# *UNIT1*

# *Overview of Nano science and Engineering*

**Nanoscience** and **Nanoengineering** are interdisciplinary fields that involve the study, manipulation, and application of materials and devices at the nanoscale, typically within the range of 1 to 100 nanometers (nm).

## Nanoscience

Nanoscience focuses on understanding the fundamental principles and phenomena that occur at the nanoscale. It encompasses several disciplines including:

**Physics**: Investigates quantum mechanics and other phenomena that occur at the nanoscale.

**Chemistry**: Studies the chemical properties and reactions of nanomaterials.

**Biology**: Examines the interactions between nanoscale materials and biological systems.

## *Overview of Nano science and Engineering*

# Nanoengineering

**Nanoengineering**

Nanoengineering applies the principles of nanoscience to design and build materials and devices with novel properties and functions. It has applications across various industries:

**Electronics**: Development of nanoscale transistors, memory devices, and quantum computers.

**Medicine**: Creation of drug delivery systems, diagnostic tools, and nanoscale therapies.

**Energy**: Enhancement of solar cells, batteries, and supercapacitors through nanomaterials.

**Environmental**: Water purification, pollution control, and energy-efficient materials.

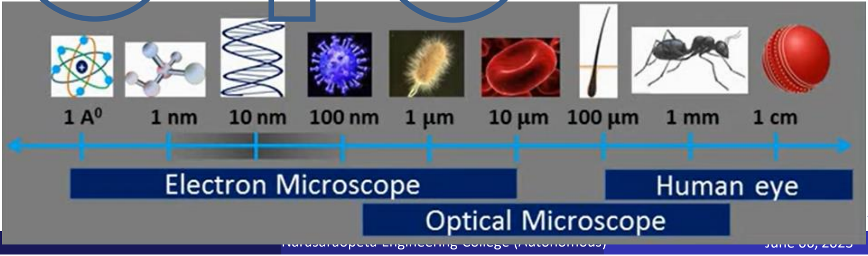
# Nano Electronics

Nano science → Nano Technology → Nano Electronics

Nano science : identification of physical and chemical properties

Nanotechnology is the term used to cover the design, construction and utilization of functional structures with at least one characteristic dimension measured in nanometers.

Nano Science + Nano Technology = Nano Electronics



# *Development Milestones in Microfabrication and the Electronic Industry*

## Early Developments in Microfabrication

**Content**:

1947: Invention of the transistor by John Bardeen, Walter Brattain, and William Shockley at Bell Labs.
1958: First integrated circuit (IC) developed by Jack Kilby at Texas Instruments.

# *Development Milestones in Microfabrication and the Electronic Industry*

Contd

## Photolithography

**Content**:

1960s: Introduction of photolithography, enabling the patterning of circuits on silicon wafers.
1970s: Advances in optical lithography techniques.

# *Development Milestones in Microfabrication and the Electronic Industry*

Contd..

## **Development of CMOS Technology**

**Content**:

1963: Invention of Complementary Metal-Oxide-Semiconductor (CMOS) technology by Frank Wanlass.

Widespread adoption due to low power consumption and high noise immunity.

## *Development Milestones in Microfabrication and the Electronic Industry*

Contd..

### Advancements in Semiconductor Manufacturing

**Content**:

1980s: Introduction of Very Large Scale Integration (VLSI) technology.

1990s: Development of Deep Submicron (DSM) technology.

# *Development Milestones in Microfabrication and the Electronic Industry*

Contd.

## Emergence of Nanofabrication

**Content**:

2000s: Transition to nanofabrication techniques.

Introduction of Extreme Ultraviolet Lithography (EUV) and FinFET transistors.

# *Development Milestones in Microfabrication and the Electronic Industry*

## Modern Microfabrication Techniques

**Content**:

Use of advanced materials such as graphene and carbon nanotubes. Techniques like Atomic Layer Deposition (ALD) and Electron Beam Lithography (EBL).

## *Development Milestones in Microfabrication and the Electronic Industry*

Contd..

### Key Applications in Electronics

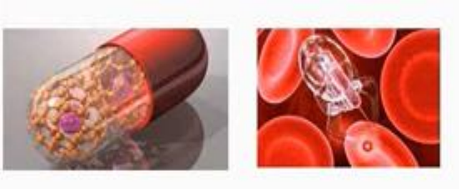
**Content**:

Microprocessors, memory devices, sensors, and MEMS (Micro-Electro-Mechanical Systems).

