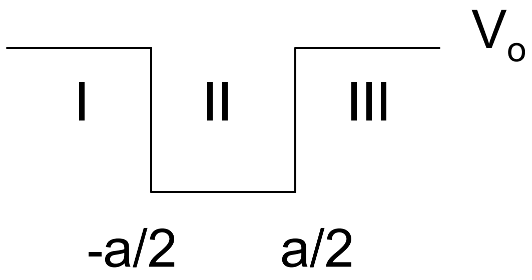
Chapter 5

Particle in finite box

$V(x) = 0, -a/2 < x < a/2$
$\quad = V_o$, for $x \geq a/2$, $x \leq -a/2$



inside box: $$\frac{d^2\psi}{dx^2} = \frac{-2mE}{\hbar^2}\psi$$

outside box: $$\frac{d^2\psi}{dx^2} = \frac{2m(V_o - E)}{\hbar^2}\psi$$

$$\text{I} \quad \psi(x) = \boxed{A'e^{-\kappa x}} + B'e^{\kappa x}$$

$$\kappa = \sqrt{\frac{2m(V_o - E)}{\hbar^2}}$$

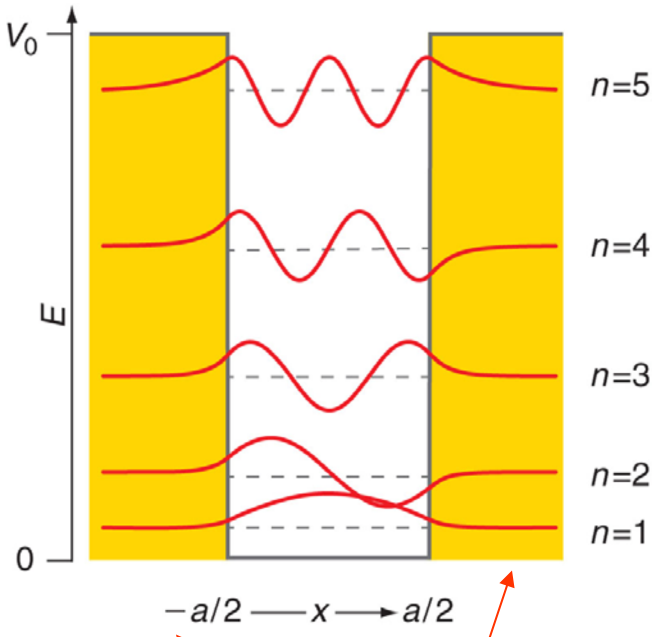
$$\text{III} \quad \psi(x) = Ae^{-\kappa x} + \boxed{Be^{\kappa x}}$$

$$\boxed{0}$$

$$\left.\begin{aligned} &\text{I} \quad \psi_I = B' e^{\kappa x} \\ &\text{III} \quad \psi_{III} = A e^{-\kappa x} \end{aligned}\right\}$$

exponentially decaying

$$\text{II} \quad \psi_{II} = C \sin kx + D \cos kx, \qquad k = \sqrt{\frac{2mE}{\hbar^2}}$$



tunneling

$$\text{I} \quad \psi(x) = B' e^{\kappa x}$$

$$\kappa = \sqrt{\frac{2m(V_o - E)}{\hbar^2}}$$

$$\text{III} \quad \psi(x) = A e^{-\kappa x}$$

The greater the mass of the particle or the deeper down in the potential, the smaller the tunneling.

How does one solve the Schrodinger Eq. for such a problem?

