the behaviour of matter at the nanoscale – particularly at the lower end - affecting the optical, electrical and magnetic behaviour of materials.
- When the particle size is comparable to the debroglie wavelength of electrons or mean free path of electrons, the energy levels of electron changes leading to an effect – quantum confinement characteristics.
- The quantum confinement effect can be observed once the diameter of the particle is of the same magnitude as then wavelength of the electron Wave function.
- Quantum confinement is responsible for the increase of energy difference between energy states and band gap.

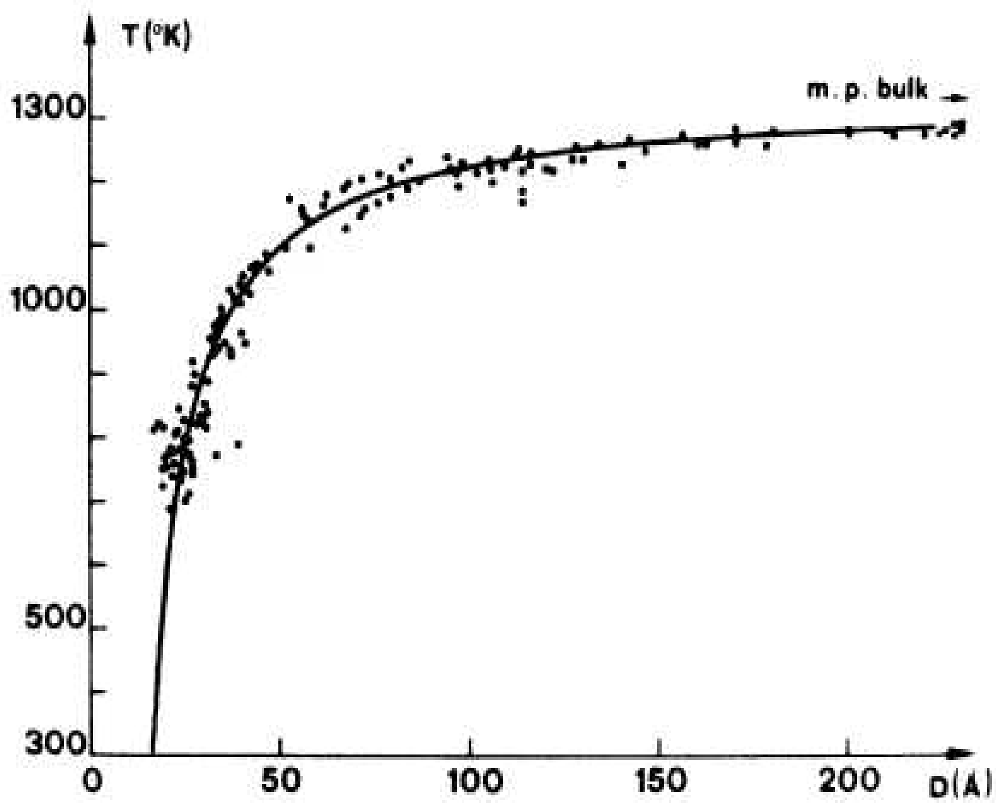
Quantum confinement

- A phenomenon tightly related with the optical and electronic properties of the materials.
- When materials are this small, their electronic and optical properties deviate substantially from those of bulk materials.(GOLD)



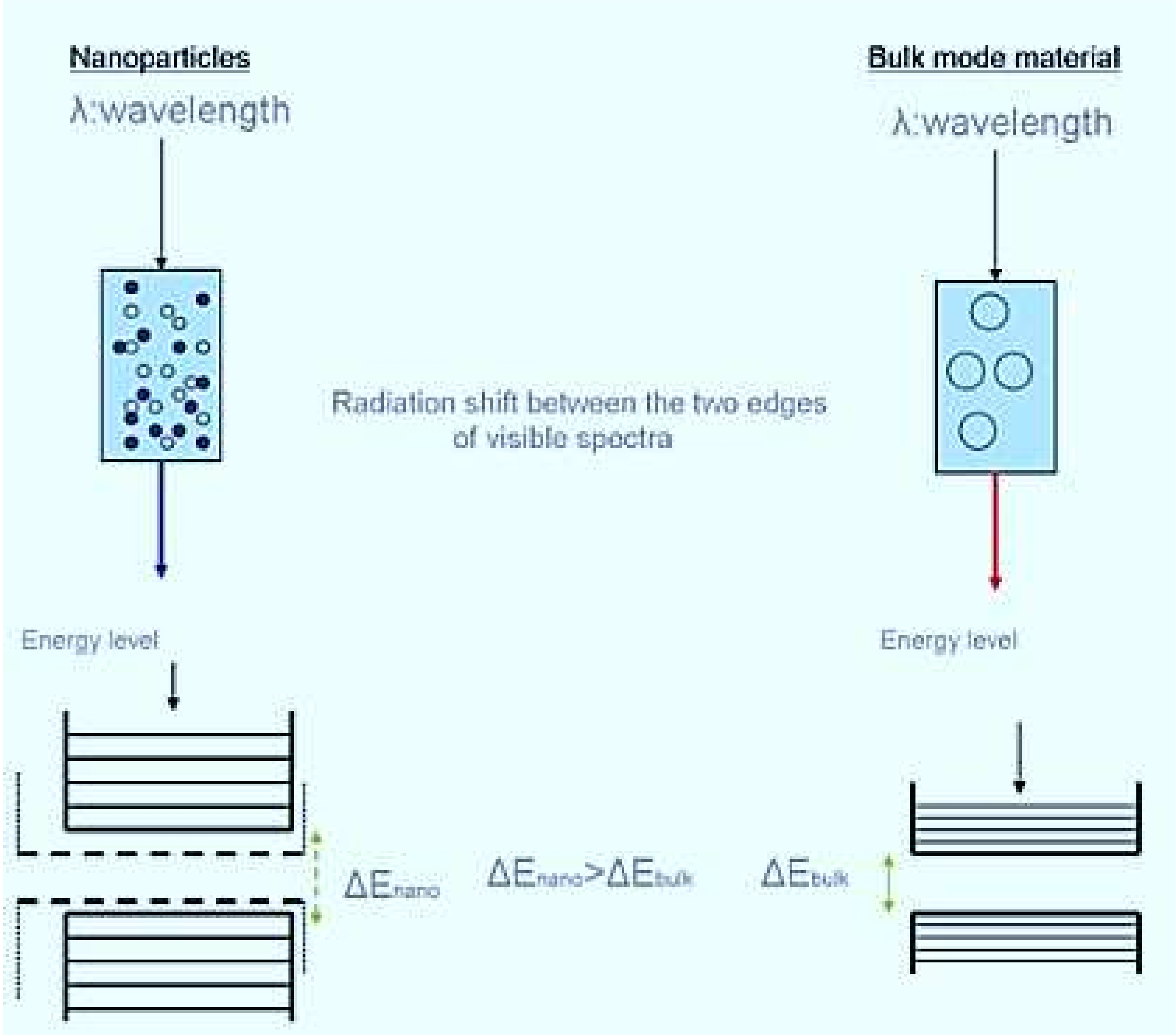
Melting point as a function of particle size

- Nanoparticles have a lower melting point than their bulk counterparts



Melting point of gold nanoparticles as a function of size.

