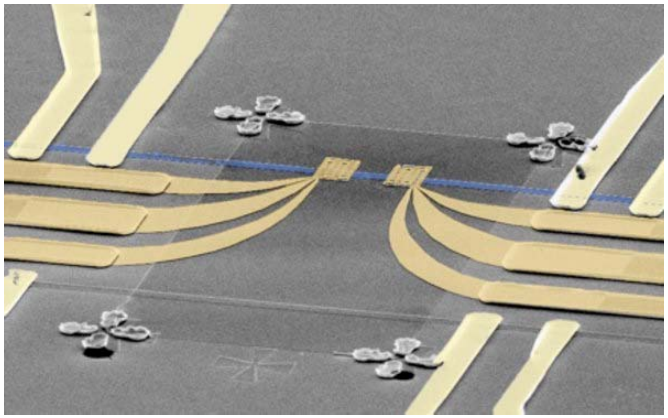
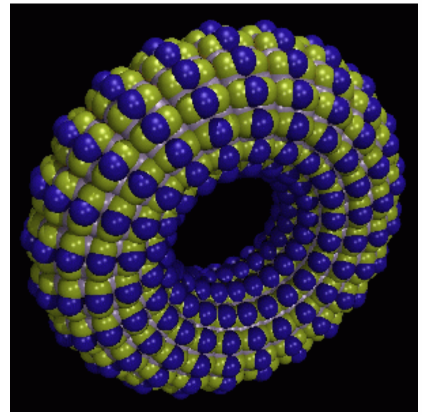
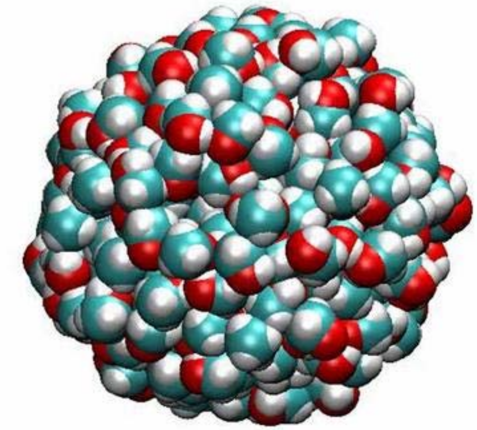
  

Nanoscience : Fundamentals and basic properties

Ulrich Hohenester

Karl–Franzens–Universität Graz, Austria

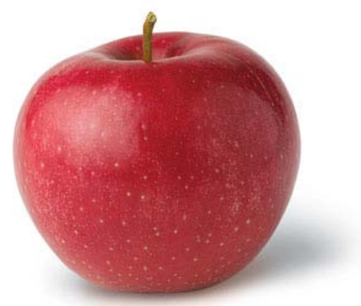
http://physik.uni-graz.at/~uxh

ASON-1, 19.-23.09.2010, Dubrovnik, Croatia

Nanometer

is the „ruler“ at the atomic scale

:



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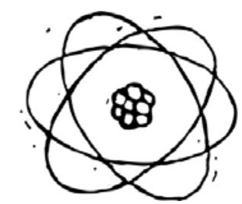
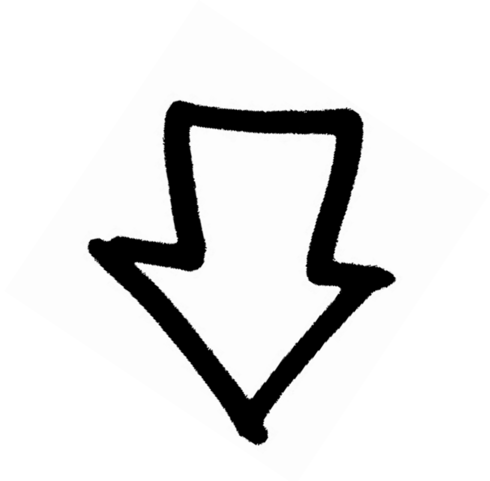
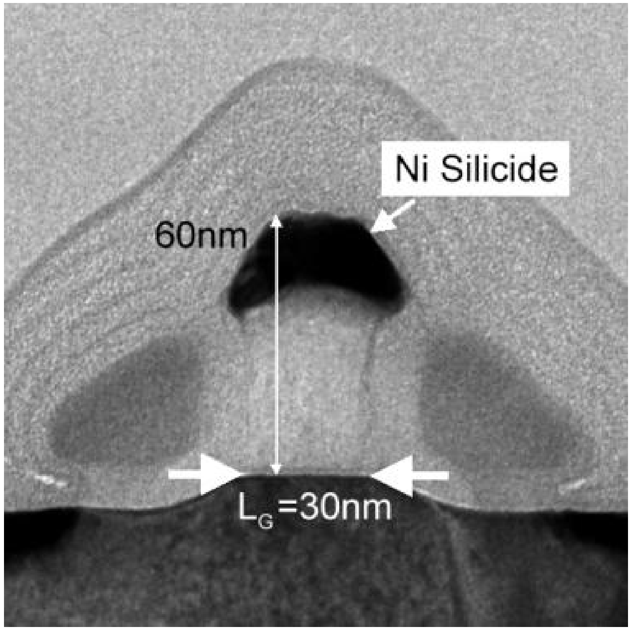
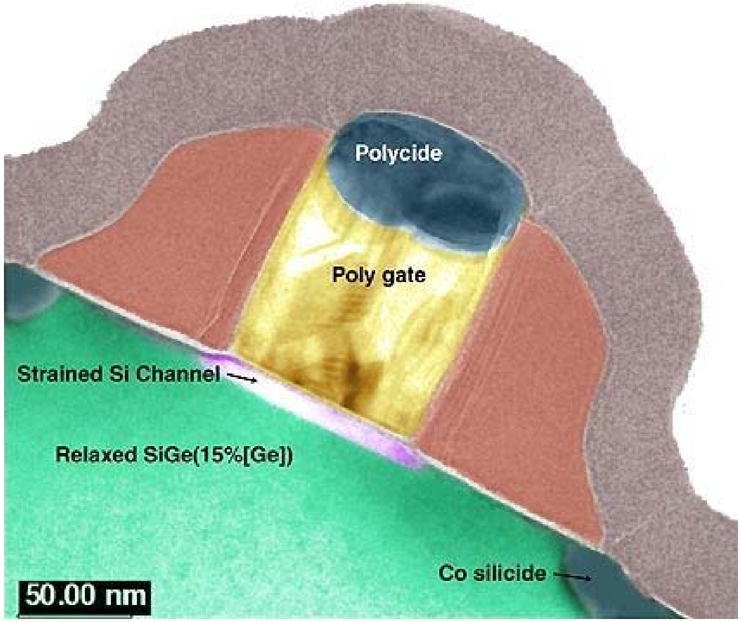


