Electronic Structures Of Quantum Wells(2d) Quantum Wires(1d) And Quantum Dot(0d) And Van Hove Singularities.

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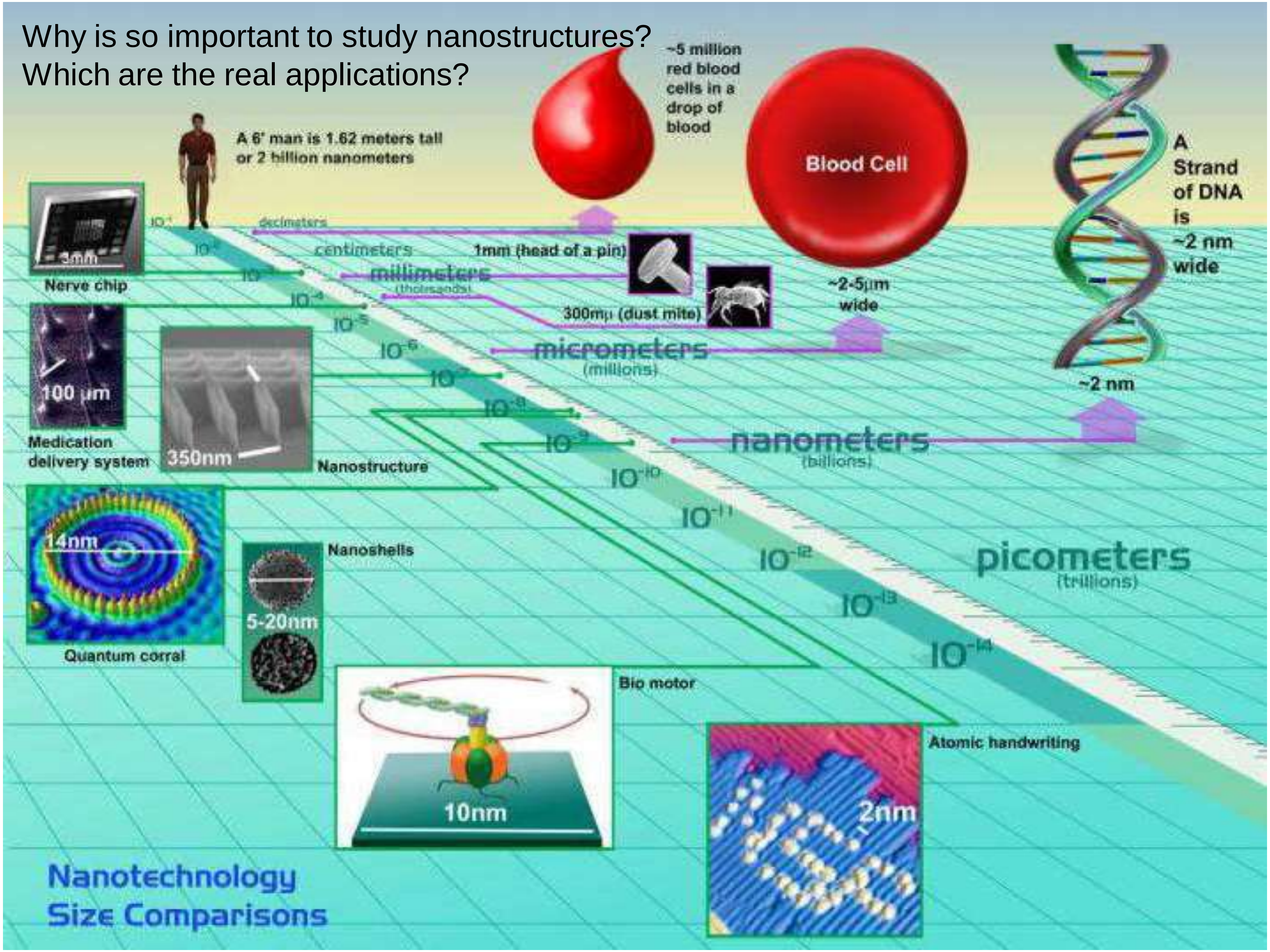
OUTLINE

Introduction
Quantum Confined Systems
Quantum Wells
Quantum Wires Qws (Nanotubes, Nanowires, Nanorods)
Quantum Dots Qds
Heterostructures

Why is so important to study nanostructures?
Which are the real applications?



Size-Dependent Properties

At the nanometer scale, properties become size-dependent.