Impact on consumer electronics, medical devices, and telecommunications.

# Introduction (Contd.)

## Applications of Nano Technology



### 1. Medicines

- ✓ Targeted drug delivery
- ✓ Reduce side effects
- ✓ Early diagnosis of

### 2. In Electronics

- ✓ Reduced power consumption
- ✓ Less size and weight of components
- ✓ Smaller and fast processors

# Introduction (Contd.)

## Applications of Nano Technology

### 3. Automobiles

✓ High strength of metal

✓ Increased fuel efficiency

✓ Quality of paints

### 4. Environmental

✓ Sensor detecting pollution level

✓ Harmful emission can be controlled

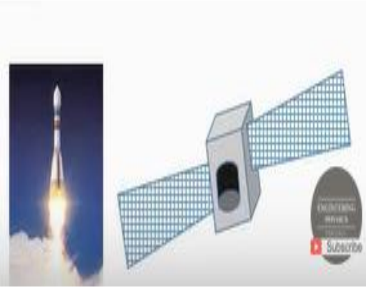
✓

# Introduction (Contd.)

## Applications of Nano Technology

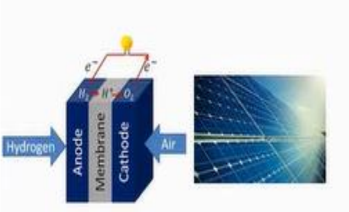
### 5. In Space Technology

- ✓ Light weight spacecraft
- ✓ Reduction in rocket fuel
- ✓ Large material strength



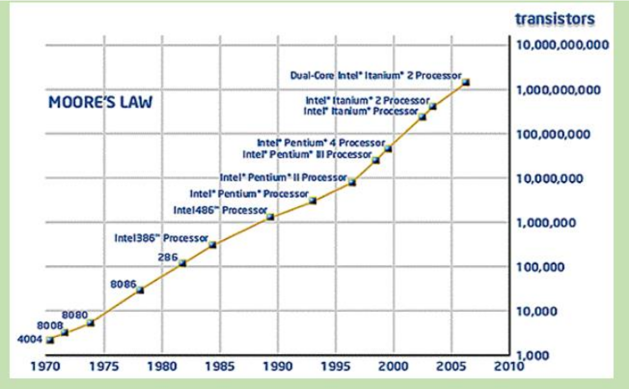
### 6. In Energy

- ✓ Reduced cost of catalysts in fuel cell
- ✓ Can increases efficiency of solar cell



# Moore’s Law

- Moore’s Law is a phenomenological observation that the number of transistors on integrated circuits doubles every two years, as shown in Figure.



Moore’s Law

# Nano Structures

Nano structure : Geometrical entity with a different shape having Nano scale dimensions(s)

Examples:

3D confinement

- Fullerenes
- Colloidal particles
- Nanoporous silicon
- Activated carbons
- Semiconductor particles in a glass matrix for non-linear optical components
- Semiconductor quantum dots (self-assembled and colloidal)
- Quasi-crystals

2D confinement

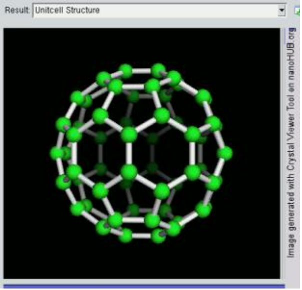
- Carbon nanotubes and nanofilaments
- Metal andmagnetic nanowires
- Oxide and carbide nanorods
- Semiconductor quantum wires

1D confinement

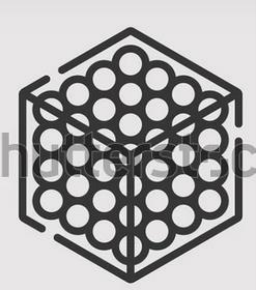
- Nanolaminated or compositionally modula materials
- Grain boundary films
- Clay platelets

# Example of Nano Structures

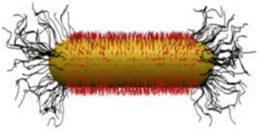
Fullerene



Nano crystals



Nano rods



It is called $C_{60}$ molecule si. It has multiple number of pentagons and hexagons. It looks like a soccer ball. It is range “nm”.