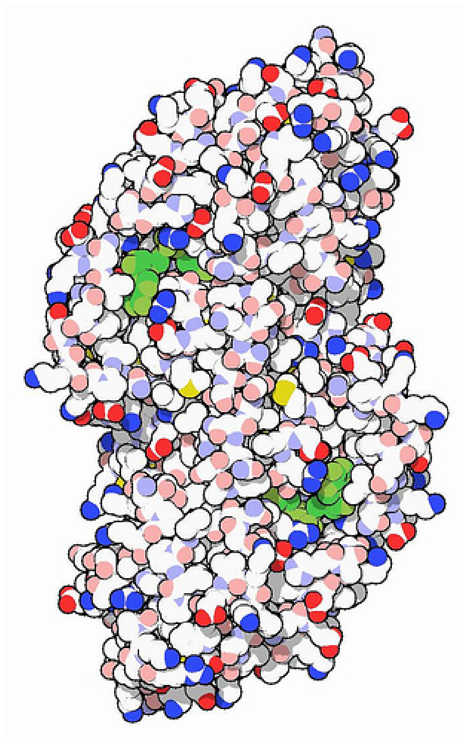


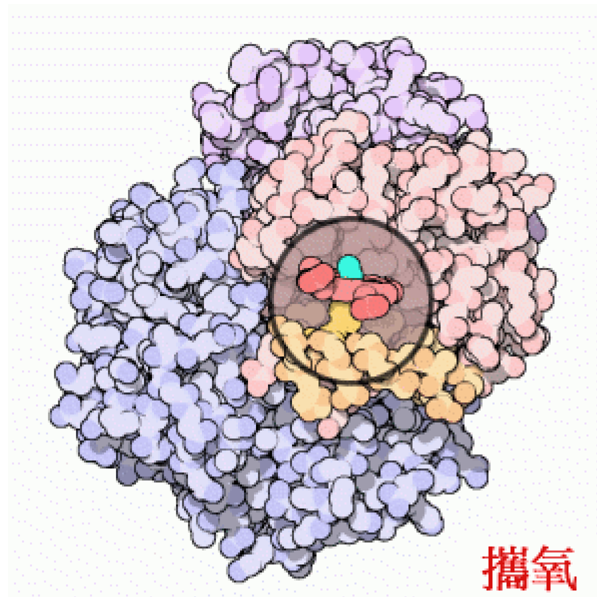


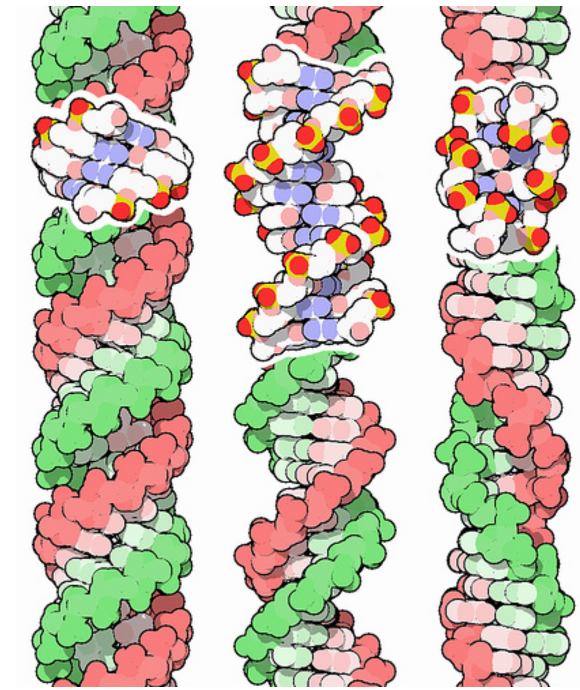


Technology is approaching nanoscale from „above“

… top – down approach







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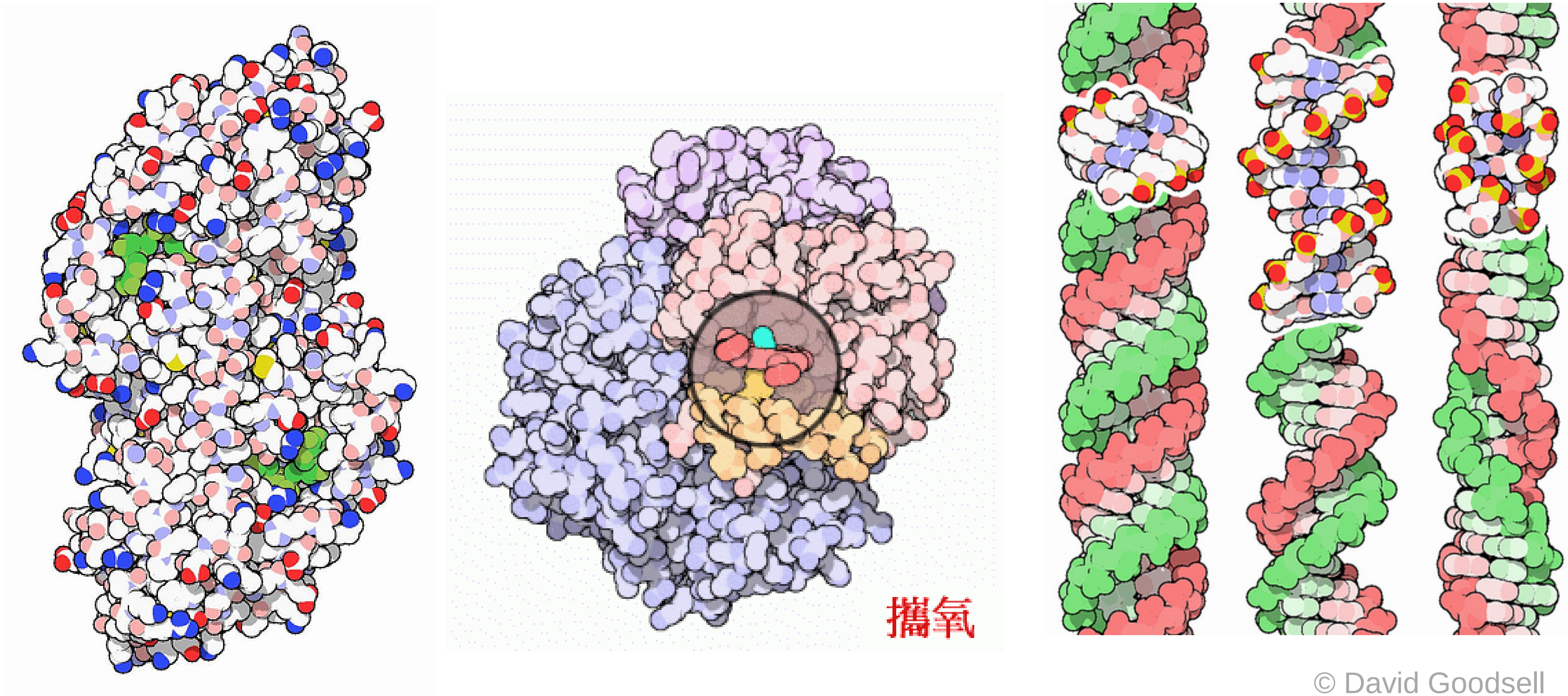
Nature uses atoms as building blocks for (bio)molecules

… bottom – up approach

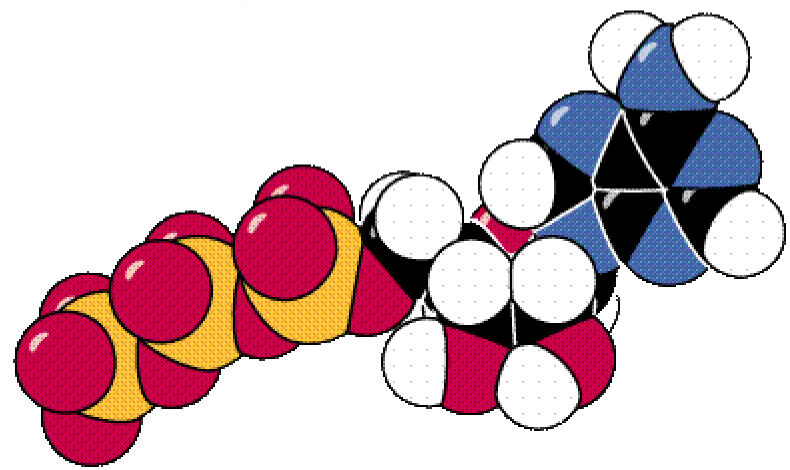


„There is plenty of room at the bottom“

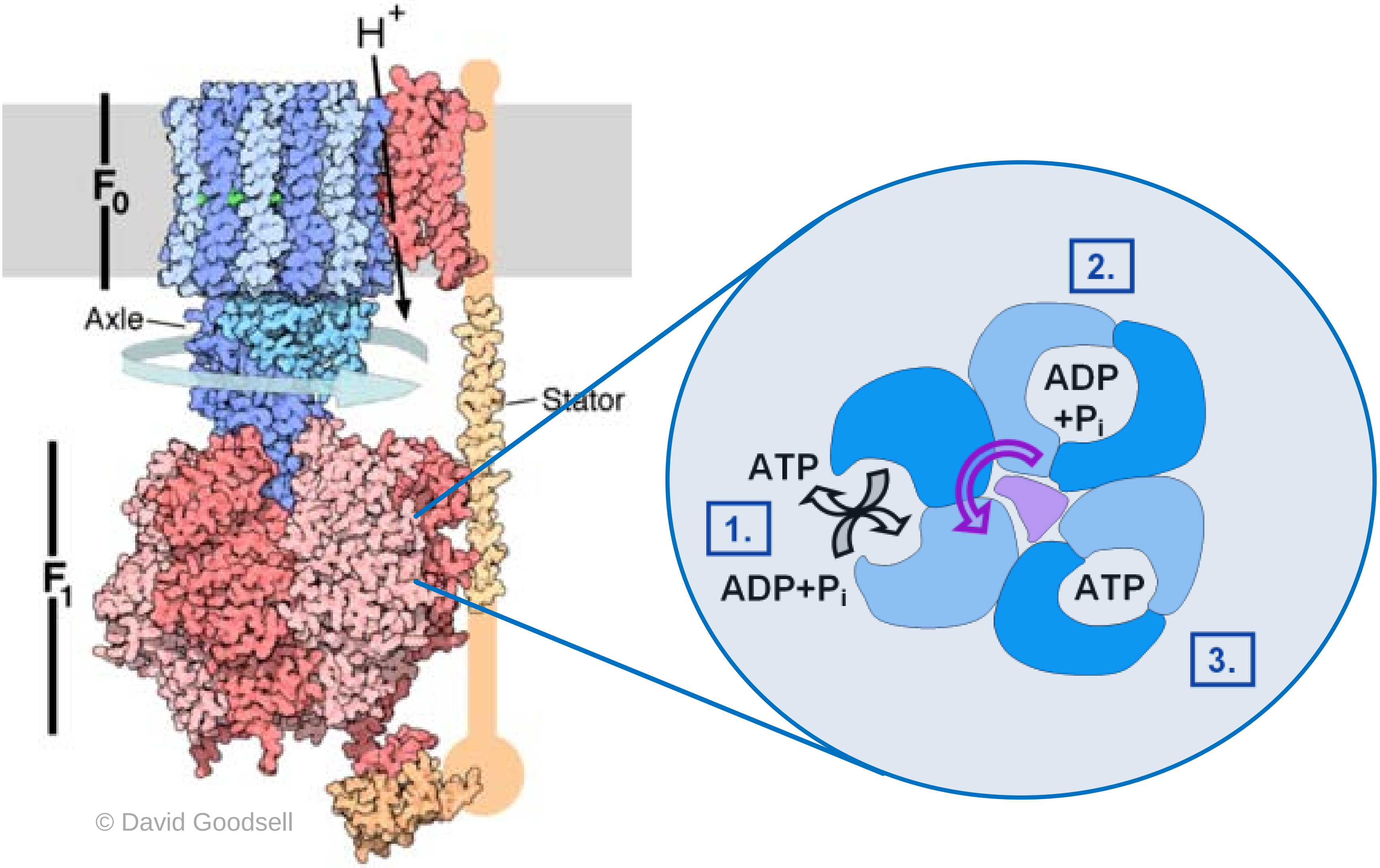
Richard Feynman, 1959

I now want to show that there is plenty of room.

I will not now discuss how we are going to do it, but only what is possible in principle — in other words, what is possible according to the laws of physics.



Example : ATP synthase



Proton pump H^+ drives "nanomotor" that drives ADP + $P_i \longrightarrow$ ATP

Agenda

What I will do in this lecture ...