For example,

(1) Thermal properties – melting temperature
(2) Mechanical properties – adhesion, capillary forces
(3) Optical properties – absorption and scattering of light
(4) Electrical properties – tunneling current
(5) Magnetic properties – superparamagnetic effect

→ New properties enable new applications

Some Applications

- Electronic (Molecular Electronics)
- Optoelectronics
- Magnetic Storage
- Catalysis
- Energetic: Solar Cells
- Energetic: Energy Harvesting
- Medical
  (Labeling Of Biomolecules For Imaging And Biosensing; Delivering Of Drugs)

Quantum Confined Systems

Quantum Mechanical Effects

1-D Time-independent Schrödinger Equation:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dz^2}+V\psi = E\psi$$

(1) Quantization of energy levels in wells

(2) Tunneling through barriers

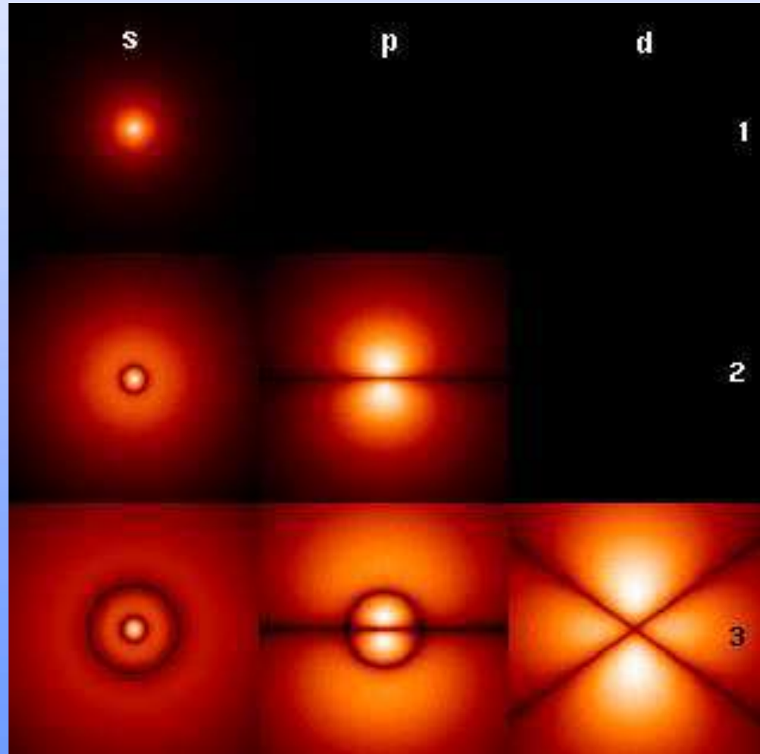
→ When heterostructures are monolayers thick, atomic level defects have a serious impact

Atomic Wavefunctions

Discrete Levels Of Energy

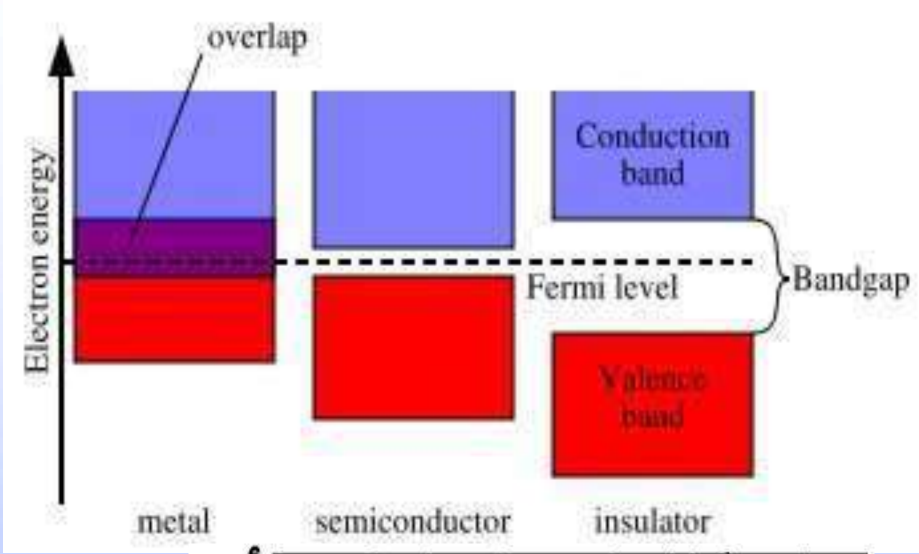
$$E_n = -\left(\frac{Z^2 \mu e^4}{32\pi^2 \epsilon_0^2 \hbar^2}\right)\frac{1}{n^2}$$

orbitals

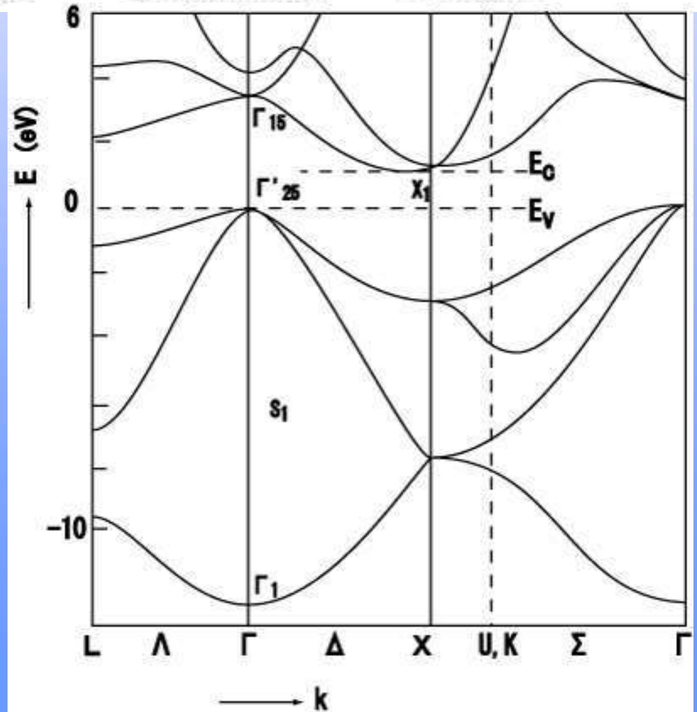


from Atoms to Solids….