# *Electronic Properties of Atoms and solids:*

**To understand effects of dimensionality in Nano systems,** it is useful to review certain topics associated with constitution of matter, ranging from the structure of the isolated atoms through to that of an extended solid

- Isolated Atom
- Bonding between Atoms
- Giant Molecular solids
- Free Electron Models and Energy Bands
- Periodicity of crystal lattices
- Electronics Conduction

# Isolated Atom

## Evolution of atomic Models

The understanding and manipulation of the atomic level have evolved significantly over the years through various scientific discoveries and technological advancements. Here's a brief overview of the evolution of atomic-level shown in Figure 3:

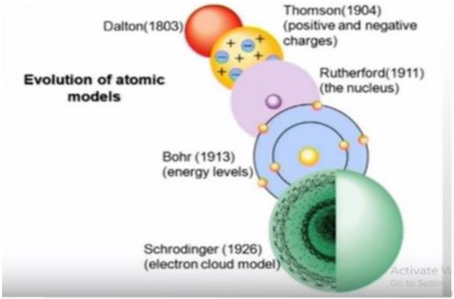


Figure1 : Evolution of Atom

# Bohr’s Model

The structure of the atom arises as a direct result of the wave–particle duality of electrons, which is summarized in the de Broglie relationship,

$$\lambda = \frac{\mathrm{h}}{m_e v} \tag{1}$$

where $\lambda$ is the (electron) wavelength, me is the $me$ (electron) mass $v$ is the velocity and $h$ = 6.63 × 10−34$J$ is the Planck constant.

V.V.IMP Point : The wave–particle duality of the electron means that an electron behaves both as a wave (i.e., it is extended over space and has a wavelength and hence undergoes wave-like phenomena such as diffraction) and a particle (i.e., it is localized in space and has a position, a velocity and a kinetic energy).

Using these ideas we come to our first model of the atom, the Rutherford–Bohr model. Here the small central nucleus of the atom consists of positively charged protons and (neutral) neutrons. Electrons orbit the nucleus in stable orbits.

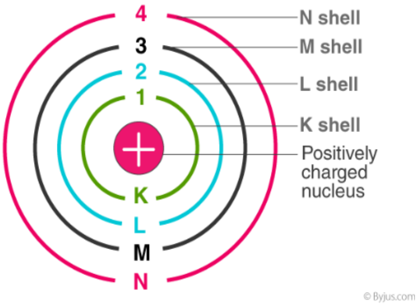
The allowed, stable orbits are those in which the electron wavelength, given by the de Broglie formula, is an

$$2\pi r = \eta\lambda = \frac{nh}{m_e v}$$

This implies that

$$m_e v\mathrm{r} = \frac{nh}{2\pi}$$

# Bohr’s Model



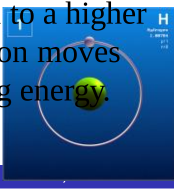
Bohr’s Model of an Atom

Bohr’s model consists of a small nucleus (positively charged) surrounded by negative electrons moving around the nucleus in orbits. Bohr found that an electron located away from the nucleus has more energy, and the electron which is closer to nucleus has less energy

# Isolated Atom

## Postulates of Bohr’s Model of an Atom

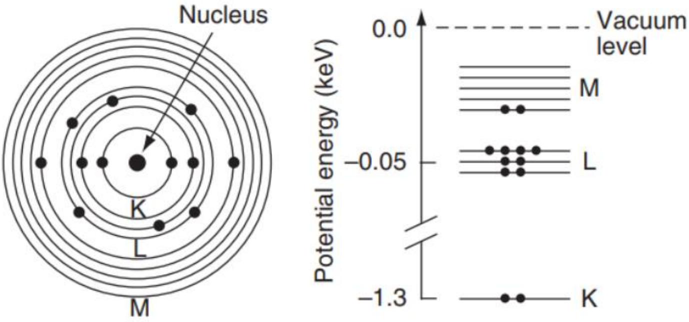
1. In an atom, electrons (negatively charged) revolve around the positively charged nucleus in a definite circular path called orbits or shells.
2. Each orbit or shell has a fixed energy and these circular orbits are known as orbital shells.
3. The energy levels are represented by an integer (n=1, 2, 3…) known as the quantum number. This range of quantum number starts from nucleus side with n=1 having the lowest energy level. The orbits n=1, 2, 3, 4… are assigned as K, L, M, N…. shells and when an electron attains the lowest energy level, it is said to be in the ground state.
4. The electrons in an atom move from a lower energy level to a higher energy level by gaining the required energy and an electron moves from a higher energy level to lower energy level by losing energy.