Electrons in solids

Confinement : from 3D to 0D

Coulomb effects at the nanoscale

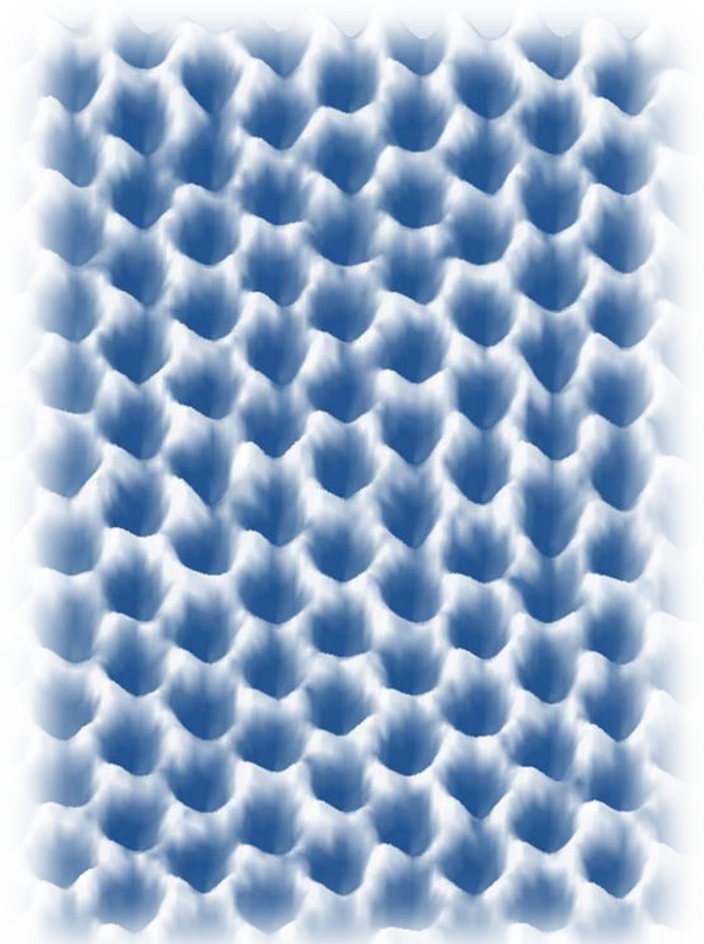
How quantum are nanostructures ?

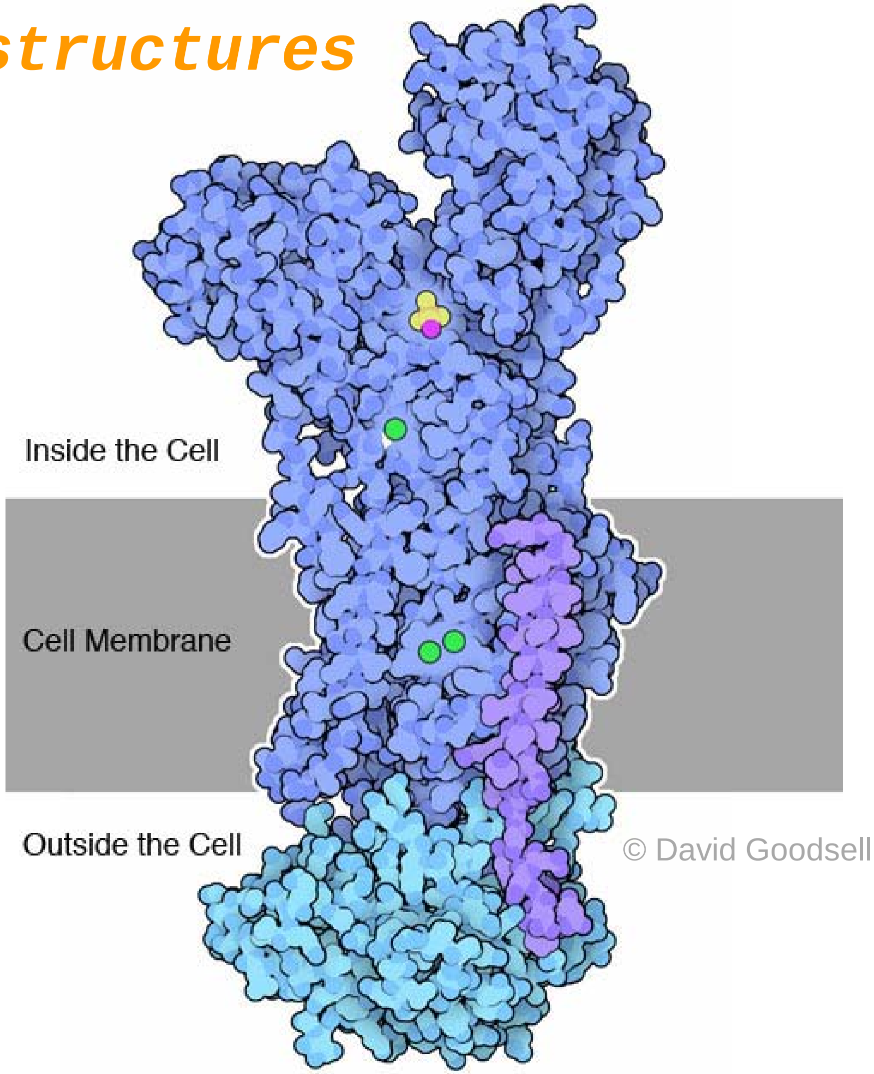
Single nanosystems, optics at the nanoscale, nanomagnetism and spintronics, forces, heat & fluids at the nanoscale

My scientific background ...

I am a theoretical physicist working in condensed matter physics, interested in plasmonic nanoparticles, semiconductor quantum dots & ultracold atoms

Charge transfer in nanostructures





(Nano)crystals:
electrons delocalized
information transfer through electrons

(Bio)molecules:
electrons localized in bonds
information transfer through ions

Quantum mechanics: Free particle

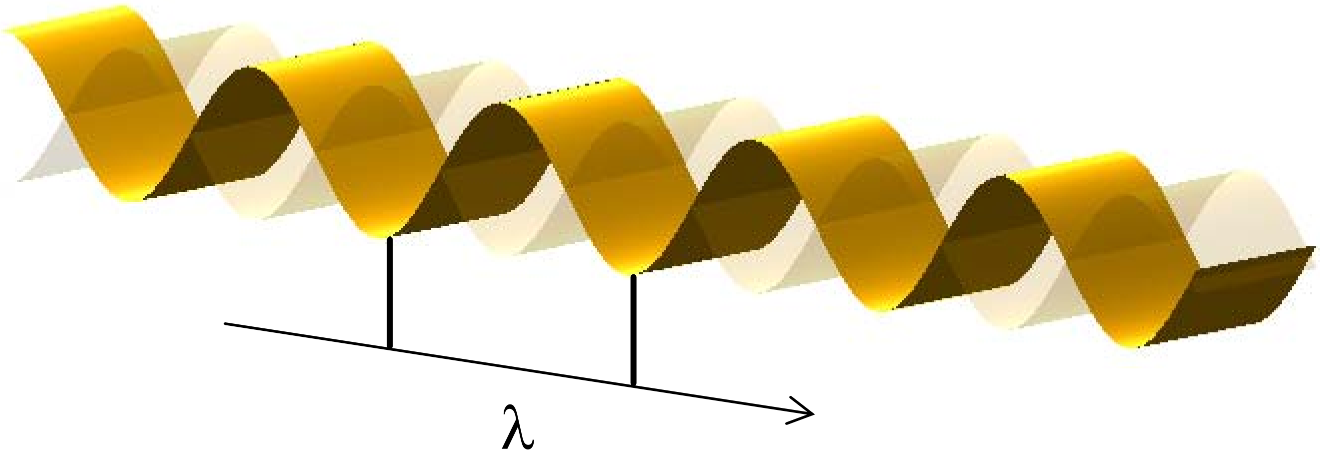
Schrödinger equation for free particle

$$-\frac{\hbar^2\nabla^2}{2m}\Psi(x) = E\,\Psi(x)$$

de Broglie wavelength $\lambda = h / p$

High momenta (energies) correspond to small wavelengths

$$\Psi(x) = e^{i\,kx}\,, \qquad p = \hbar k = \frac{h}{\lambda}$$



Quantum mechanics: Free particle

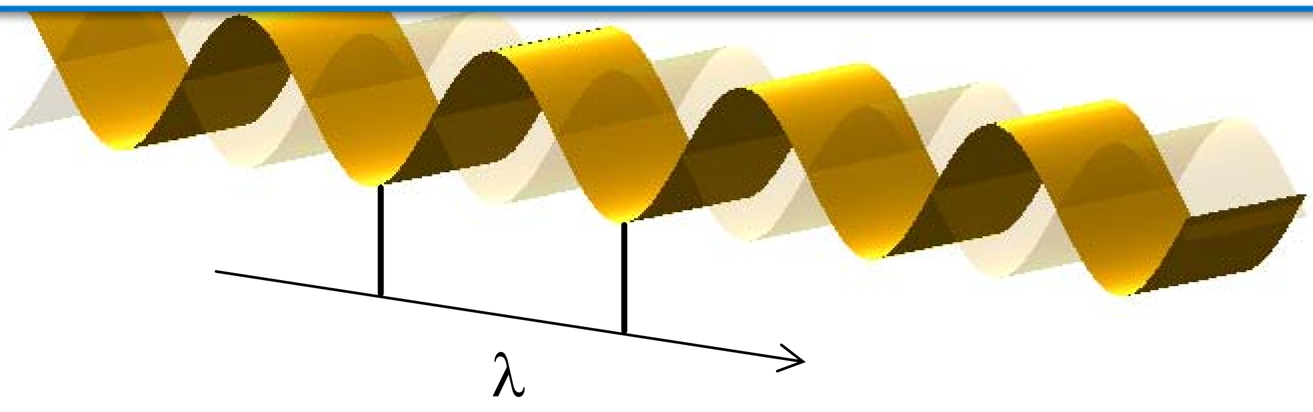
Schrödinger equation for free particle

$$-\frac{\hbar^2\nabla^2}{2m}\Psi(x) = E\,\Psi(x)$$

Finite differences

Coupling to left and right „neighbours“

$$\nabla^2\Psi(x) \approx \frac{\Psi(x+\Delta x) - 2\Psi(x) + \Psi(x-\Delta x)}{(\Delta x)^2}$$