require that ψ and $\dfrac{d\psi}{dx}$ continuous at the boundaries

$$\psi_I(-a/2) = \psi_{II}(-a/2) \qquad \psi_{II}(a/2) = \psi_{III}(a/2)$$

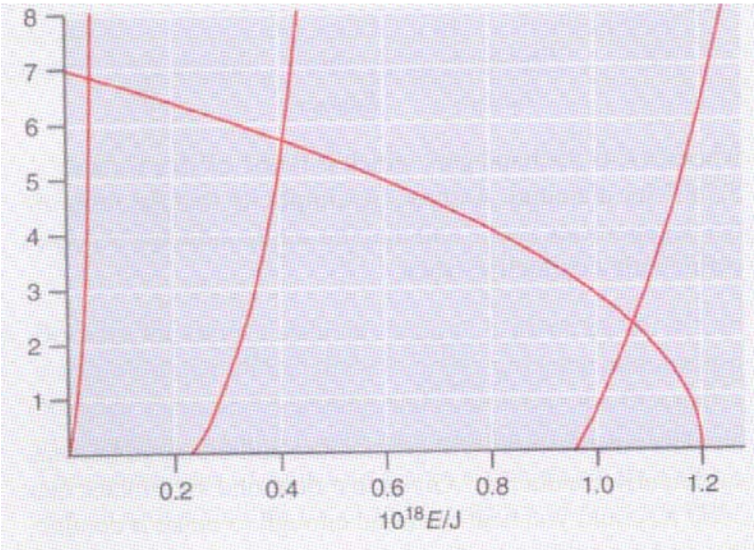
$$\psi_I'(-a/2) = \psi_{II}'(-a/2) \qquad \psi_{II}'(a/2) = \psi_{III}'(a/2)$$

The resulting equations can be manipulated to give

$$\sqrt{Vo - E} = \sqrt{E}\,\tan\left(\sqrt{mEa^2/2\hbar^2}\right)$$

Can be solved graphically

- Only a finite number of solutions
- If V_o is high, low-lying levels very close to solutions of problem with infinite potential outside box.



Consider the case of two finite square-well potentials next to one another as shown to the right.

The levels near the bottom of the potential show little or no overlap.

As one goes to higher energy levels, overlap increases.

Each pair of levels is split into a bonding and an antibonding combination

Do you see how this could model H2+?

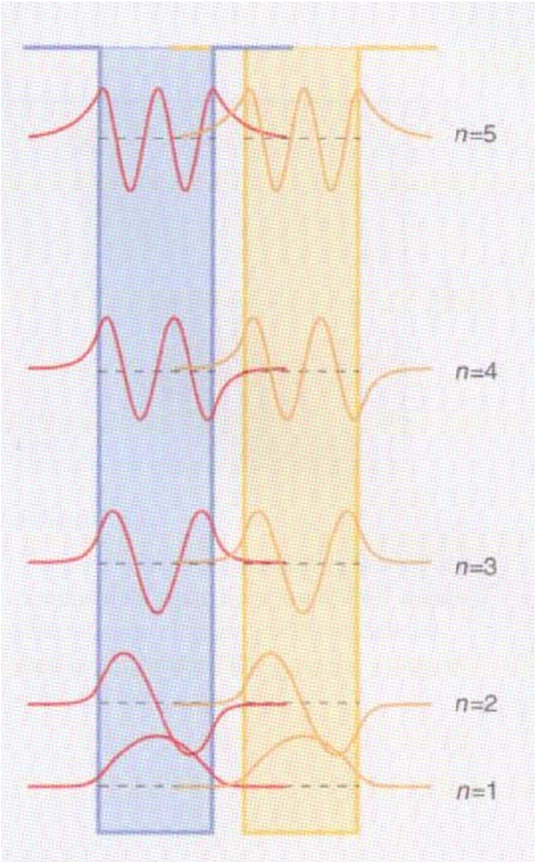
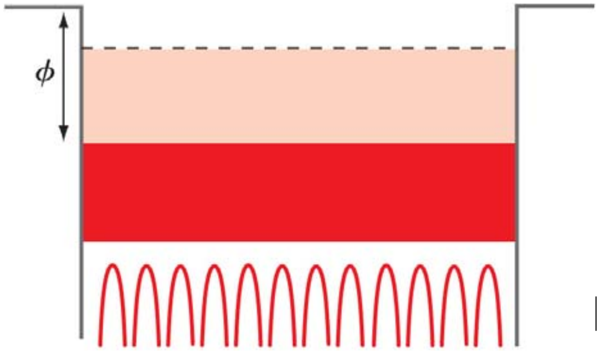