# *Isolated Atom*

## Example : Mg atom

Such a simplified picture of the structure of an isolated Mg atom and the associated energy level diagram are shown in Figure 4.



# *Isolated Atom*

A much more sophisticated model of the atom considers the **wave-like nature of the electrons** from the very beginning. This uses wave **mechanics or quantum mechanics**.

- Here each electron is described by a wave function $\psi$ which is a function of spatial position (x,y,z) and, in general, of time. Physically $|\psi|^2$ represents the probability of finding the electron at any point.

- To work out the energy of each electron, we need to solve the Schro¨dinger equation which, in the time-independent case, takes the form

$$-\frac{\hbar^2}{2m_e}\nabla^2\psi + V(x,y,z)\psi = E\psi\,, \tag{1.3}$$

where V(x,y,z) describes the potential energy function in the environment of the electron. Solution of the Schro¨dinger equation, under certain boundary conditions, leads to a set of solutions for the allowed wave functions n of the atomic electrons together with their associated energies En

# Isolated Atom

The allowed wavefunctions form the electron orbitals, which we term 1s, 2s, 2p, 3s, 3p, 3d, etc. (here 1, 2, 3, ... are alternative labels for K, L, M, ...). These allowed wavefunctions now depend on not just one quantum number but four: n, l, m and s. **These numbers may be summarized as follows:**

**n** is the principal quantum number; it is like the quantum number used for the case of Bohr shells (n = 1, 2, 3, ... ).

l is the angular momentum quantum number; it can vary from l = 0, 1, 2, ... , (n-1). The value of l governs the orbital shape of the subshell: l=0 is an s orbital, which is spherical; l = 1 is a p orbital, which has a dumbbell shape; while l = 2 is a d orbital, which has a more complex shape such as a double dumbbell. .

**m** is the magnetic quantum number; it can vary from 0, $\pm 1, \ldots \ldots \ldots \pm l$. The value of m governs the spatial orientation of the different orbitals within a subshell; i.e., there are three p orbitals (l = 1) px, py, and pz corresponding to the three values of m which are 0, $+1$ and $-1$. In the absence of a magnetic field, all these orbitals within a particular subshell will have the same energy.

**s** is the spin quantum number which, for an electron, can take the values $\pm\frac{1}{2}$. Each (n, l, m) orbital can contain two electrons of opposite spin due to the Pauli exclusion principle, which states that no two electrons can have the same four quantum numbers.

# Bonding Between Atoms

One way to picture the bonding between atoms is to use the concept of Molecular Orbital (MO) Theory

- MO theory considers the electron wavefunctions of the individual atoms combining to form molecular wavefunctions (or molecular orbitals as they are known).

- A simple one-electron molecule is the $h_2^+$ ion, where we have to consider the interactions (both attractive and repulsive) between the single electron and two nucleii.

# Bonding Between Atoms

Contd..

- For the $h_2^+$ion, the two lowest-energy solutions are known as $1s\sigma_g$ and$1s\sigma_u$. Here 1s refers to the original atomic orbitals; the subscripts g and u refer to whether the MO is either symmetrical or non-symmetrical with respect to inversion about a line drawn between the nucleii (viz. an even or odd mathematical function). This is shown in figure 1.3

- As can be seen the **electron density** is concentrated between the nuclei for the $1s\sigma_g$ MO, which is known as a bonding orbital since the energy of the molecular wavefunction is lower (i.e., more stable) than the corresponding isolated atomic wavefunctions.