Delocalized electronic states continuum of energies

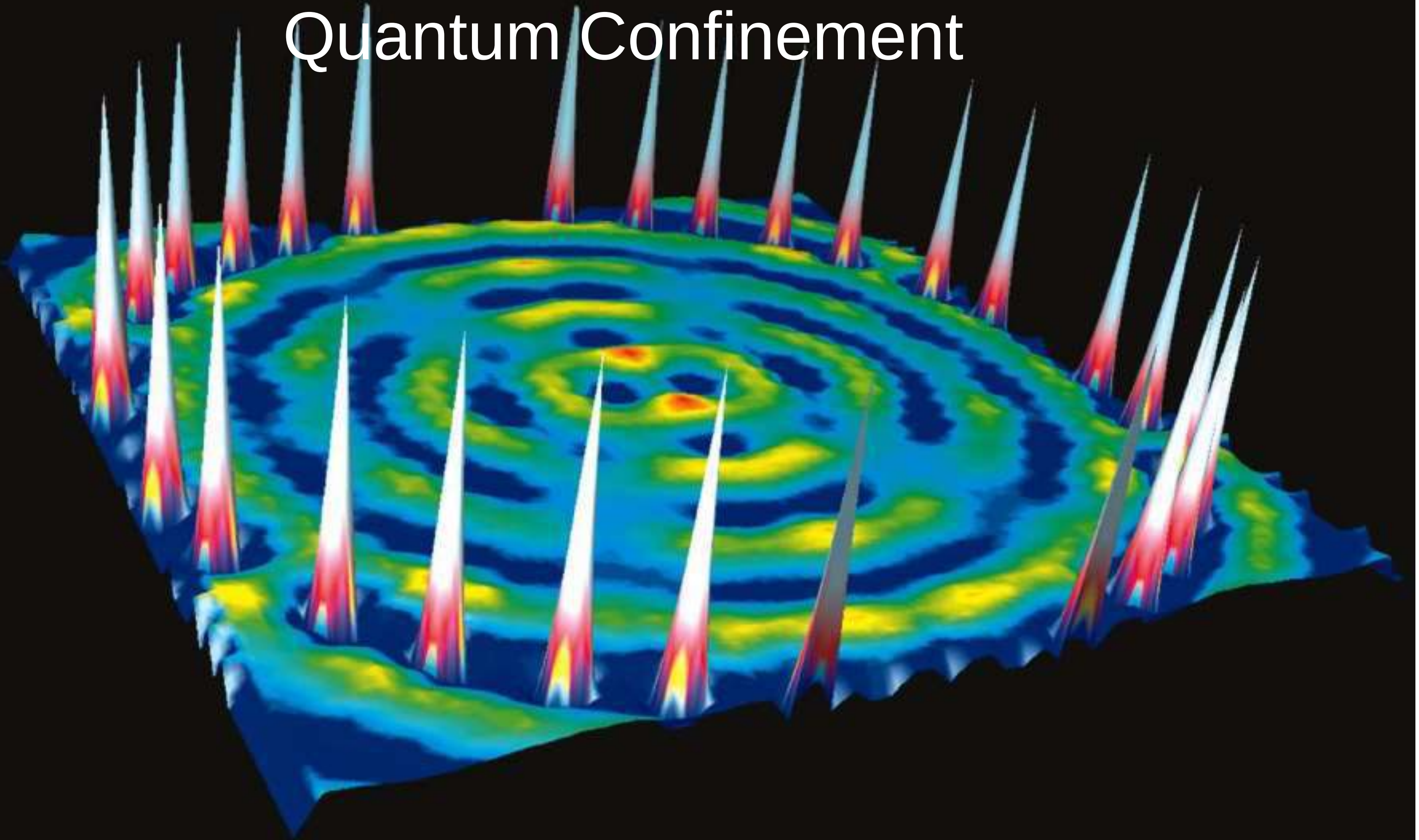


If several atoms are brought together into a molecule, their atomic orbitals split like in a coupled oscillation. This produces a number of molecular orbitals proportional to the number of atoms. In solids, there are so many atoms that the difference in energy between them becomes very small, so the levels form *bands* of energy rather than the discrete energy levels of The isolated atoms



The energy of the bands depends on the propagation direction of the electron in the solid