Tight binding model

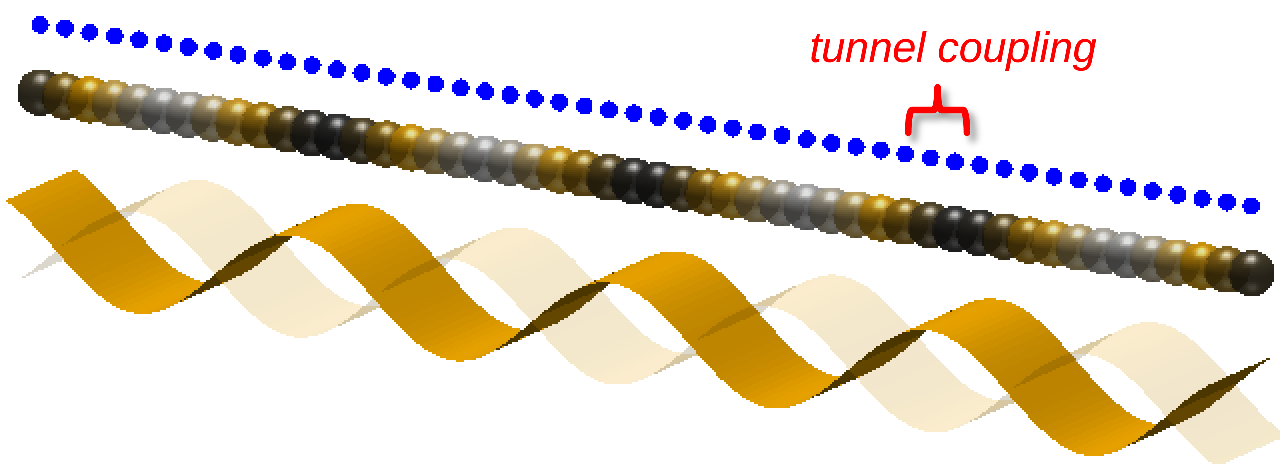
Wavefunction of electron in a linear chain of atoms

$$\Psi(x) = \sum_{\ell} C_{\ell}\, \underbrace{\phi(x - \ell a)}_{\text{localized atomic orbital}} = \sum_{\ell} \underbrace{e^{ik\ell a}}_{\text{plane wave modulation}} \phi(x - \ell a)$$

localized atomic orbital *plane wave modulation*

Tight-binding model for tunnel – coupled atoms in 1D

$$\epsilon_0 C_{\ell} + t \left(C_{\ell+1} + C_{\ell-1} \right) = E\, C_{\ell}$$



Tight binding model

Wavefunction of electron in a linear chain of atoms

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localized atomic orbital *plane wave modulation*

Tight-binding model for tunnel – coupled atoms in 1D

$$\epsilon_0 C_{\ell} + t \left(C_{\ell+1} + C_{\ell-1} \right) = E \, C_{\ell}$$

Energy dispersion

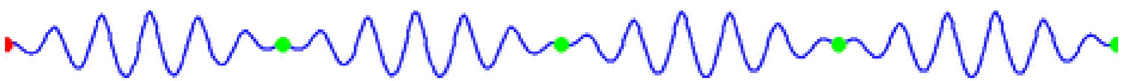
Relation between frequency and wavelength

$$E(k) = \epsilon_0 - 2|t| \cos ka$$

Energy dispersion

Energy dispersion determines how a wavepacket propagates

$$v_g = \frac{d\omega}{dk} = \frac{1}{\hbar}\frac{dE(k)}{dk}$$



© wikipedia

- *phase velocity*
- *group velocity*

Energy dispersion for tunnel – coupled atoms in 1D

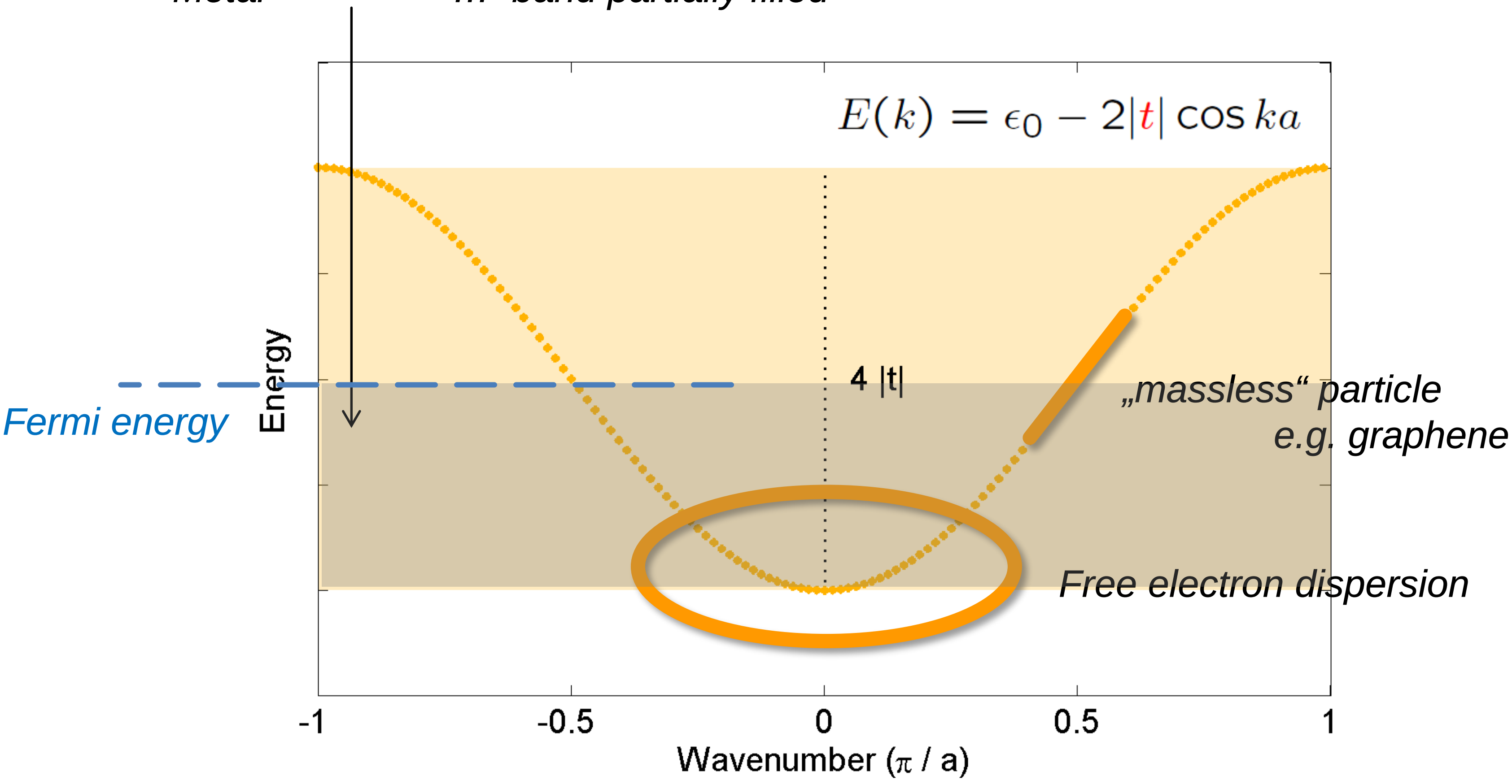
$$E(k) = \epsilon_0 - 2|t|\cos ka \longrightarrow \text{const} + |t|a^2k^2$$

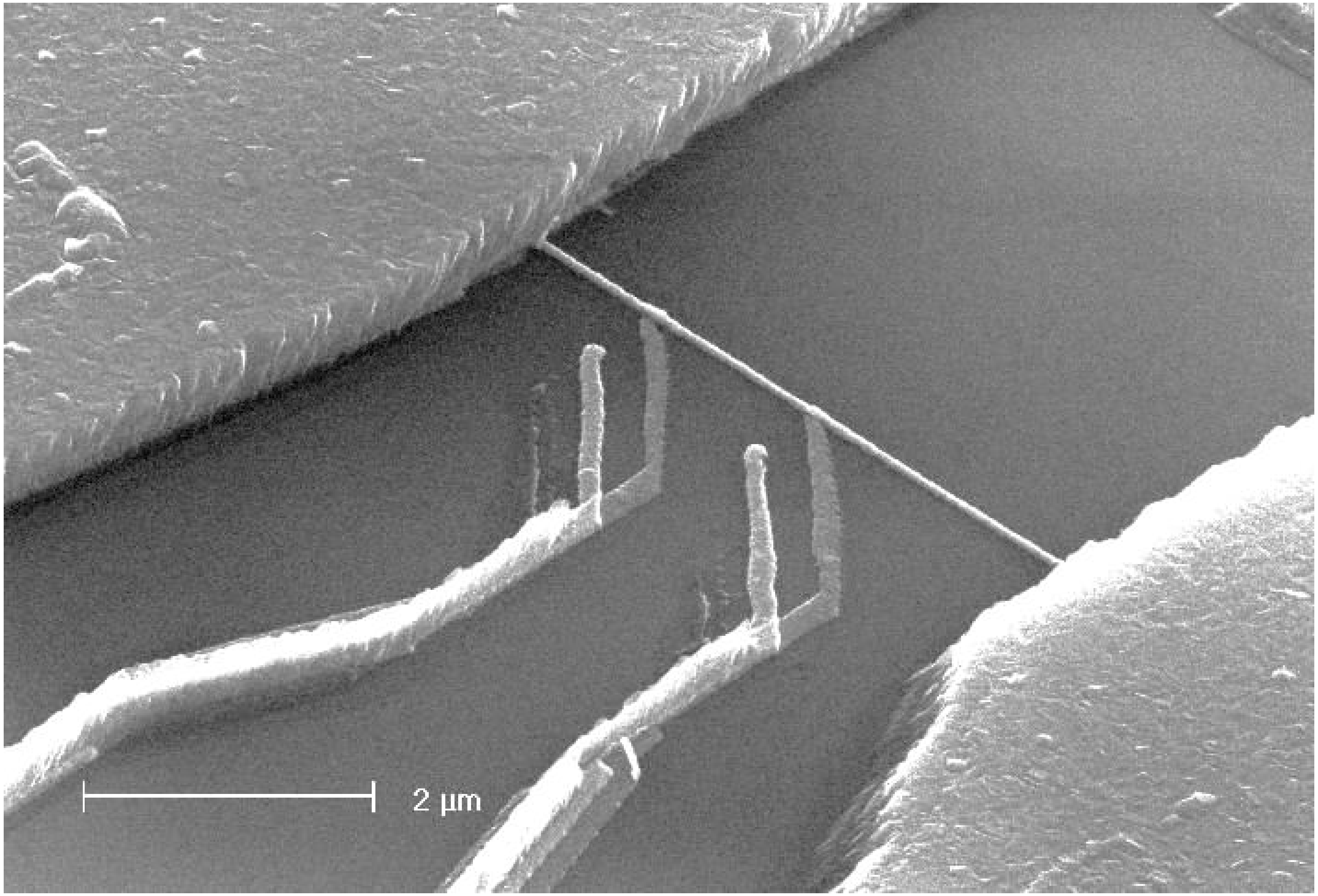
For long wavelengths (small k values) the dispersion is similar to that of a free electron, however, with an <u>effective mass</u> which is governed by the hopping t