- Conversely, the **electron density** is diminished between the nuclei for$1s\sigma_u$, which is known as an antibonding orbital since the energy of the molecular wavefunction is higher (i.e., less stable) than the corresponding isolated atomic wavefunction

# Bonding Between Atoms

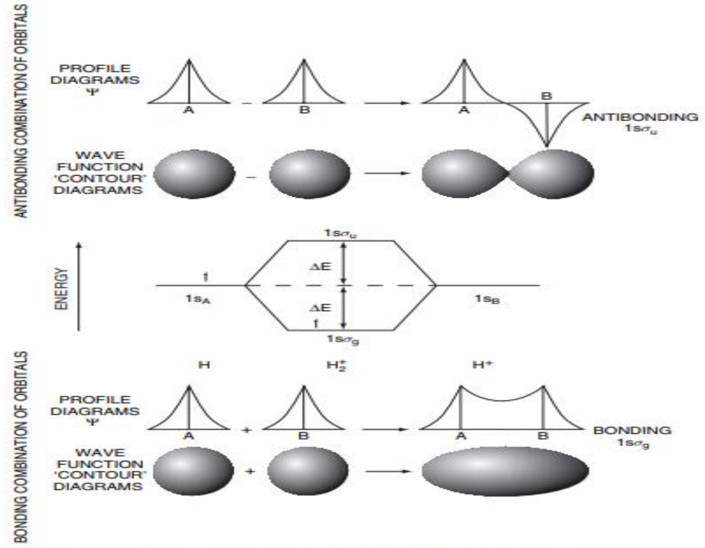


**Figure 1.3** Molecular orbital description and energy level diagram for an $H_2^+$ ion

# Bonding Between Atoms

Contd..

we can then construct a set of molecular orbitals from a linear combination of atomic orbitals (LCAO).

For instance, as shown in Figure 1.4, the $1s\sigma_g$ bonding MO is formed from the in-phase overlap (i.e., addition) of two 1s atomic orbitals, whereas the $1s\,\sigma_u$ anti-bonding MO is formed from the out of-phase overlap (i.e., subtraction) of two 1s atomic orbitals.

Similar considerations apply to overlap of **p** orbitals, although now these may form both $\sigma$ and $\pi$ bonding and antibonding Mos

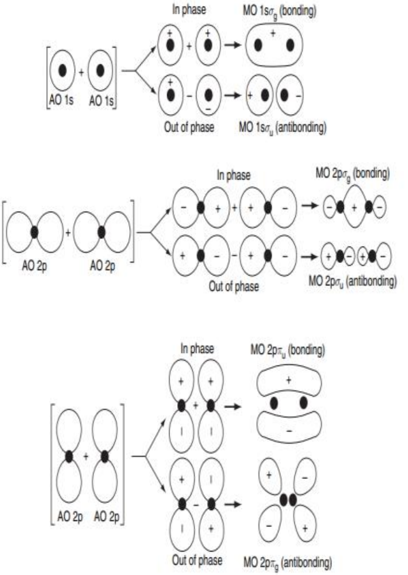


**Figure 1.4** Formation of molecular orbitals from a linear combination of atomic orbitals; the + and − signs indicate the signs (phases) of the wavefunctions

# *Giant molecular solids*

- When atoms come into close proximity with other atoms in a solid, most of the electrons remain localized and may be considered to remain associated with a particular atom.

- However, some outer electrons will become involved in bonding with neighbouring atoms.

- . Upon bonding the atomic energy level diagram is modified. Briefly, the well-defined outer electron states of the atom overlap with those on neighbouring atoms and become broadened into energy bands

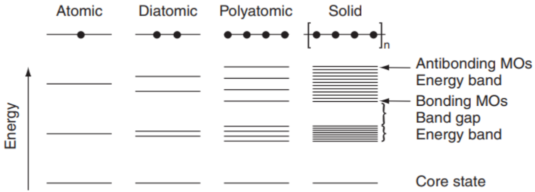


**Figure 1.5** Electron energy level diagram for a progressively larger linear chain of atoms showing the broadening of molecular orbitals into energy bands for a one-dimensional solid

# *The free electron model and energy bands*

Contd..

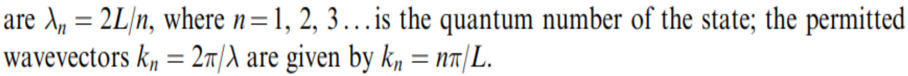
- the free electrons in metals quantum mechanically and consider their wave-like properties

- Here the free valence electrons are assumed to be constrained within a potential well which essentially stops them from leaving the metal (the ‘particle-in-a-box’ model).