Quantum confinement



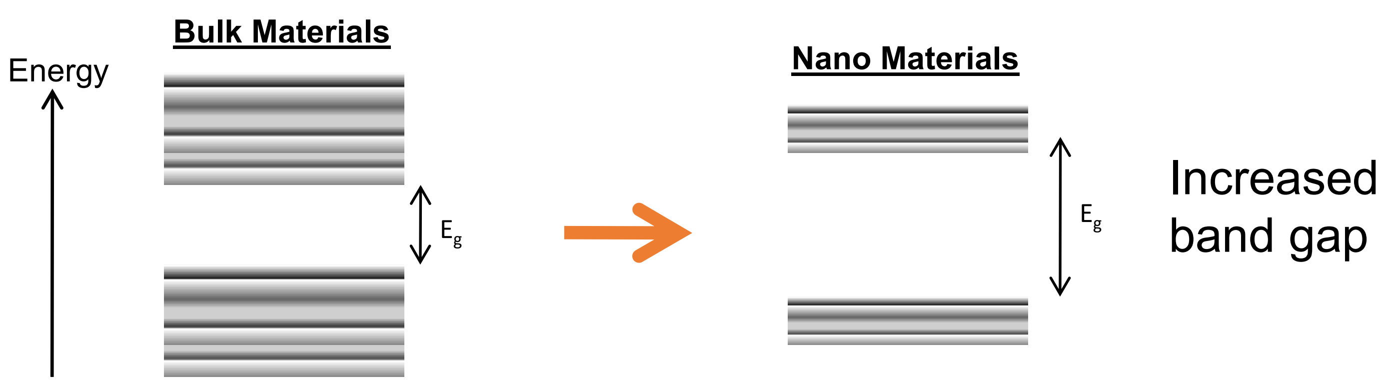
Quantum confinement

Definition:

- Quantum Confinement is the spatial confinement of electron-hole pairs (excitons) in one or more dimensions within a material.
  - 1D confinement: Quantum Wells
  - 2D confinement: Quantum Wire
  - 3D confinement: Quantum Dot
- Quantum confinement is more prominent in semiconductors because they have an energy gap in their electronic band structure.
- Metals do not have a bandgap, so quantum size effects are less prevalent. Quantum confinement is only observed at dimensions below 2 nm.

Quantum confinement

- Energy level spacing and 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 dimensions of a nanoparticle approach the de Broglie wavelength of electrons in the conduction band.
  - As a result the spacing between energy bands of semiconductor or insulator is **increased** (Similar to the *particle in a box* scenario, of introductory quantum mechanics.)