Energy band

Number of k states depends on number of atoms in the chain

Semiconductor … no or only a few states of band filled
Metal … band partially filled





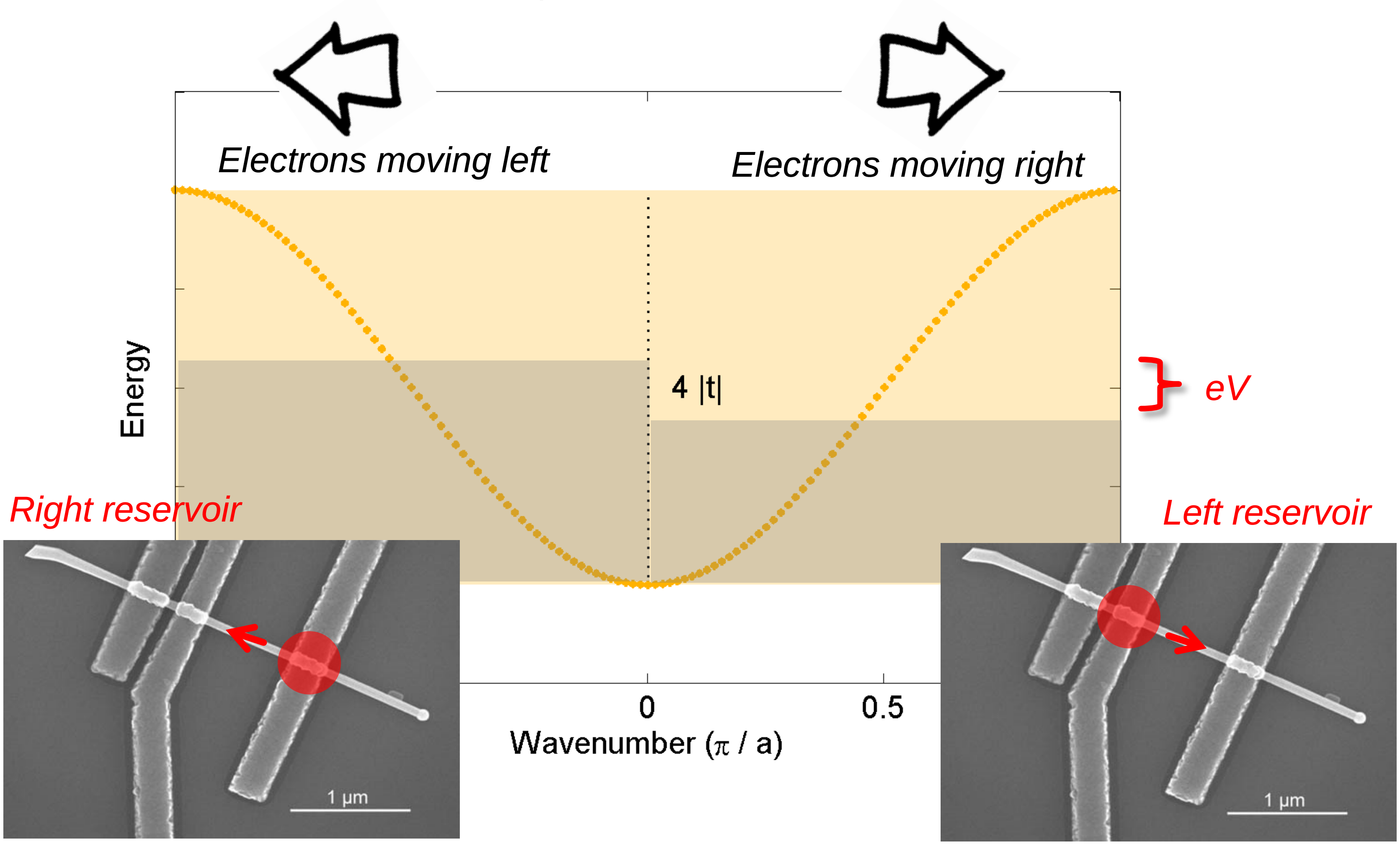
© quantronics, Sacley

Resistance of a ballistic nanowire

Transport through a nanowire

Nanowire connected to contacts

Short nanowire … ballistic transport



Current through a nanowire

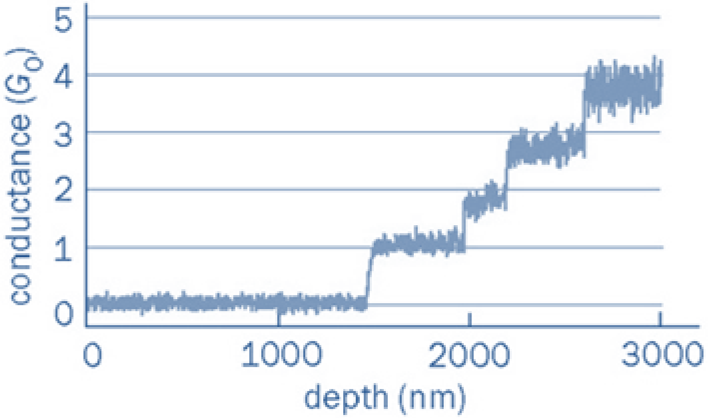
Current = spin x (electron density) x (sum of electron velocities)

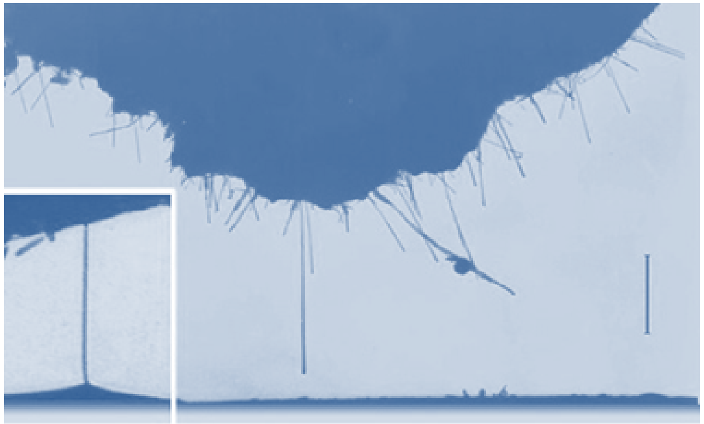
$$I = \frac{2e}{L}\sum_k v_k$$
$$= \frac{2e}{L}\frac{L}{2\pi}\int dk\,\frac{1}{\hbar}\frac{\partial E(k)}{\partial k} = \frac{2e}{h}\int_{E_F}^{E_F+eV} dE = \frac{2e}{h}eV$$

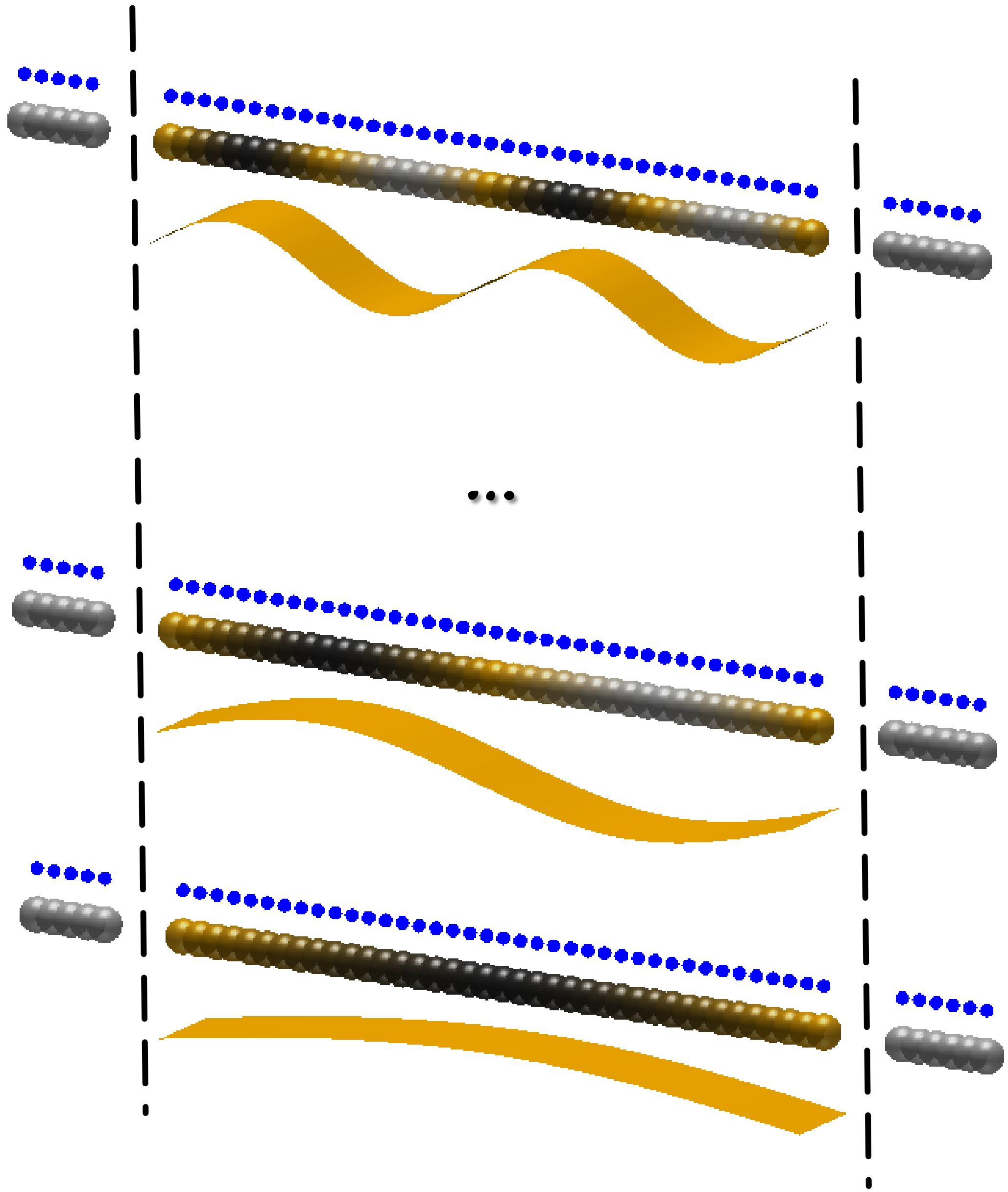
Resistance R and conductance G = 1/R depend only on natural constants