- The box boundary conditions require the wavefunctions to vanish at the edges of the crystal (or ‘box’)

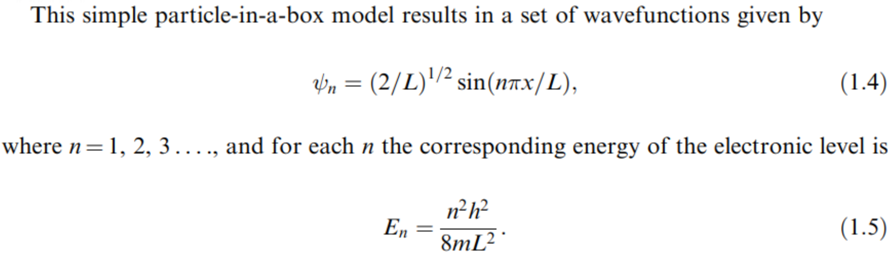
- The allowed wave functions given by the Schrödinger equation then correspond to certain wavelengths as shown in Figure 1.6.

- For a one-dimensional box of length L, the permitted wavelengths are $\lambda_n$= 2L/n,



are $\lambda_n = 2L/n$, where $n = 1, 2, 3 \ldots$ is the quantum number of the state; the permitted wavevectors $k_n = 2\pi/\lambda$ are given by $k_n = n\pi/L$.

# The free electron model and energy bands

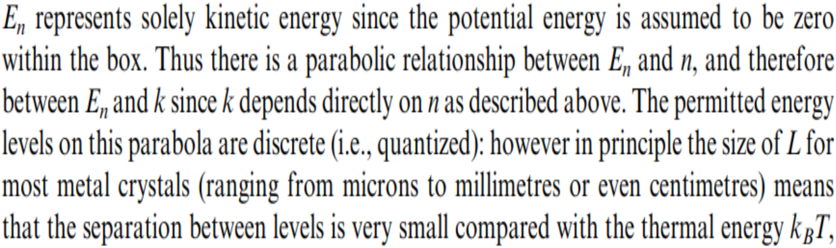


This simple particle-in-a-box model results in a set of wavefunctions given by

$$\psi_n = (2/L)^{1/2} \sin(n\pi x/L), \tag{1.4}$$

where $n = 1, 2, 3 \ldots.$, and for each $n$ the corresponding energy of the electronic level is

$$E_n = \frac{n^2 h^2}{8mL^2}. \tag{1.5}$$



$E_n$ represents solely kinetic energy since the potential energy is assumed to be zero within the box. Thus there is a parabolic relationship between $E_n$ and $n$, and therefore between $E_n$ and $k$ since $k$ depends directly on $n$ as described above. The permitted energy levels on this parabola are discrete (i.e., quantized): however in principle the size of $L$ for most metal crystals (ranging from microns to millimetres or even centimetres) means that the separation between levels is very small compared with the thermal energy $k_B T$,

# The free electron model and energy bands

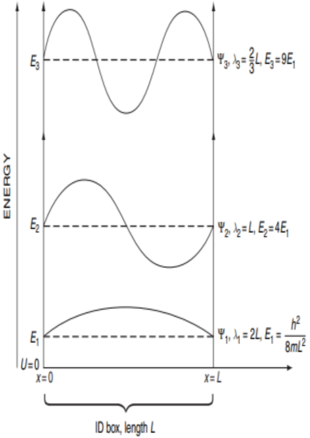


**Figure 1.6** Energy level diagram also showing the form of some of the allowed wavefunctions for an electron confined to a one-dimensional potential well

Note that as the electron becomes more localized (i.e., $L$ decreases), the energy of a particular electron state (and more importantly the spacing between energy states) increases; this has important implications for bonding and also for reduced-dimensionality or quantum-confined systems which are discussed later.