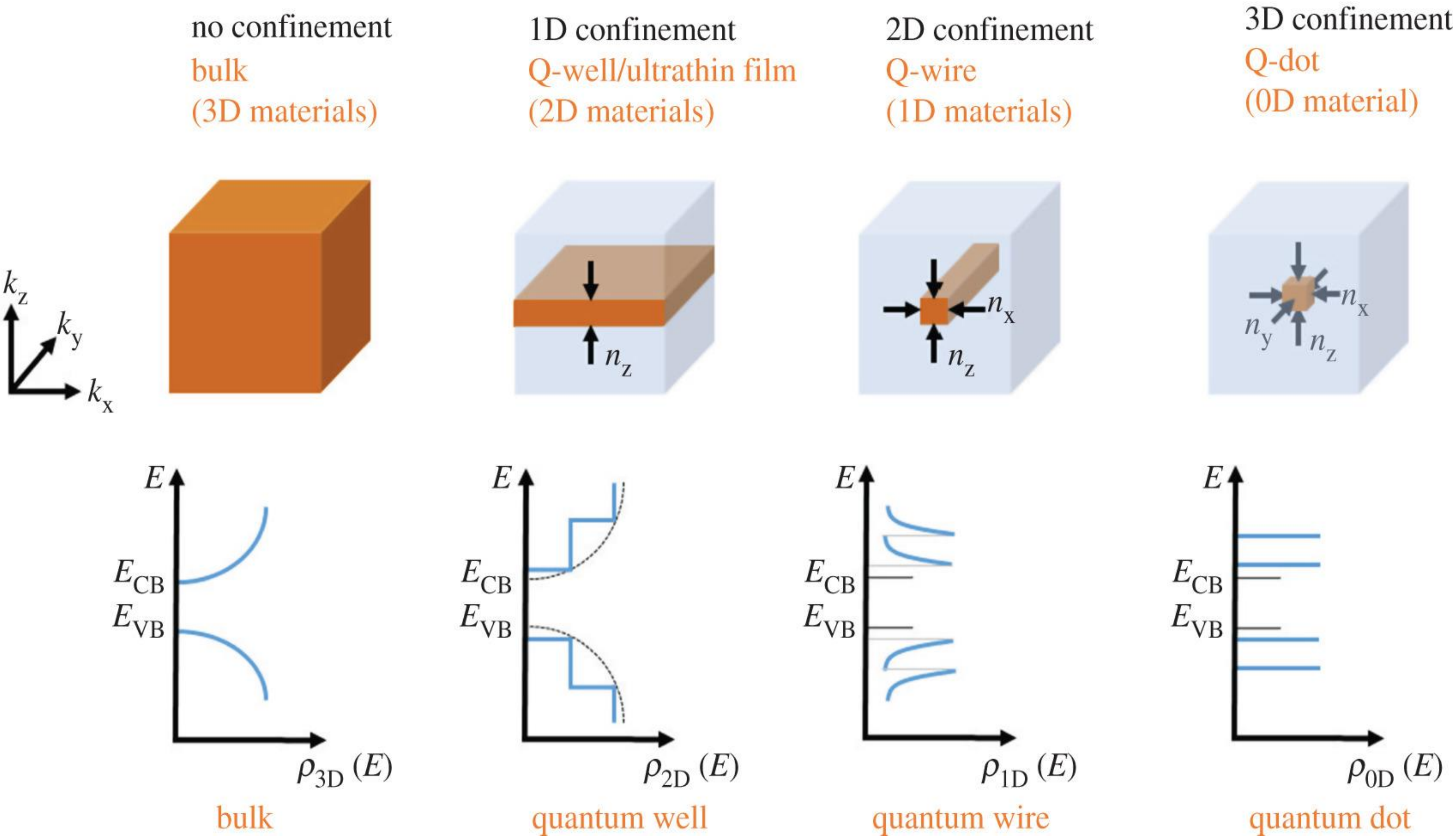


Quantum confinement

- Recall that when atoms are brought together in a bulk material the number of energy states increases substantially to form nearly continuous bands of states.

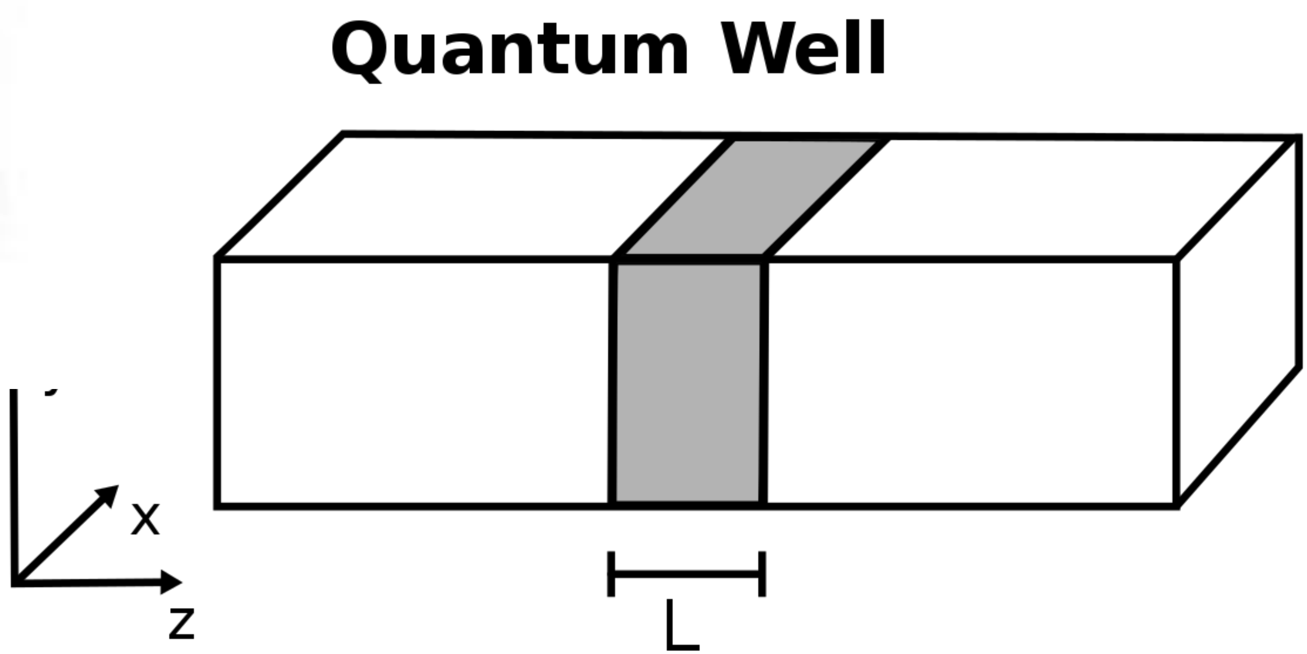
Quantum confinement

- This is very similar to the famous particle-in-a-box scenario and can be understood by examining the Heisenberg Uncertainty Principle.
- The Uncertainty Principle states that the more precisely one knows the position of a particle, the more uncertainty in its momentum (and vice versa).
- Therefore, the more spatially confined and localized a particle becomes, the broader the range of its momentum/energy.
- This is manifested as an increase in the average energy of electrons in the conduction band = increased energy level spacing = larger bandgap
- The bandgap of a spherical quantum dot is increased from its bulk value by a factor of $1/R^2$, where R is the particle radius.*