Conductance quantization

$$G_0 = \frac{2e^2}{h}, \quad h/e^2 \approx 25\ \mathrm{k\Omega}$$





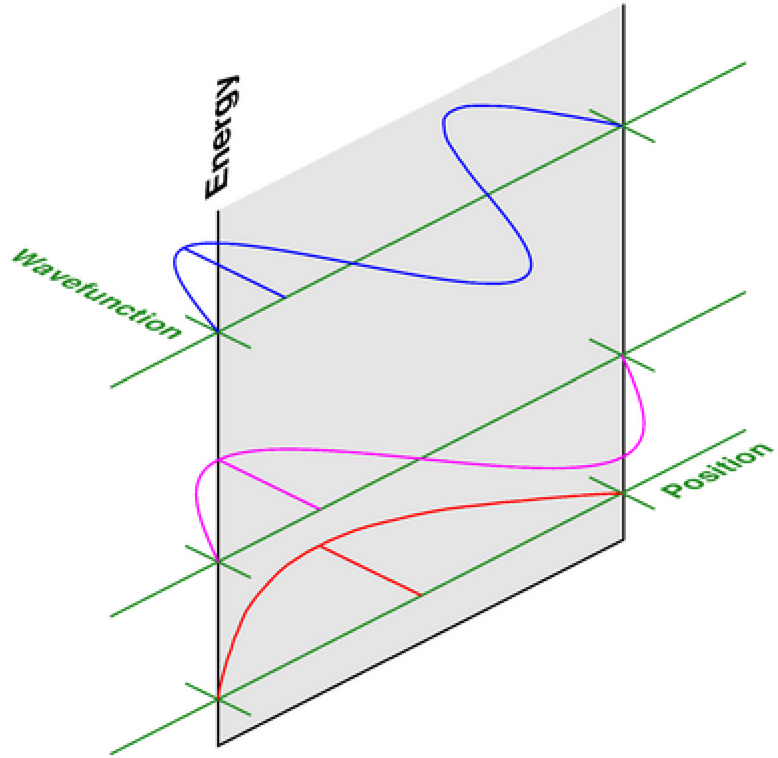


Quantum confinement: From 3D to 0D

Particle in a box

Motion of particle confined in a box

$$\psi(x) = \sin kx\,, \qquad kL = n\pi$$



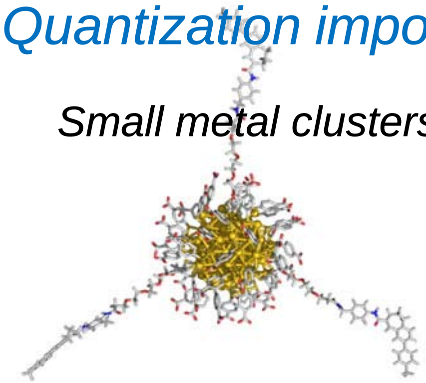
Energy quantization

Confinement results in discrete energy levels

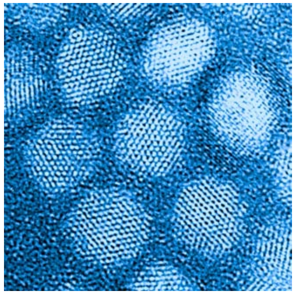
$$E_n = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2 \pi^2 n^2}{2mL^2}$$

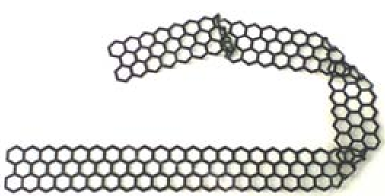
Quantization important if de Broglie wavelength comparable to NP size

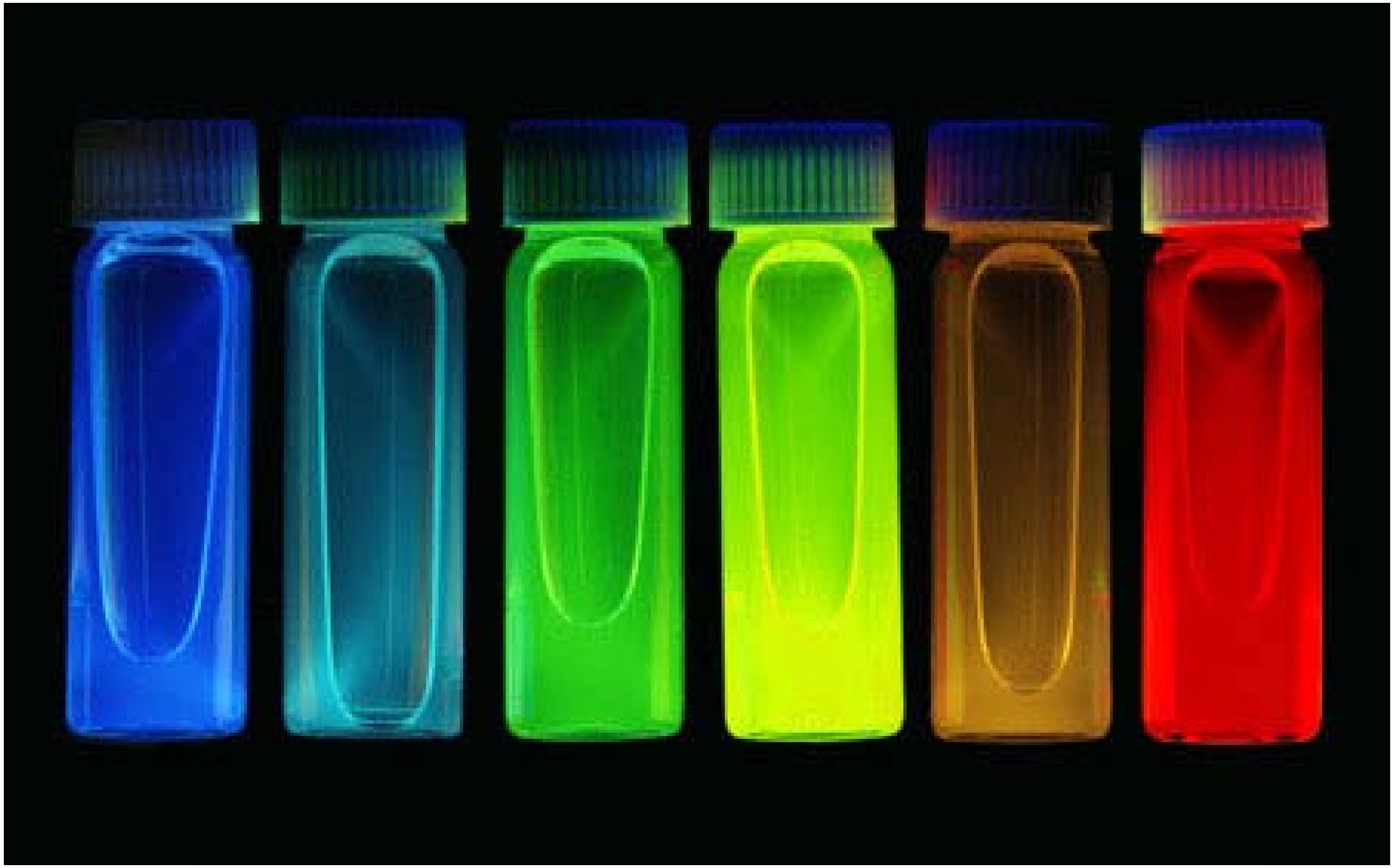
Small metal clusters (λ ~ nm)



Semiconductor nanocrystals





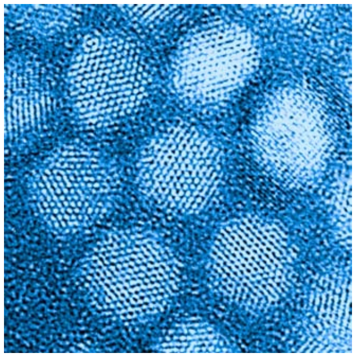


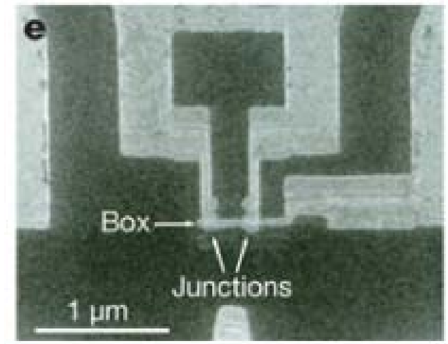
Small dots

large dots

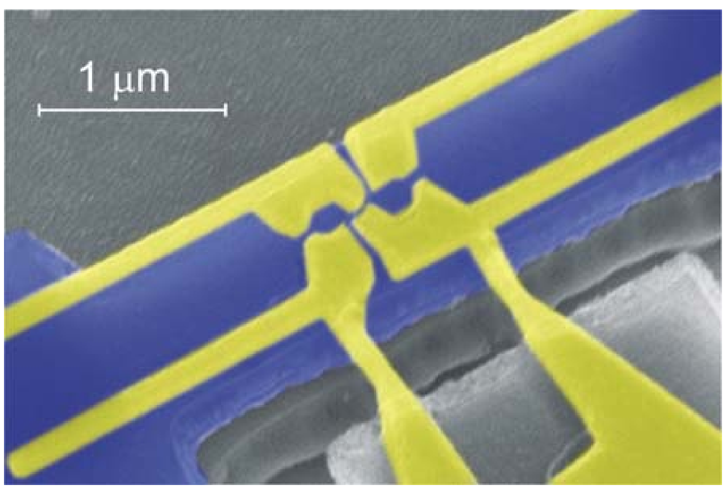
How to confine electrons ?