Quantum Confinement

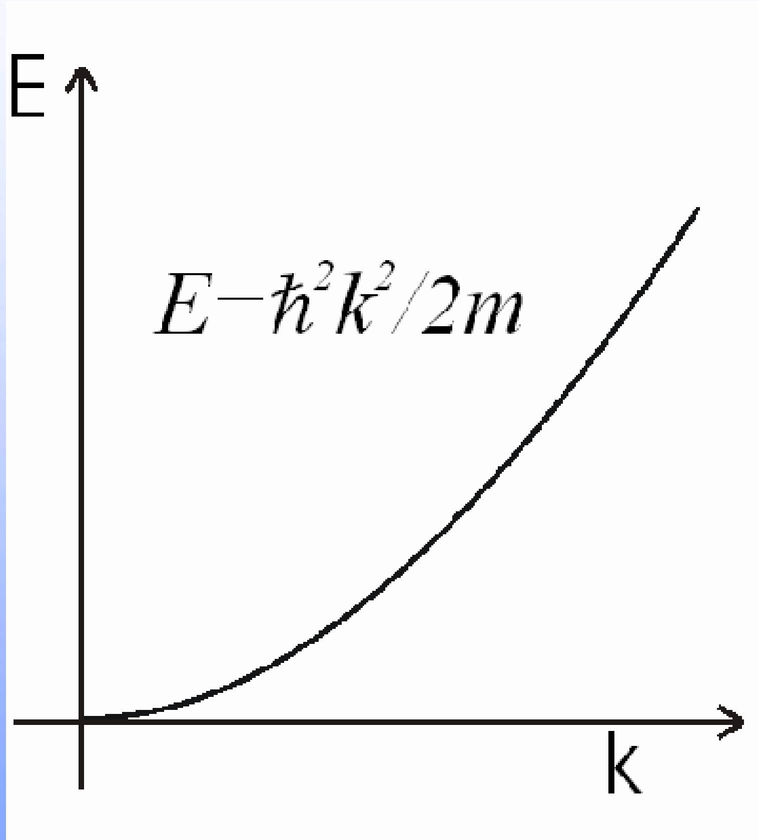


Quantum confinement in a quantum corral.
In the STM image, the surface-state electrons are localized in the circular area made-up from ad-atoms (peaks), showing concentric charge-density oscillations.

Quantum Coherence

Specific phase relations of the electronic wavefunctions are preserved in a nanostructure, giving rise to interference effects if the phase-coherence length is larger than the nanoscale dimension.

Free Particle in One Dimension



Density of States

In general, the density of states in *d*-dimensions is:

$$D(E) = \left(\frac{L}{2\pi}\right)^d \int \frac{\delta(k(E)-k)\,dk^d}{\left|\nabla_k(E)\right|}$$

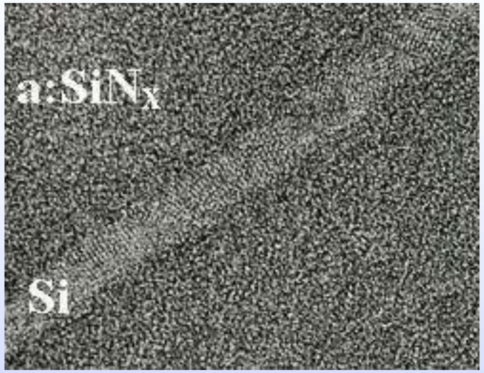
At band edges, $\left|\nabla_k(E)\right| = 0$

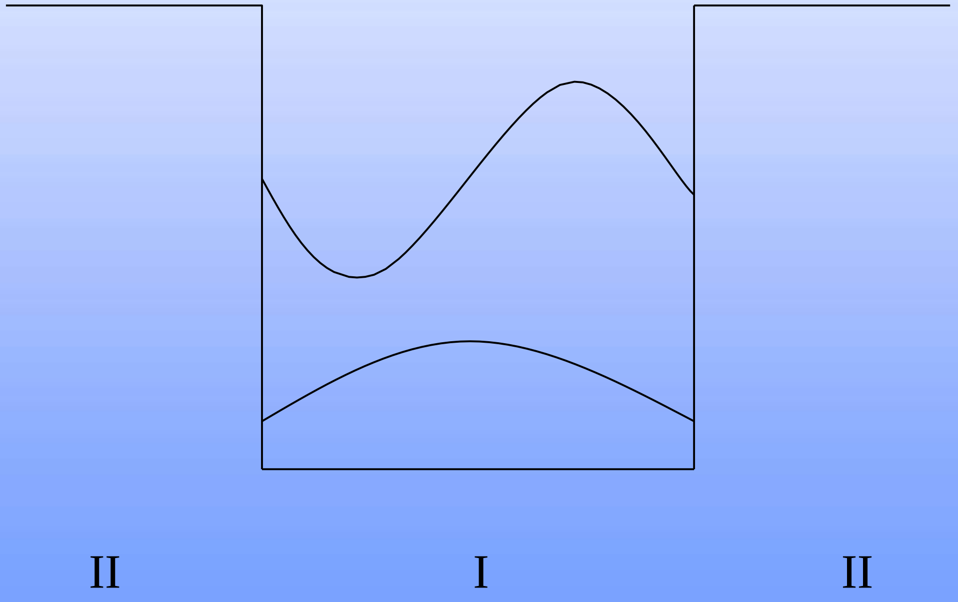
→ van Hove singularities in the density of states