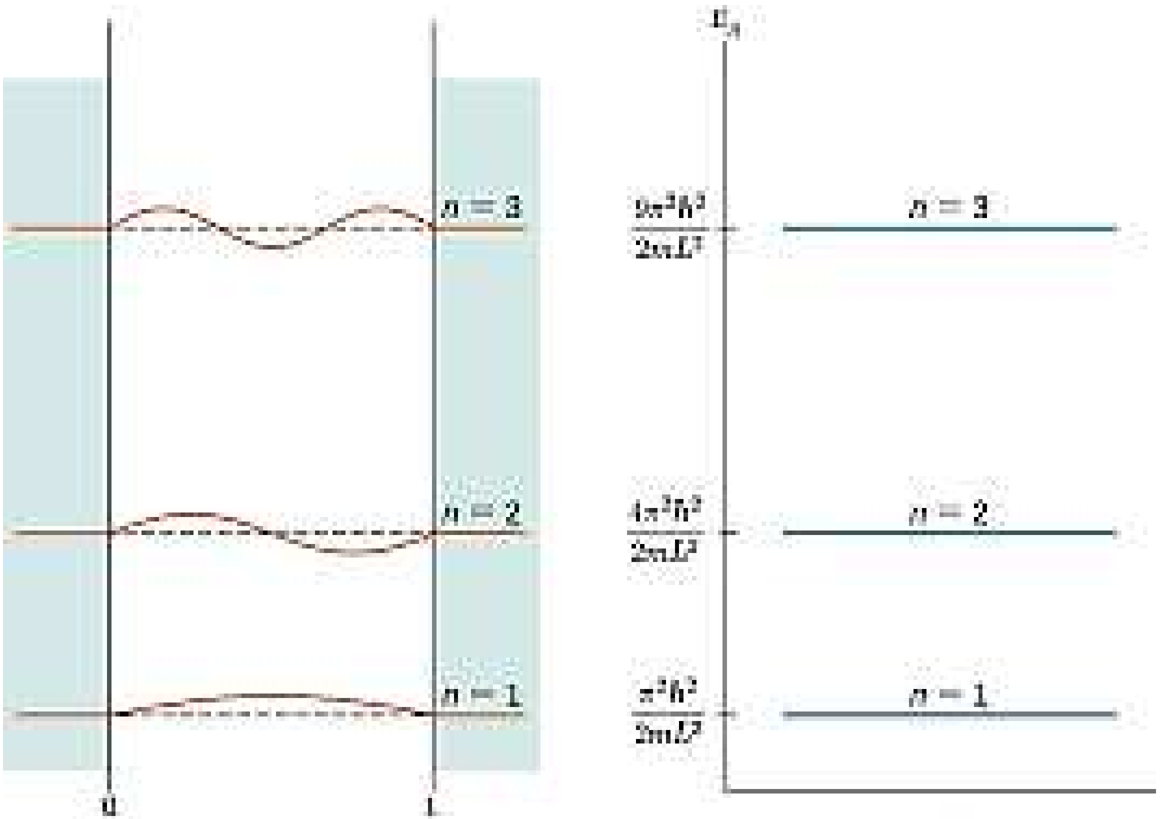

no confinement
bulk
(3D materials)
1D confinement
Q-well/ultrathin film
(2D materials)
2D confinement
Q-wire
(1D materials)
3D confinement
Q-dot
(0D material)
k_z
k_y
k_x
n_z
n_x
n_z
n_x
n_y
n_z
E
E_{CB}
E_{VB}
$\rho_{3D}(E)$
bulk
$\rho_{2D}(E)$
quantum well
$\rho_{1D}(E)$
quantum wire
$\rho_{0D}(E)$
quantum dot

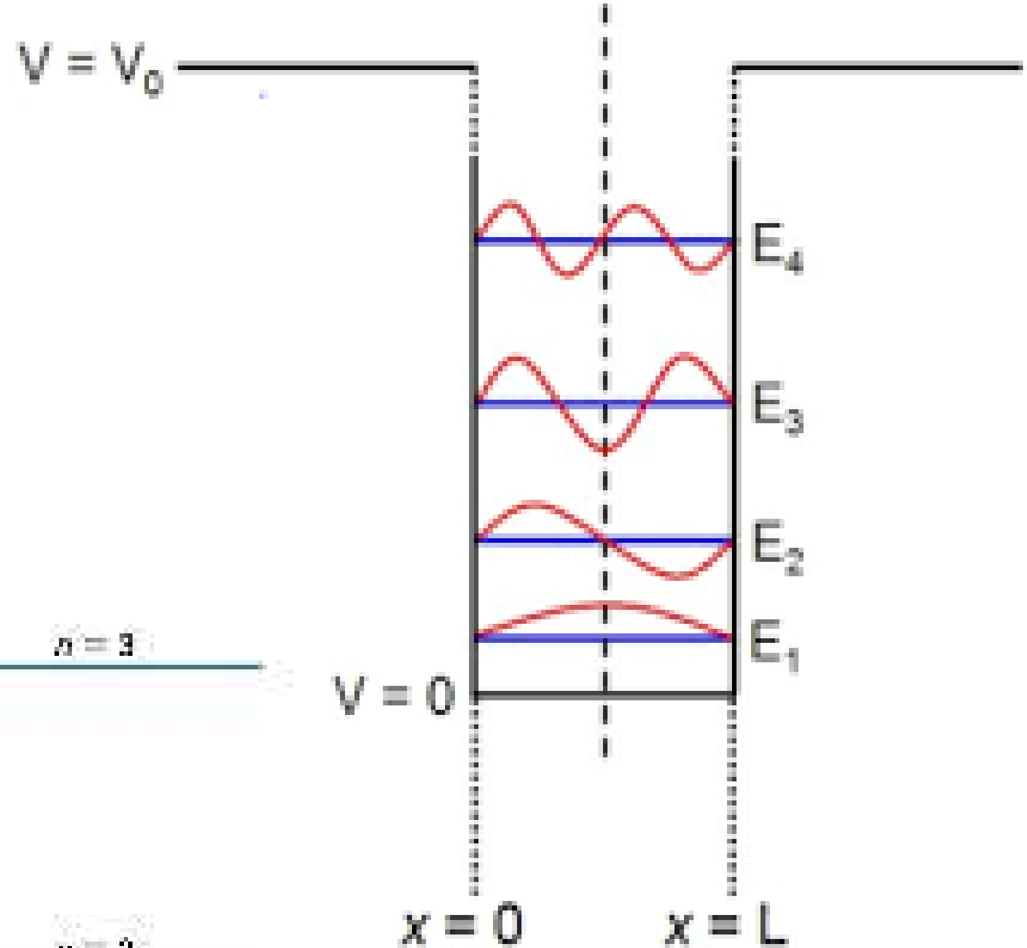
Quantum Well

- Quantum effects arise in systems which confine electrons to regions comparable to their de Broglie wavelength.
- When such confinement occurs in one dimension only (say, by a restriction on the motion of the electron in the z-direction), with free motion in the x- and y-directions, a two-dimensional system is created.