FIGURE 5.3



empty levels

filled levels

a^{+} cores

zero energy gap ⇒ metal
large energy gap ⇒ insulator

small gap → semiconductor

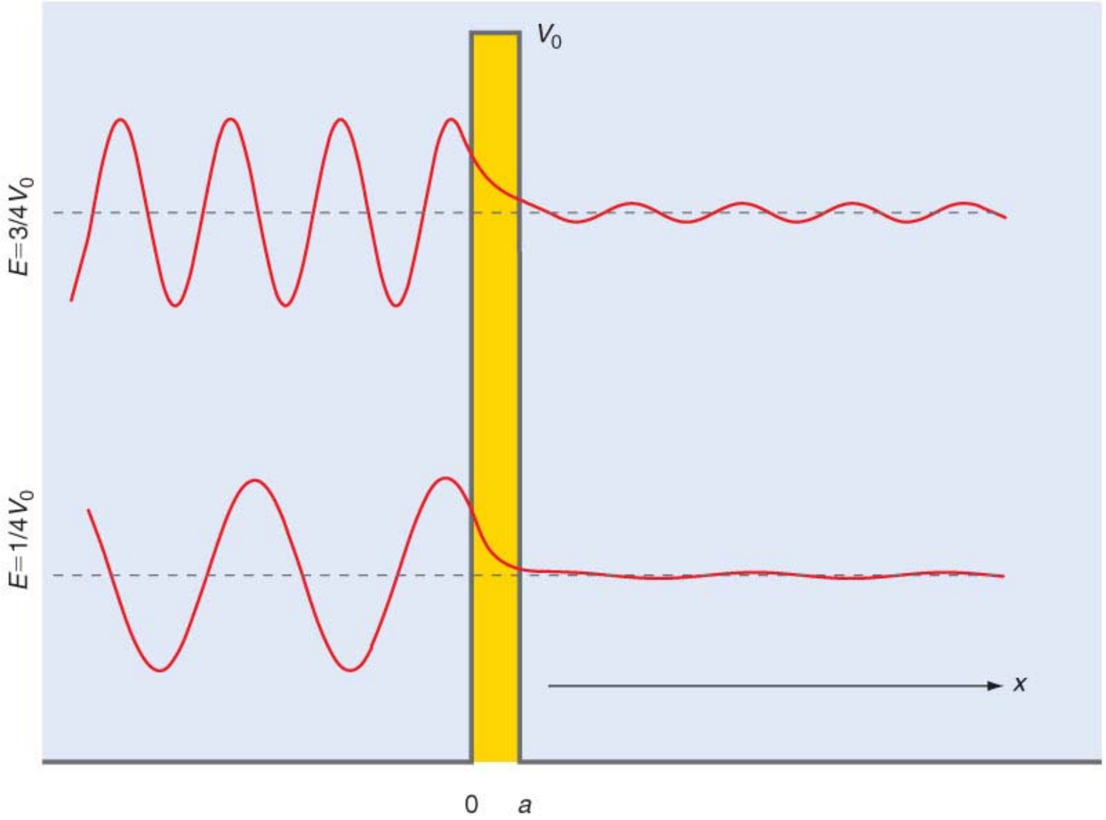
Apply electrical potential → charge will flow (for metal)

Tunneling through barrier

Can show tunneling is proportional to

$$e^{-2a\sqrt{2m(V_o - E)/\hbar^2}}$$

Solve Schrodinger Eq. using the same sort of strategy that was used for the particle in the finite box.