T. W. Odom, *et al.*, *J. Phys. Chem. B*, **104**, 2794 (2000).

Quantum wells

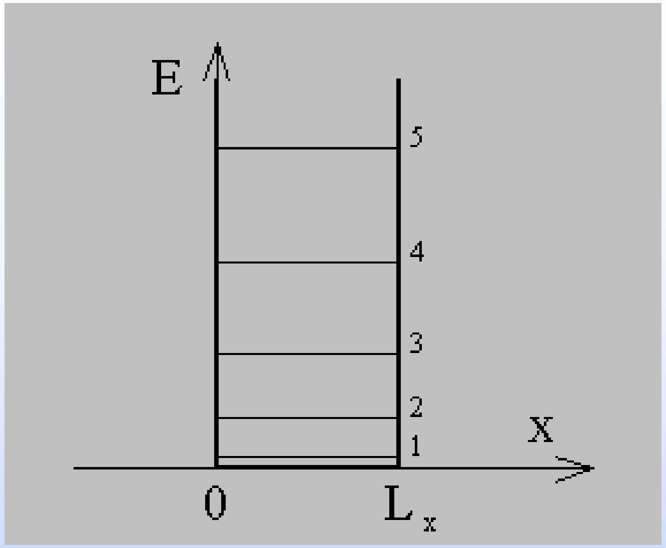
Square qws (epitaxial techniques)





Quantum well. In the transmission electron microscope (TEM) picture the Si quantum well appears as bright area, surrounded by SiN (dark).

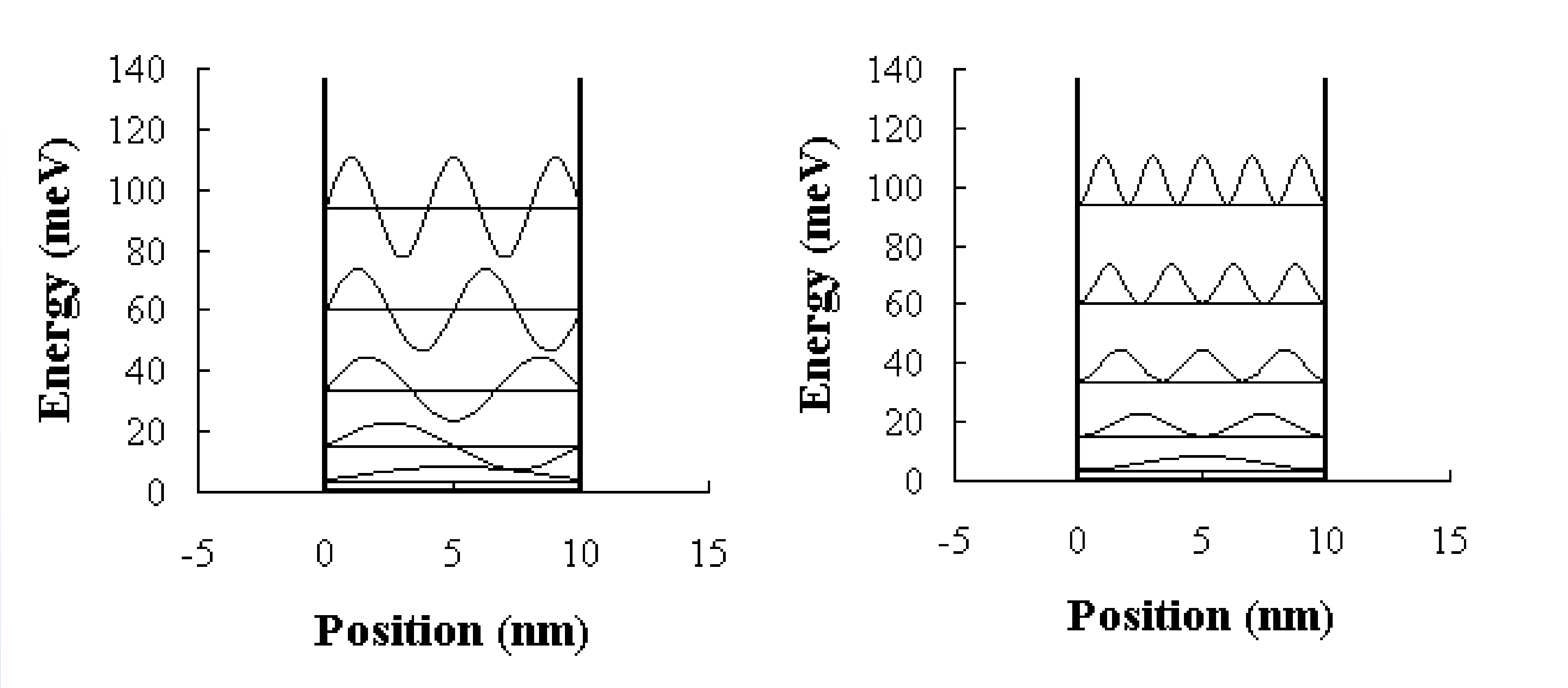
The simplest model is based on idealized nanostructures, using effective mass approximation (EMA)