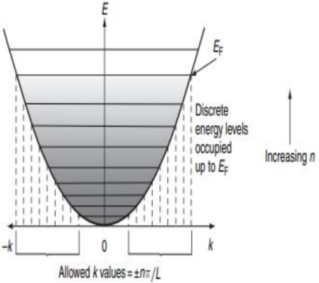


**Figure 1.7** Schematic version of the parabolic relationship between the allowed electron wave vectors and the their energy for electrons confined to a one-dimensional potential well. Shaded energy regions represent those occupied with electrons

# *Electron Conduction*

Figure 1.10 shows schematic energy diagrams for insulators, metals and semiconductors respectively

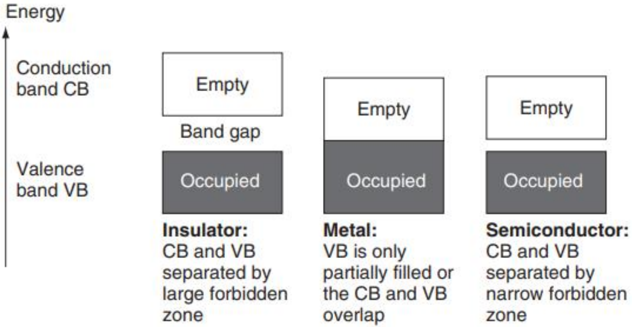


**Figure 1.10** Electron energy band diagram for an insulator, a conductor and a semiconductor

# *Electron Conduction*

**Metals:** Metals are highly conductive materials. They have a large number of free electrons that are loosely bound to their atomic nuclei. These free electrons can move easily throughout the material, facilitating the flow of electric current. Metals typically have high electrical conductivity and low electrical resistivity. Examples of metals include copper, aluminum, and gold.

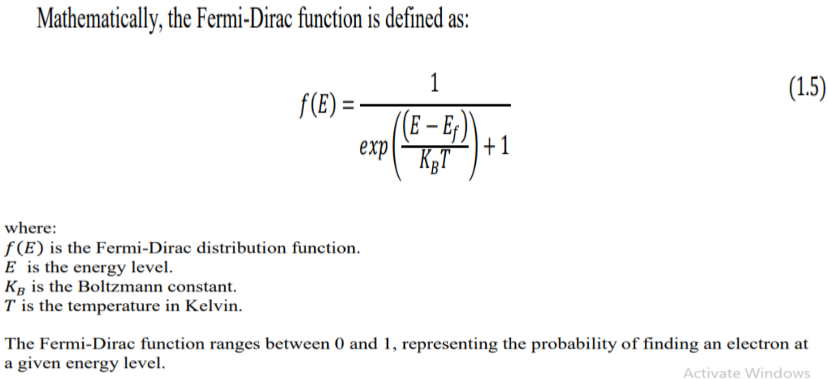
**Semiconductors:** Semiconductors have intermediate conductivity compared to metals and insulators. They have a partially filled valence band, which means that some electrons are free to move. However, their conductivity is relatively low at room temperature compared to metals. The conductivity of semiconductors can be significantly increased by introducing impurities or by applying external influences such as temperature or electric fields. This process is known as doping. Semiconductors are crucial in electronic devices such as transistors and diodes. Silicon and germanium are commonly used semiconducting materials.

**Insulators:** Insulators are materials with very low conductivity. They have a completely filled valence band, which means that electrons are tightly bound to their atomic nuclei and cannot move freely. Insulators have high electrical resistivity and do not conduct electricity easily. Examples of insulators include rubber, glass, and wood. However, it's important to note that under certain conditions, insulators can exhibit some degree of conductivity, although it is significantly lower compared to metals or semiconductors

# Electron Conduction

**Fermi-Dirac function**: The Fermi-Dirac function is used to describe the probability of finding an electron at a particular energy level in a system that obeys Fermi-Dirac statistics. These statistics account for the exclusion principle, which states that no two identical fermions (particles with half-integer spin, such as electrons) can occupy the same quantum state simultaneously.

Mathematically, the Fermi-Dirac function is defined as:



Mathematically, the Fermi-Dirac function is defined as:

$$f(E) = \frac{1}{exp\left(\frac{(E - E_f)}{K_B T}\right) + 1} \qquad (1.5)$$

where:
$f(E)$ is the Fermi-Dirac distribution function.
$E$ is the energy level.
$K_B$ is the Boltzmann constant.
$T$ is the temperature in Kelvin.

The Fermi-Dirac function ranges between 0 and 1, representing the probability of finding an electron at a given energy level.