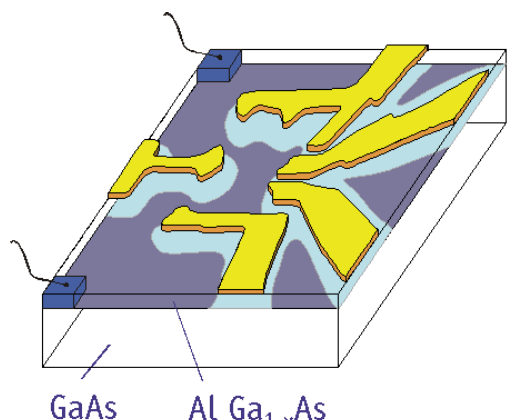
Structural confinement

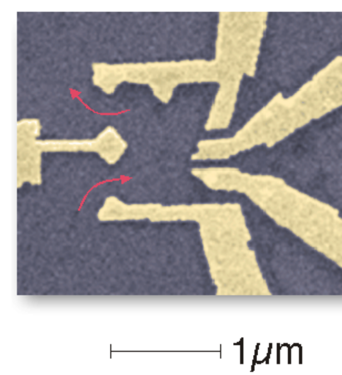


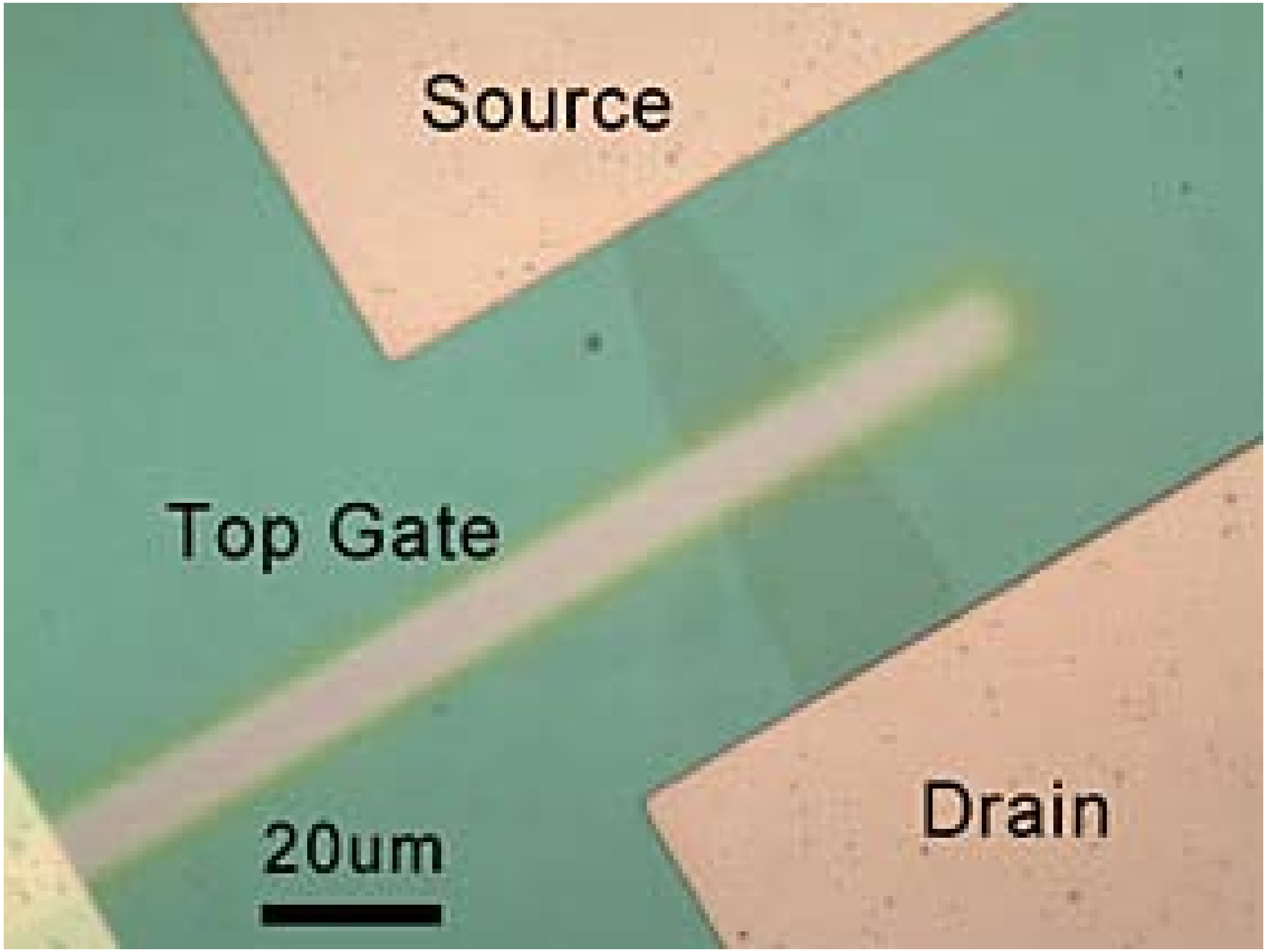


Gate control



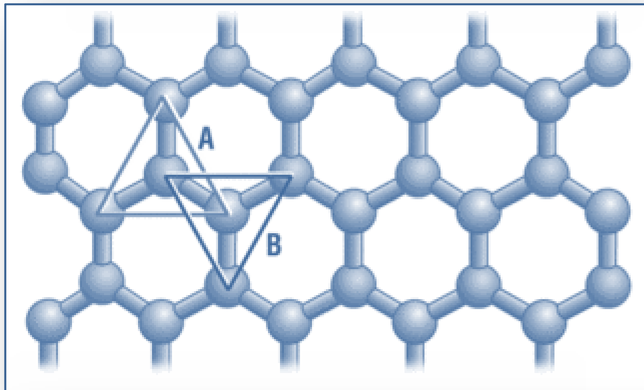


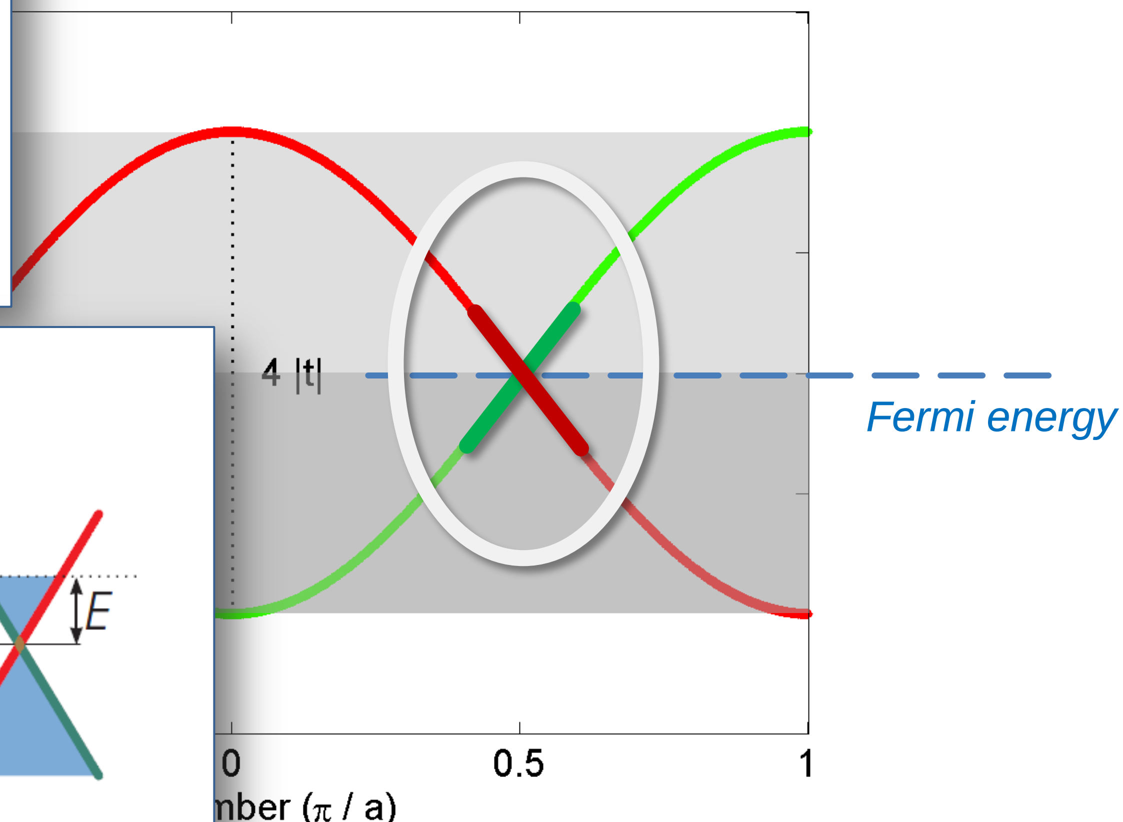


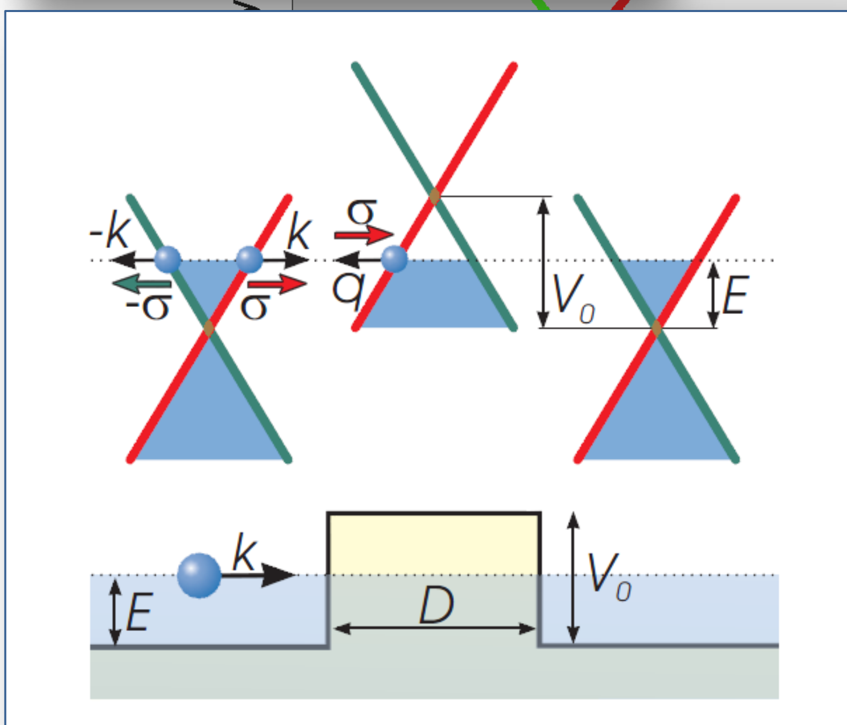


Electron confinement in graphene