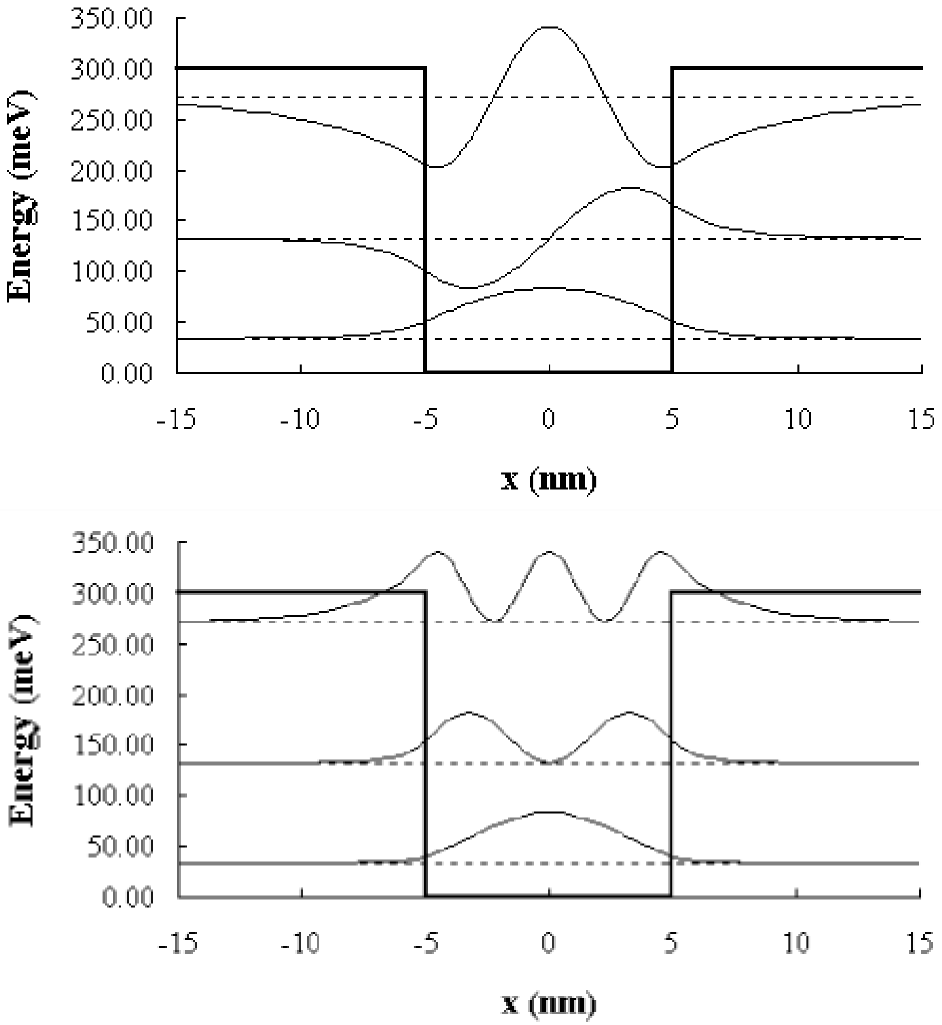
- Two-dimensional (2D) electron system
- Electrons confined in one dimension

realizations

- Interface between two semiconductors (gaalas/gaas)
- Ultra-thin film on a substrate (ag/fe)



Energies, wavefunctions (left), and probability densities (right) of a quantum well with extension 10nm and walls of infinite height.
The five lowest energy levels are shown.
Note the symmetry and the number of nodes of the wavefunctions.



Energies, wavefunctions (up), and probability densities (down) of a quantum well with extension 10 nm and walls of finite height (300 meV). The first three lowest energy levels are shown (bound states).