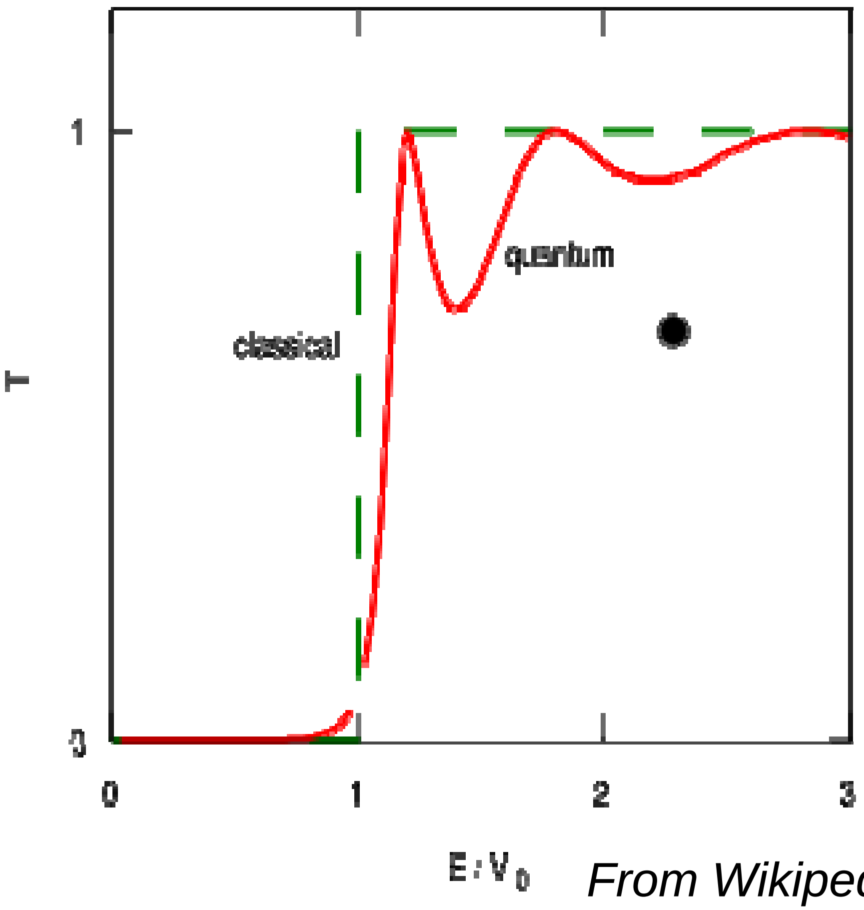


tunneling most important when:
- particle light
- energy near top of barrier
- barrier width is small

Check out: http://www.youtube.com/watch?v=4-PO-RHQsFA&feature=related

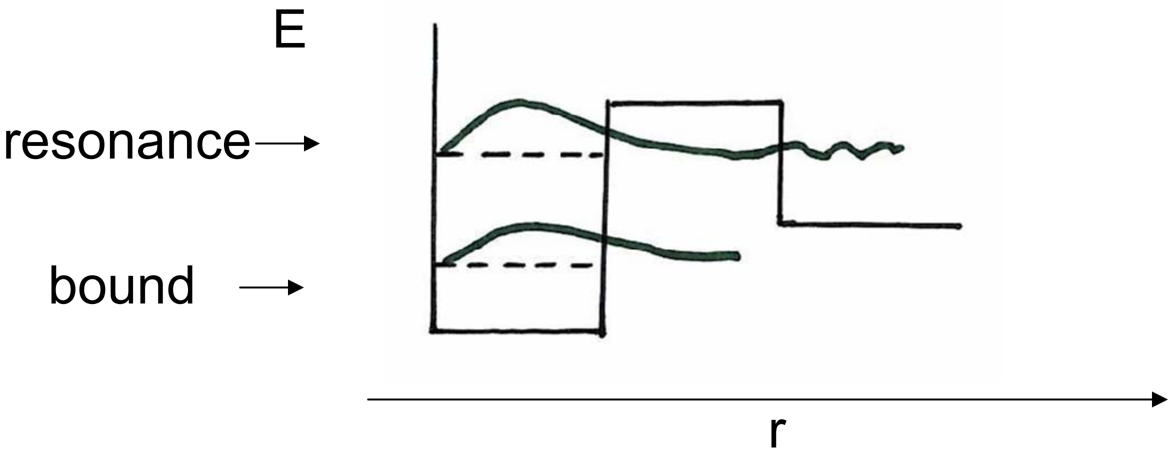
Probability of transmission through the barrier as a function of the incident energy