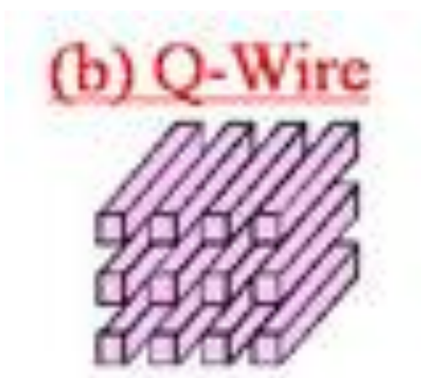
Quantum Well

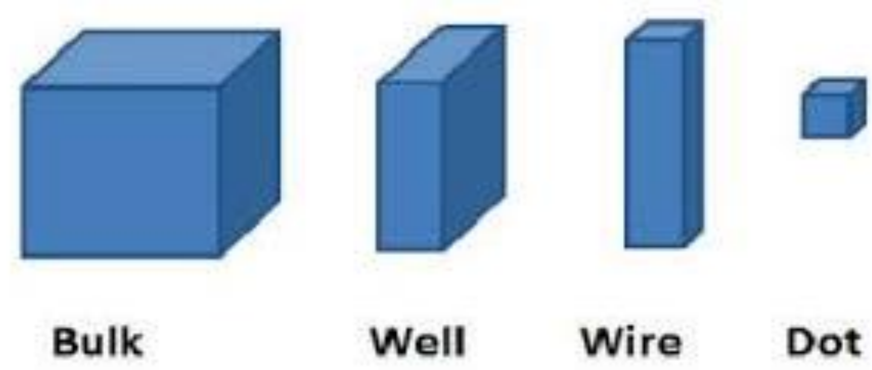




Quantum wire

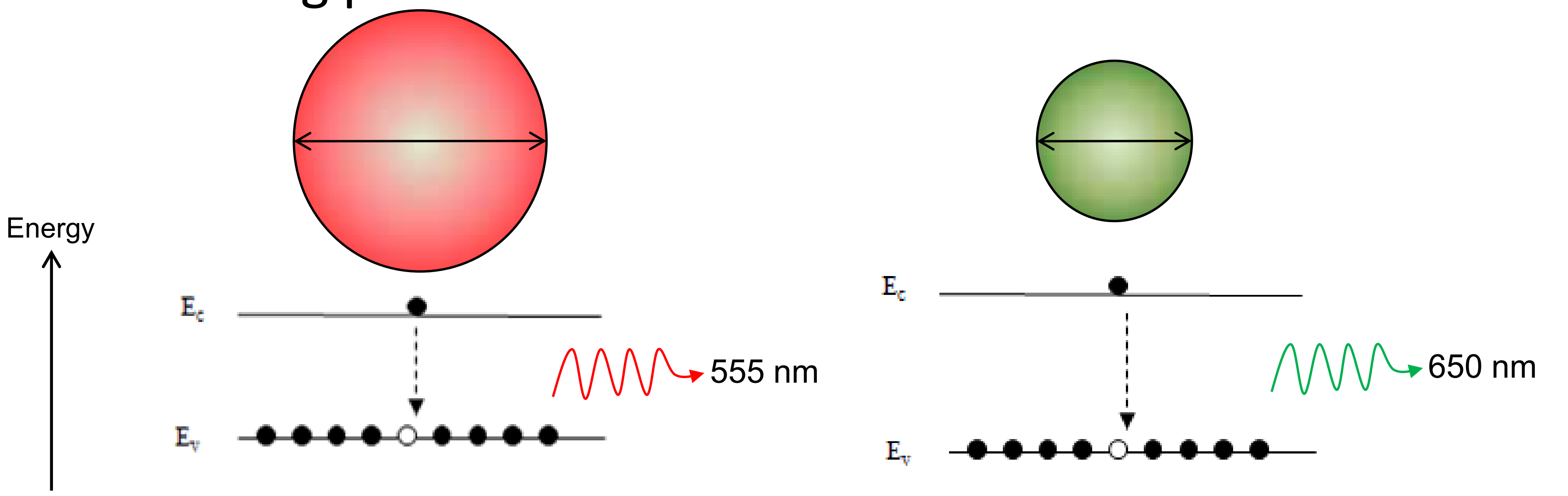
- Quantum effects in systems which confine electrons to regions comparable to their de Broglie wavelength.
- When such confinement occurs in two dimensions only (say, by two restrictions on the motion of the electron in the z- and y-directions), with free motion in the x-direction, a one dimensional electron is created.



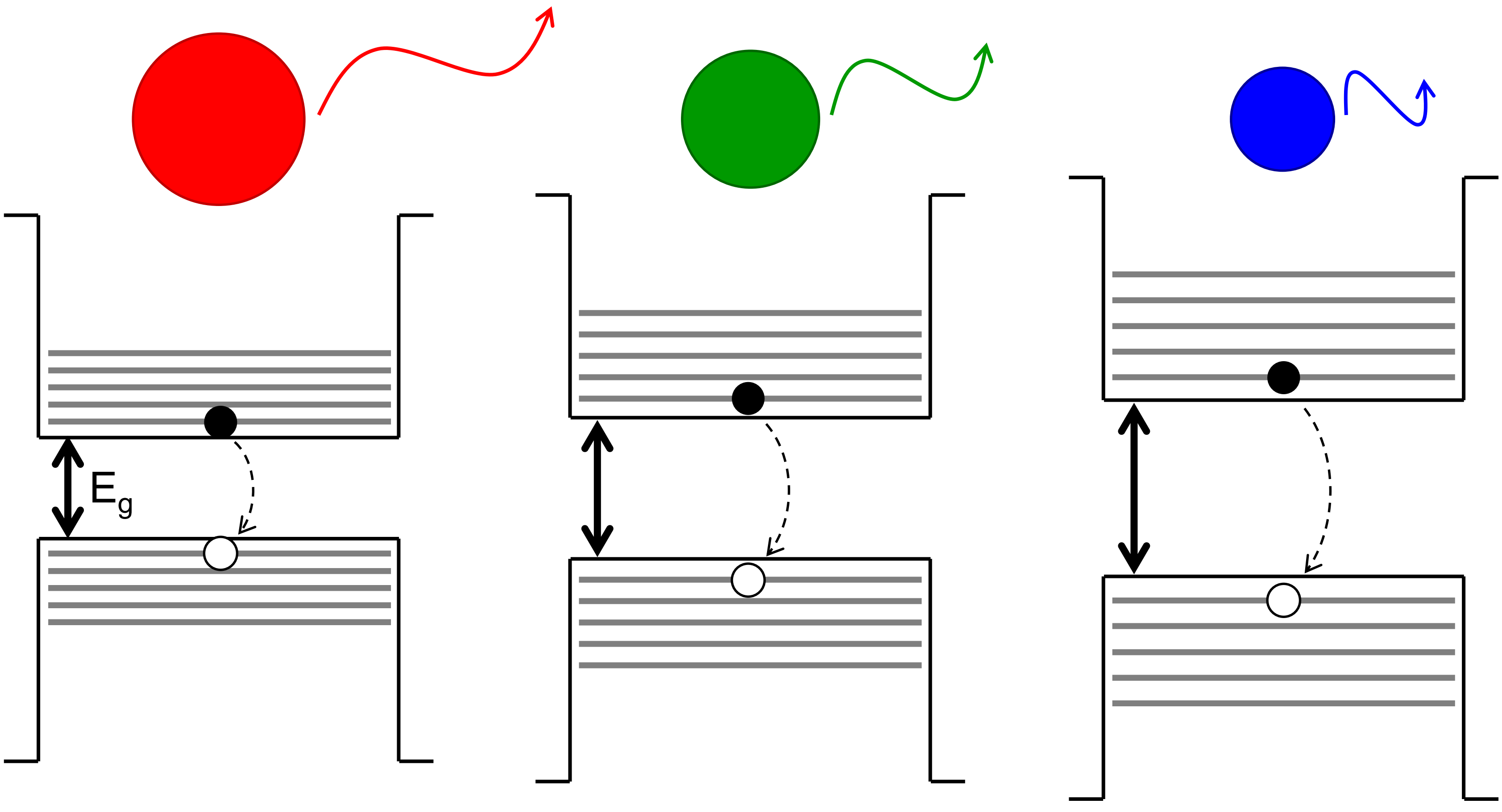


What does this mean?