NANOWIRES
NANOTUBES
NANORODS

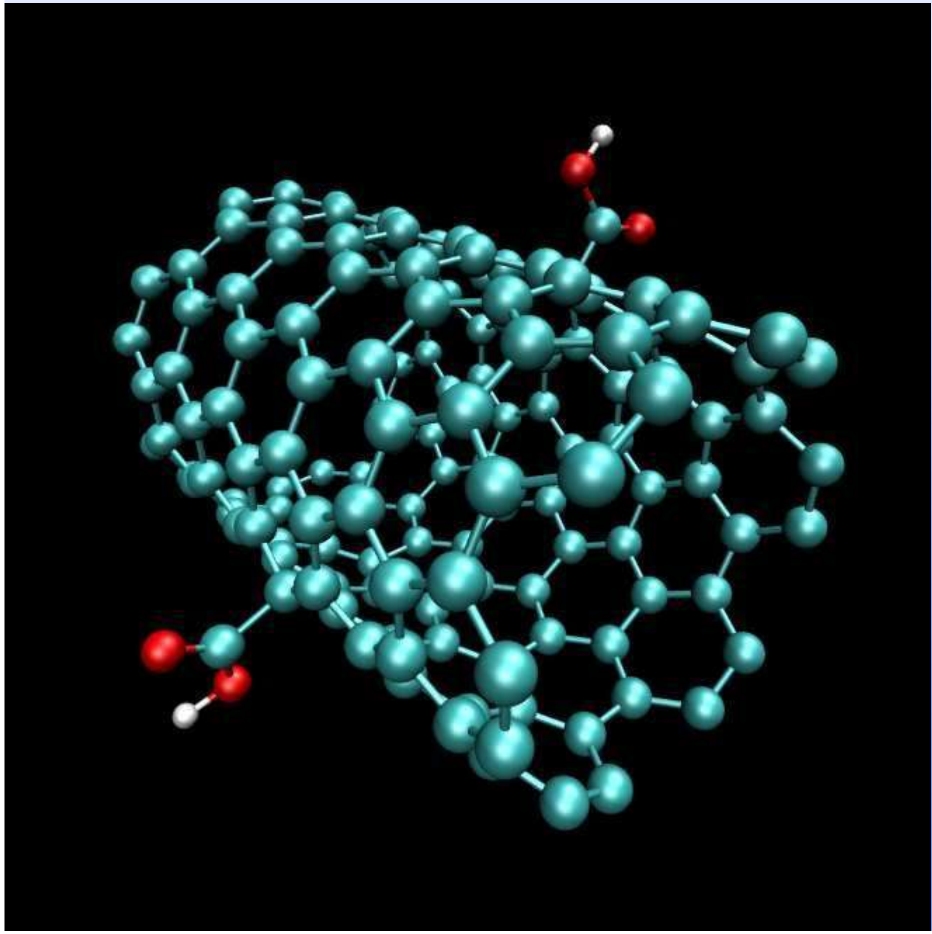
Quantum wire. A chain of atoms is formed between two semi-infinite leads.

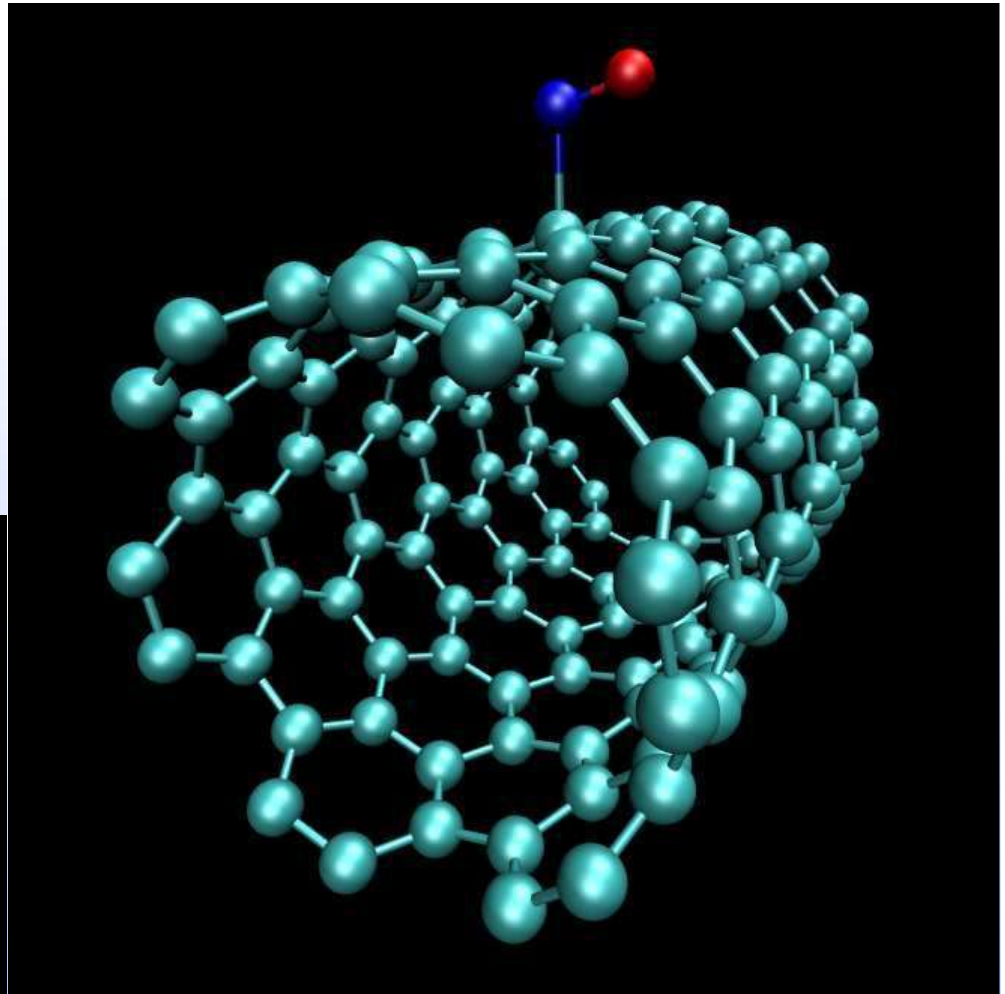
- one-dimensional (1D) electron system
- electrons confined in two dimensions