Note if $E > V_o$, the particle can be reflected by the barrier

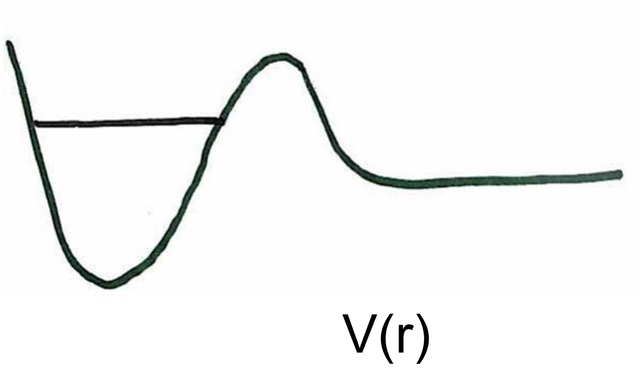


From Wikipedia

resonances:
particle can
escape by
tunneling



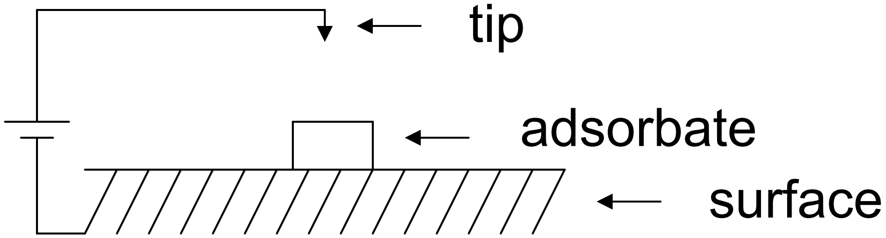
Examples:
- radioactive decay
- temporary anions: Be^-, N_2^-, benzene$^-$ electron falls off in ≈10^{-14} sec



How can one measure something with such a short lifetime?

Chapter 5, continued

Scanning tunneling microscopy (STM) – invented ~20 years ago at IBM Research Labs, Zürich



Apply voltage – measure current

often run so that as the tip is scanned over the surface, the height is varied so as to keep the current constant

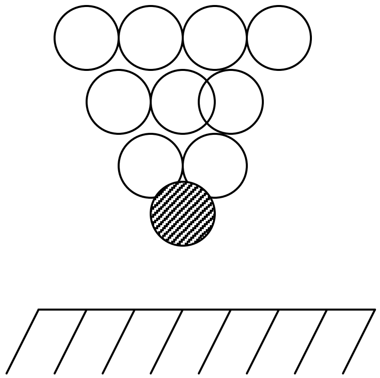
the tip does not actually touch the surface

electrons tunnel between tip and surface

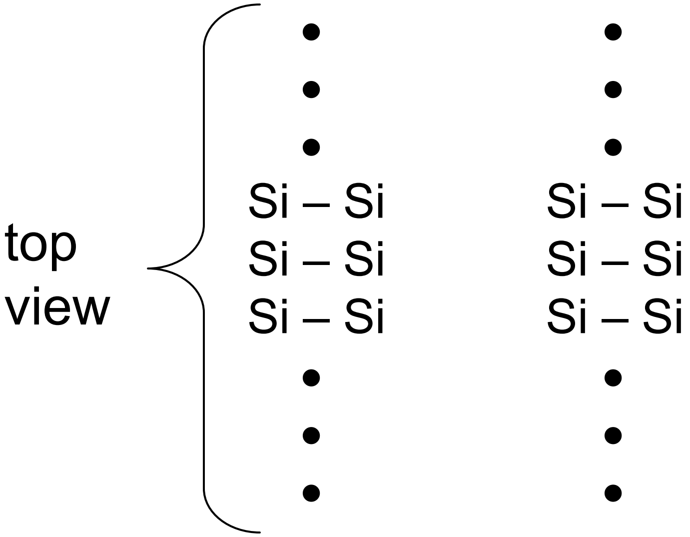
Atomic resolution

tunneling dominated by single atom
at the end of the tip

Why?