- Quantum dots are bandgap tunable by size. We can engineer their optical and electrical properties.
- Smaller QDs have a large bandgap.
- Absorbance and luminescence spectrums are blue shifted with decreasing particle size.

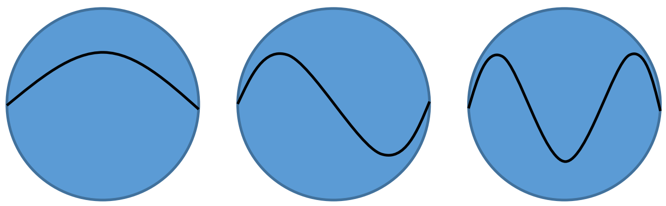


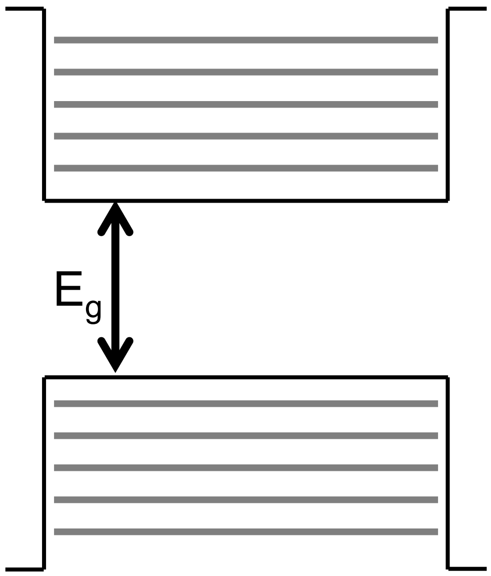
- Absorption and emission occur at specific wavelengths, which are related to QD size.



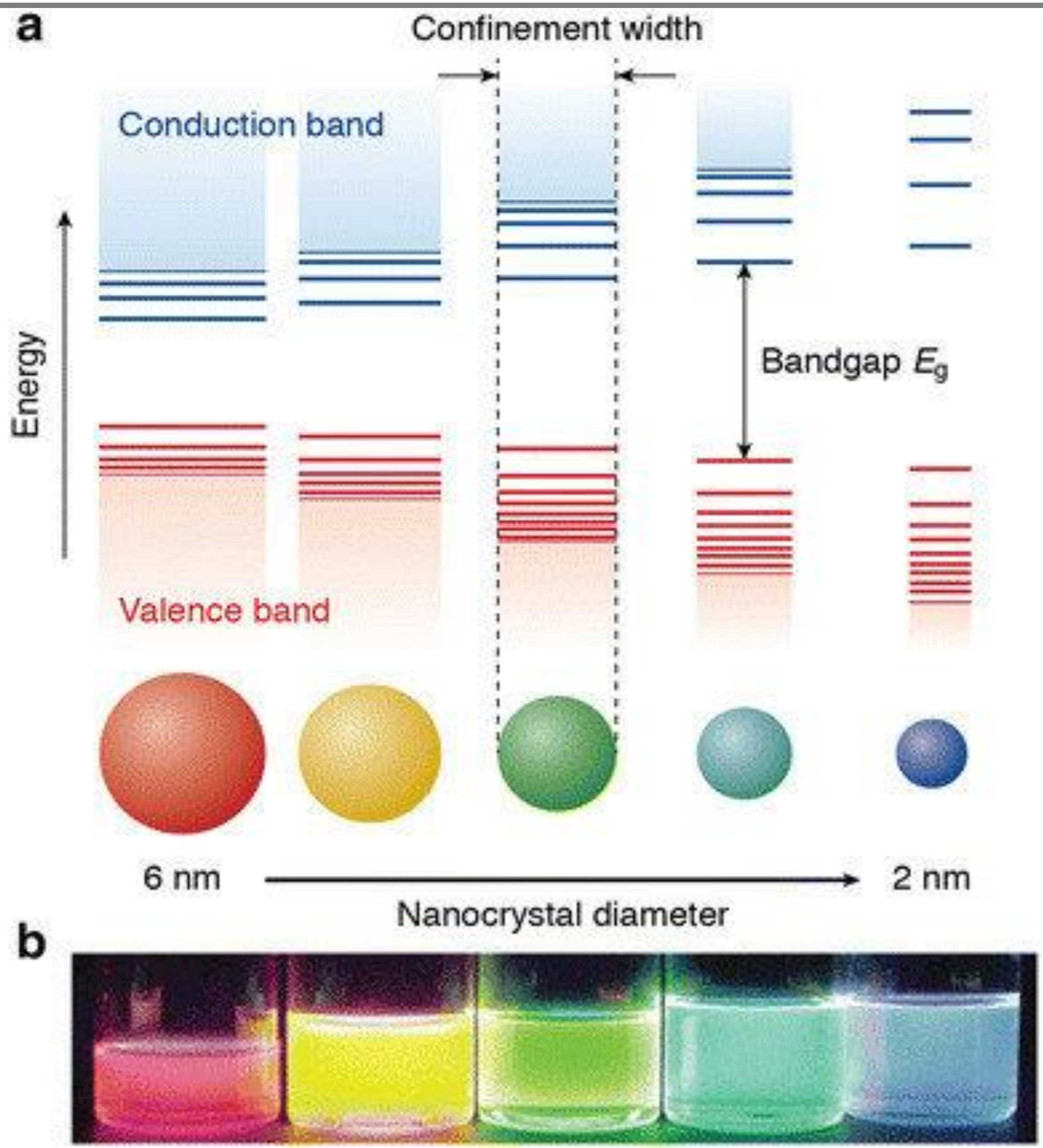
Quantum Dots

- Quantum dots are usually regarded as semiconductors by definition. Similar behavior is observed in some metals.
- Therefore, in some cases it may be acceptable to speak about metal quantum dots.
- Typically, quantum dots are composed of groups II-VI, III-V, and IV-VI materials.
- QDs are bandgap tunable by size which means their optical and electrical properties can be engineered to meet specific applications.
- Nanocrystals (2-10 nm) of semiconductor compounds
- Small size leads to confinement of excitons (electron-hole pairs)
- Quantized energy levels and altered relaxation dynamics
- Examples: CdSe, PbSe, PbTe, InP