Realizations

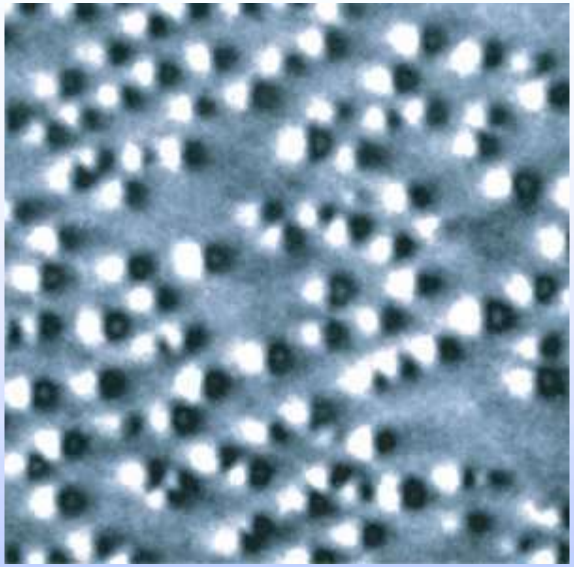
- atomic point contact (`quantum point contact')
- atomic chains deposited on a stepped surface
- carbon nanotubes
- polymers on a substrate

Functionalized
Nanotubes





courtesy Dr. Y. Pouillon



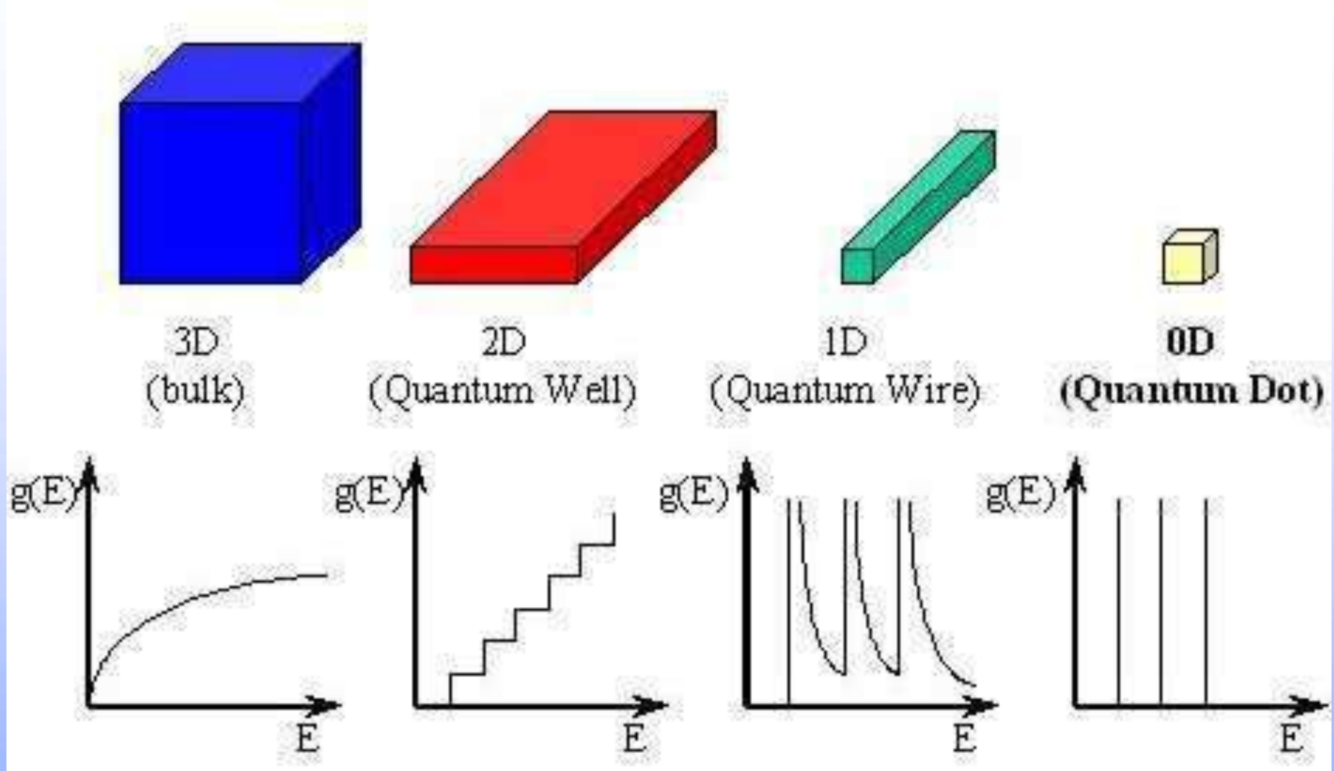
quantum dots (nanocrystallites on a surface)

Zero-dimensional (0D) electron system (`artificial atoms’)

•electrons confined in three dimensions

Realizations

- clusters or crystallites on a surface
- clusters embedded in a crystal
- colloidal nanoclusters



density of states of free electrons confined
in various dimensions (0D –3D).

Thank-You