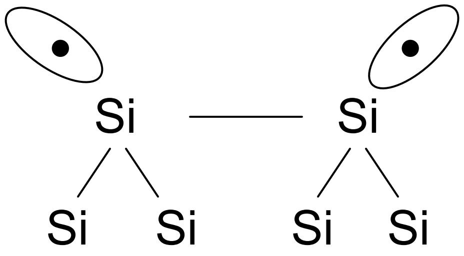
Used to study defects and adsorbed molecules on surfaces



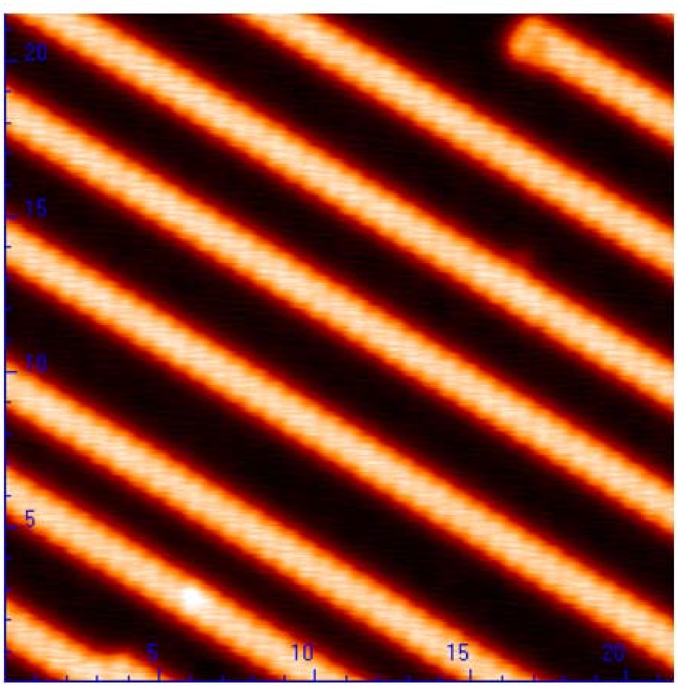
top
view

Si – Si   Si – Si
Si – Si   Si – Si
Si – Si   Si – Si

Si(100) surface –
rows of silicon dimers

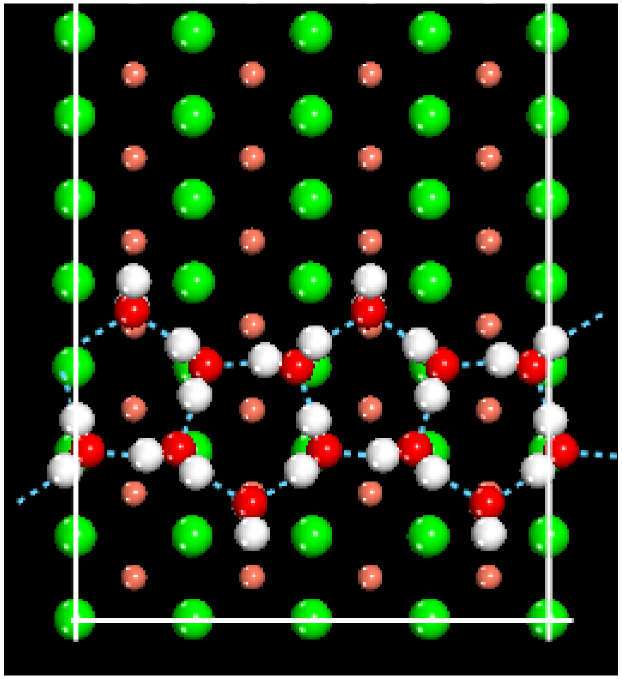


On surfaces and in confining environments as well as in clusters, water can assemble into structures with very different arrangements than found in ice or the liquid