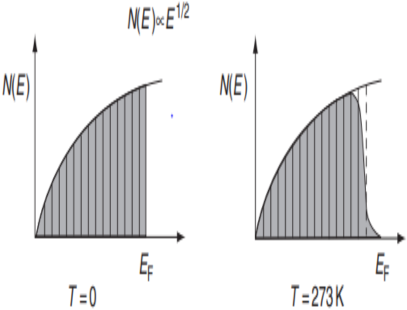


**Figure 1.11** The density of electron states for free electrons and the occupation of electron energy levels (shaded region) at zero and room temperature

# *Effects of nanometer length scale*

The effects of the nanometre length scale are profound and **significant across various fields, including physics, chemistry, biology, and materials science**. Here are some of the key effects:

1. Quantum Effects

•**Quantum Confinement**: At the nanometre scale, the behavior of electrons is governed by quantum mechanics. Electrons are confined in small spaces, which quantizes their energy levels. This is prominent in quantum dots, where the electronic properties can be tuned by changing the size of the dots.

•**Tunneling**: At nanoscale distances, electrons can tunnel through barriers, a phenomenon that is not significant at larger scales. This is the principle behind scanning tunneling microscopy (STM) and certain types of transistors.

## 2. Surface Area to Volume Ratio

**Increased Surface Area**: Nanomaterials have a high surface area to volume ratio, which significantly affects **their physical and chemical properties**

# *Effects of nanometer length scale*

### 3. Mechanical Properties

•**Strength and Elasticity**: Materials at the nanoscale often exhibit enhanced mechanical properties. Nanowires and nanotubes, for example, can have significantly higher tensile strength and elasticity compared to their bulk counterparts.

•**Defects and Grain Boundaries**: The small size of nanoparticles means fewer defects and grain boundaries, which can improve the material's mechanical properties.

### **4.** Optical Properties

•**Plasmonics**: Nanoparticles of metals like gold and silver can exhibit surface plasmon resonance, where conduction electrons on the surface oscillate in resonance with incident light. This leads to unique optical properties, useful in sensors and imaging.

•**Quantum Dots**: Due to quantum confinement, quantum dots can emit light of specific wavelengths based on their size, leading to applications in displays, bioimaging, and photovoltaics.

# Effects of nanometer length scale

Contd

## 5. Electrical Properties

**Conductivity**: Nanomaterials can exhibit different electrical properties compared to their bulk forms. For instance, carbon nanotubes can be either metallic or semiconducting depending on their chirality and diameter.

**Electron Mobility**: Reduced dimensions can lead to high electron mobility, which is beneficial in the development of high-speed electronic devices.

## 6. Thermal Properties

**Thermal Conductivity**: The thermal conductivity of nanomaterials can be significantly different from their bulk counterparts. For example, carbon nanotubes have very high thermal conductivity along their length but lower across their diameter.

**Thermal Stability**: Nanomaterials can exhibit enhanced thermal stability due to their size and the absence of defects.

# Effects of nanometer length scale

## 7. Magnetic Properties

**Superparamagnetism**: At the nanoscale, ferromagnetic materials can become superparamagnetic, where they exhibit magnetism only in the presence of an external magnetic field and do not retain magnetization in its absence. This property is useful in applications like magnetic resonance imaging (MRI) contrast agents and data storage.

## 8. Chemical Reactivity

**Enhanced Reactivity**: The high surface area and the presence of more reactive surface atoms lead to enhanced chemical reactivity, making nanomaterials ideal for catalysis.

**Stability and Self-Assembly**: Nanoparticles can exhibit unique behaviors like self-assembly into ordered structures, which can be utilized in creating novel materials and devices.

## 9. Biological Interactions

**Biocompatibility**: Nanomaterials can interact with biological systems in unique ways, leading to applications in drug delivery, imaging, and diagnostics.

**Cellular Interactions**: Due to their small size, nanoparticles can enter cells easily, facilitating targeted drug delivery and molecular imaging.

## Conclusion

The nanometre length scale brings about a range of unique and tunable properties that are not present in bulk materials. These effects enable the development of new technologies and enhance existing ones, spanning across various scientific and engineering disciplines.

# *Thank You*

# *Thank You*