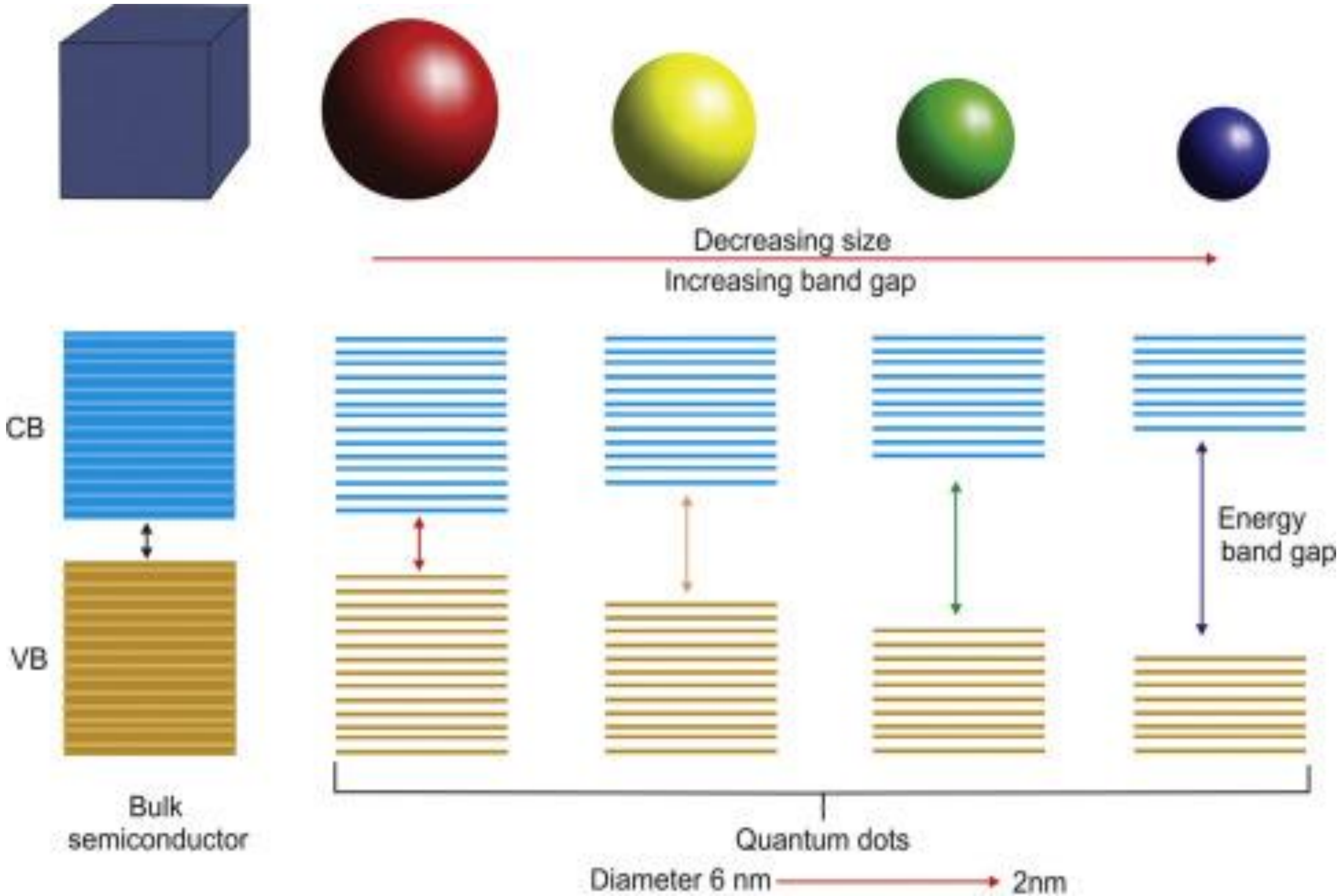




Quantum Dots

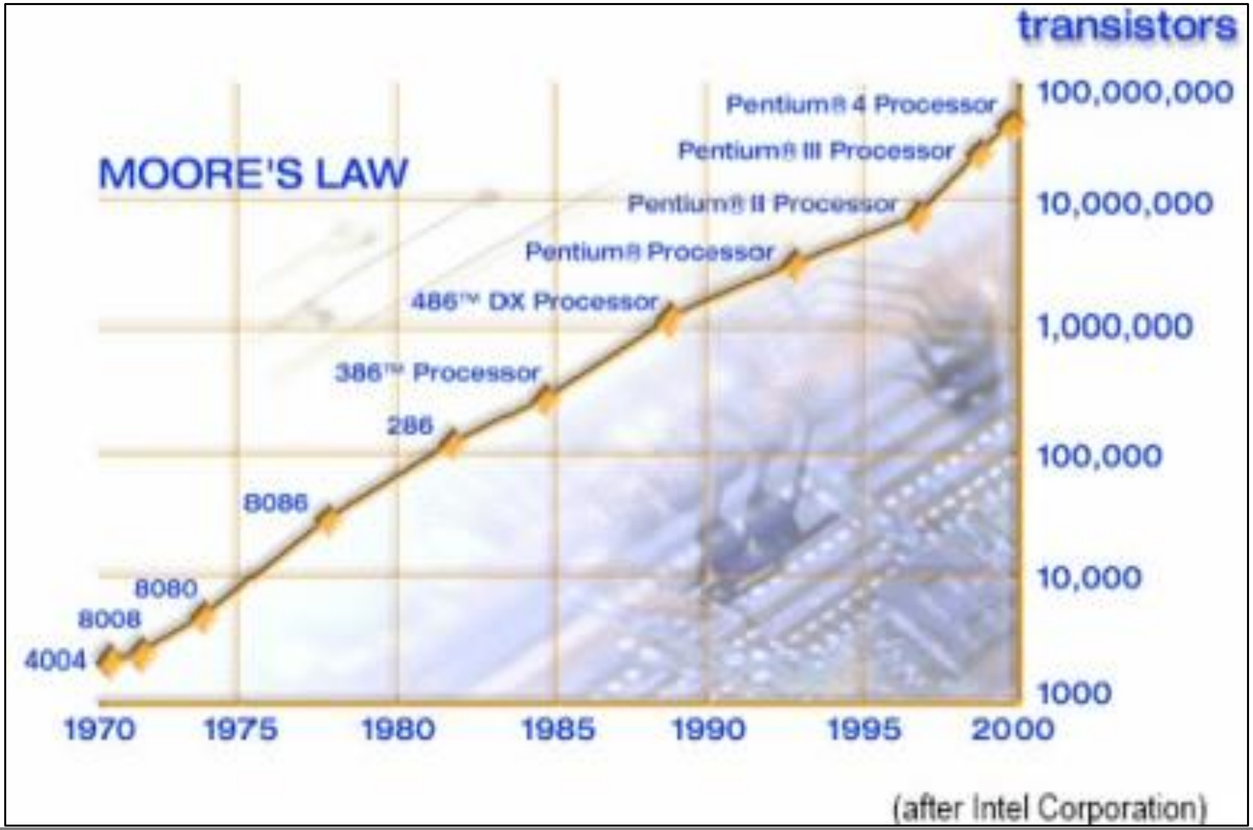


Quantum Dots

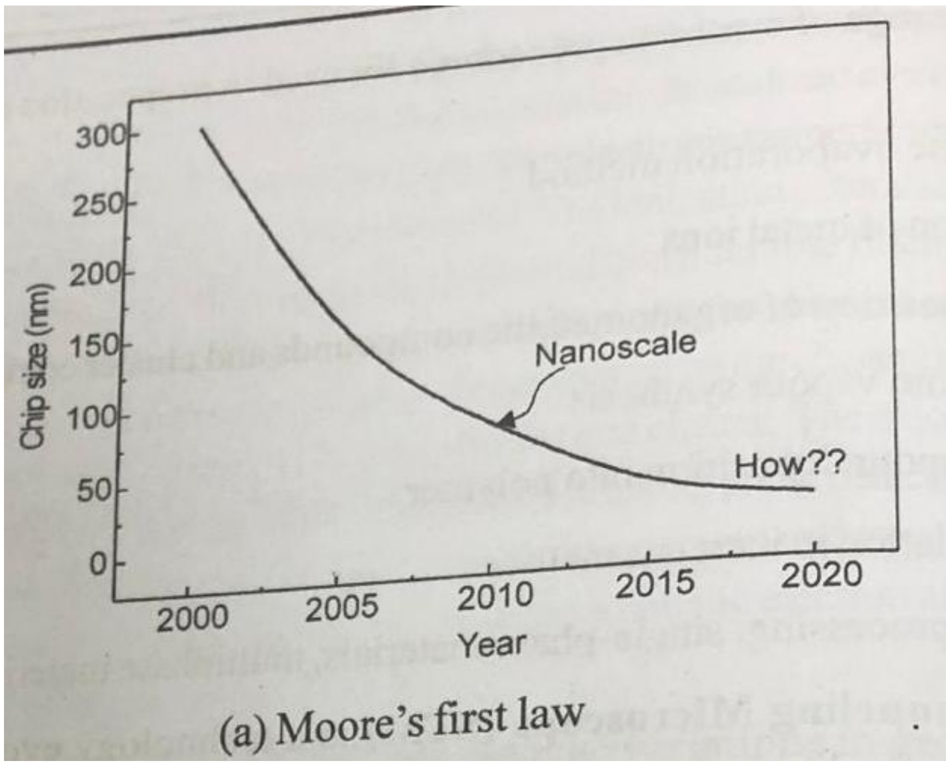


Moore’s Law

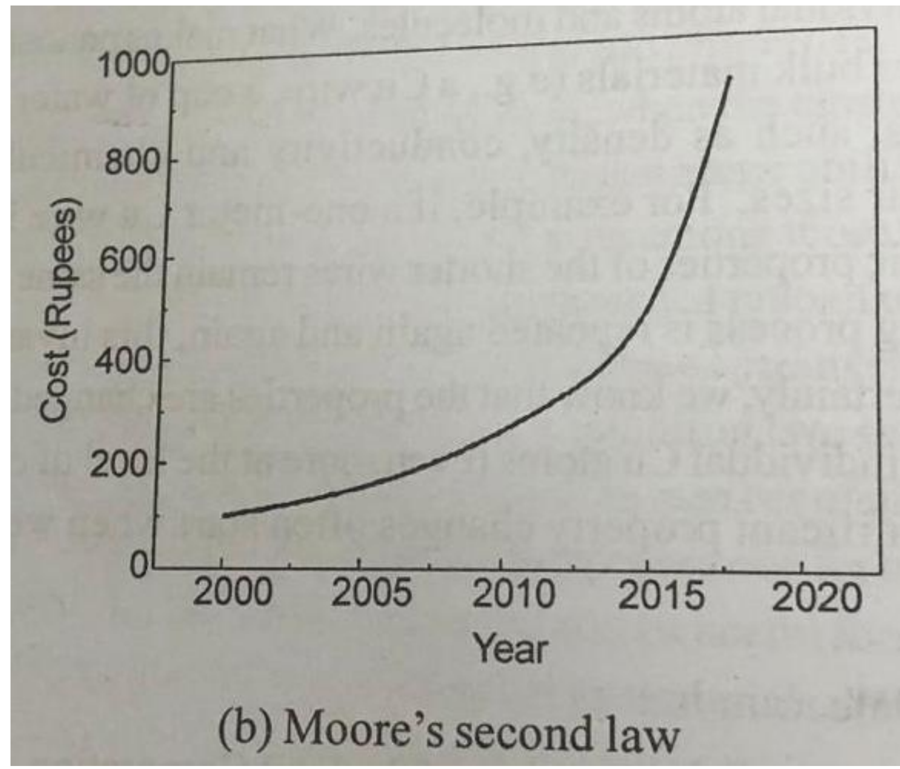
- The number of transistors on a chip will approximately double every 18 to 24nmonths (Moore’s Law).
- This law has given chip designers greater incentives to incorporate new features on silicon.
- Moore's Law works largely through shrinking transistors, the circuits that carry electrical signals.
- By shrinking transistors, designers can squeeze more transistors into a chip



- Moore's second law predicts that the cost of building a chip manufacturing plant doubles with every other chip generation or roughly every 36 months.



(a) Moore's first law



(b) Moore's second law