22 x 22nm^2

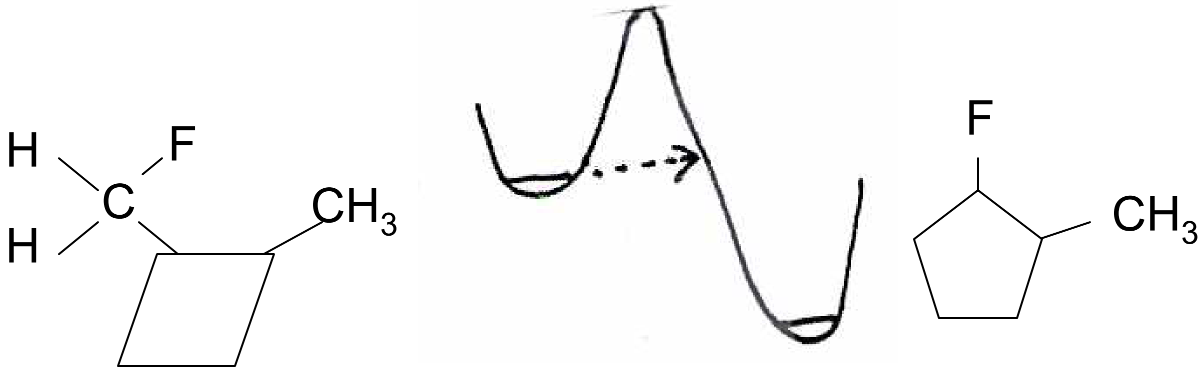
STM image of water chains on the Cu(110) surface: width ~ 9 Å (J. Lee and J. Yates)



Many groups tried to explain the structure in terms of fused hexagons. However, Carrusco et al., showed that it is due to fused pentagons [Nature Materials (2008)]

Consequence of more favorable interactions with Cu atoms

Reaction is 10^{152} times faster than expected at T = 10 K.



It proceeds *via* tunneling rather than going over the barrier

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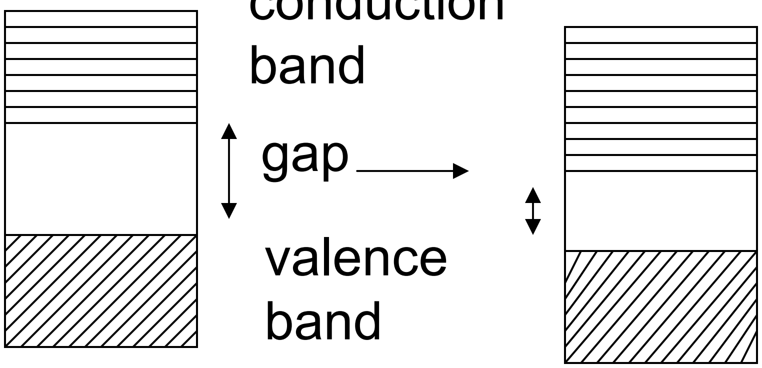
quantum wells



conduction band

gap

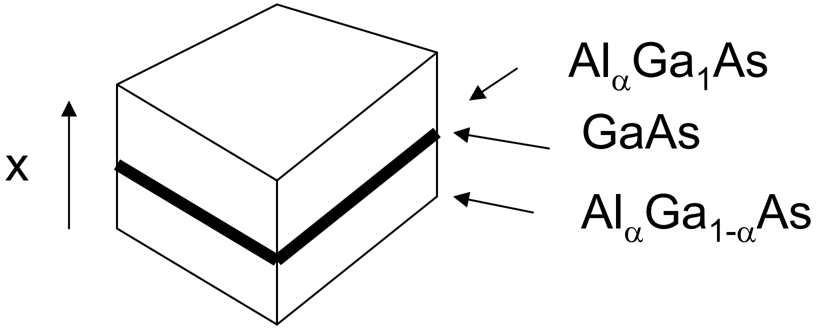
valence band

$Al_{\alpha}Ga_{1-\alpha}As$

GaAs

GaAs has a smaller band gap

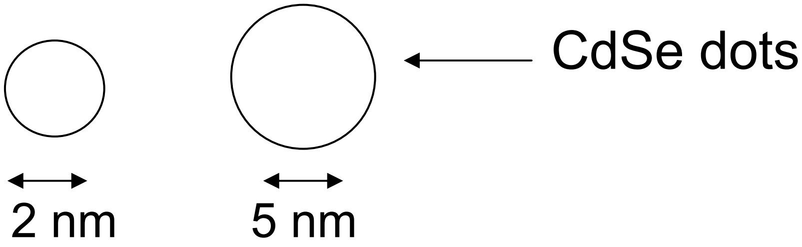
Make a layered device



Electron is free in y, z directions and confined in the x direction

Such systems can act as lasers

quantum dots



emits green red ← fluorescence

used as tags to study processes in cells