Electron confinement in graphene

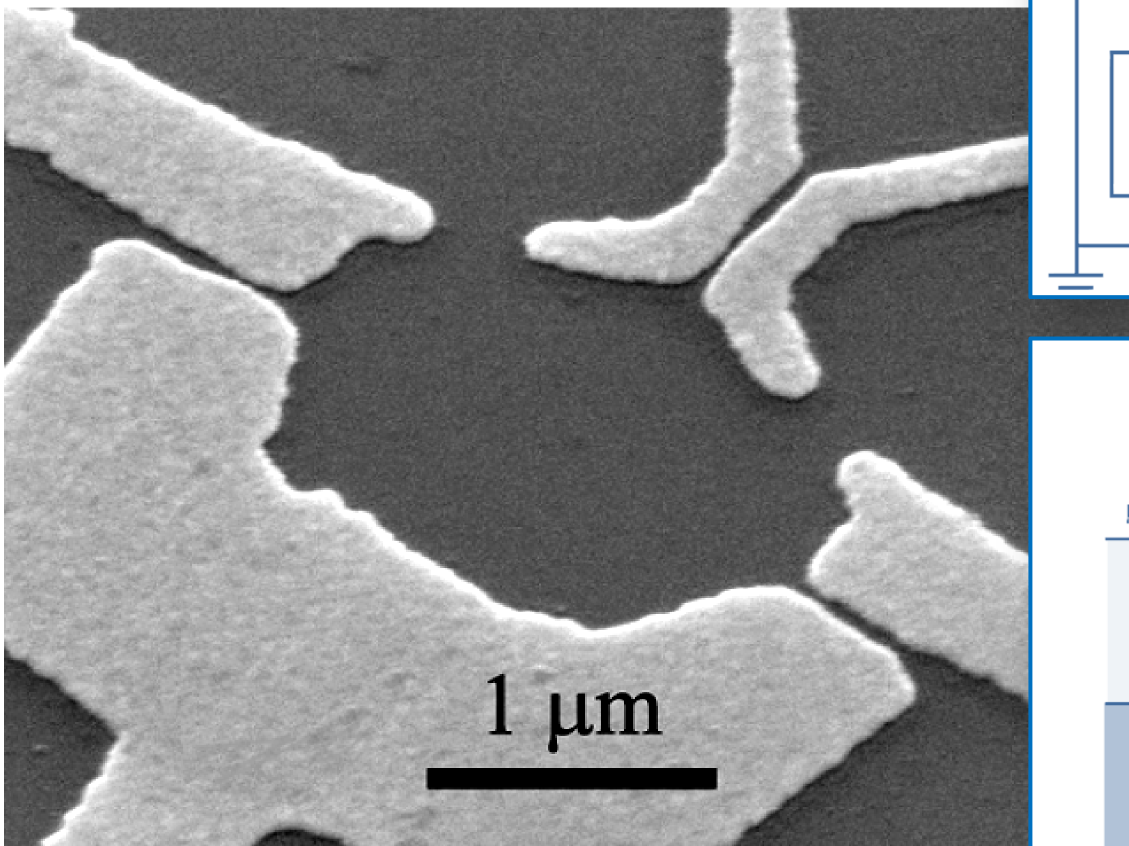


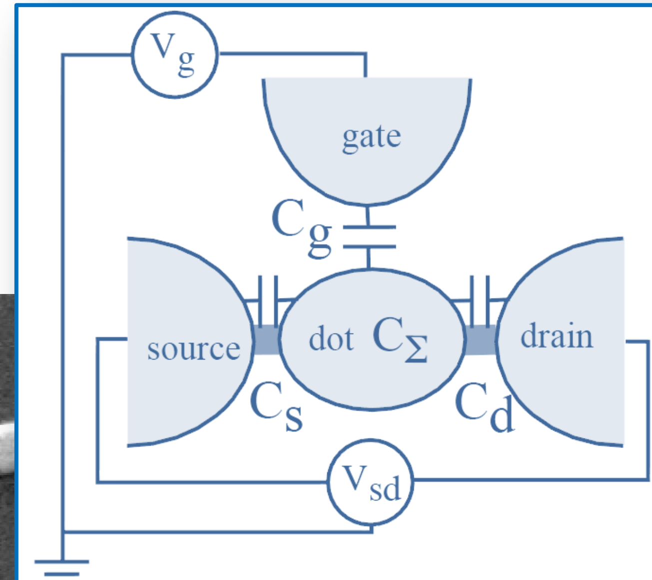


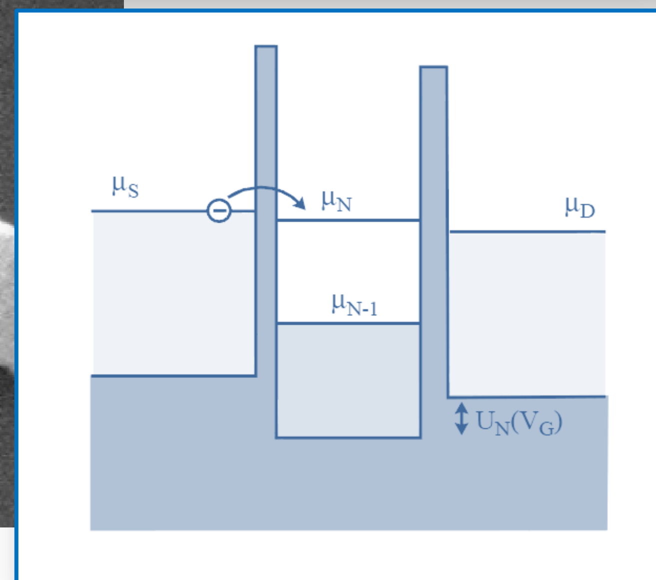


No confinement in graphene with gates !!!

Confinement through nanoribbons, double layer graphene



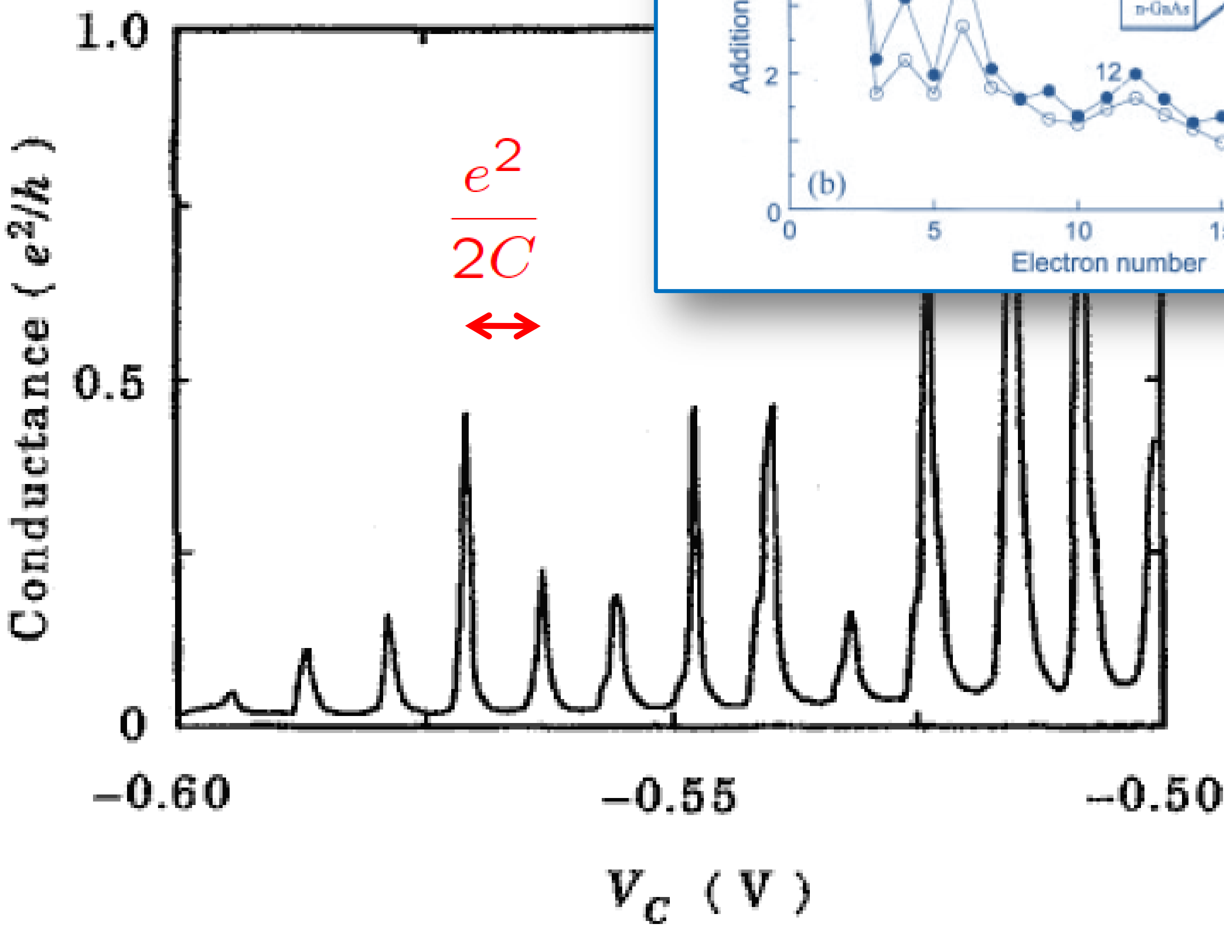


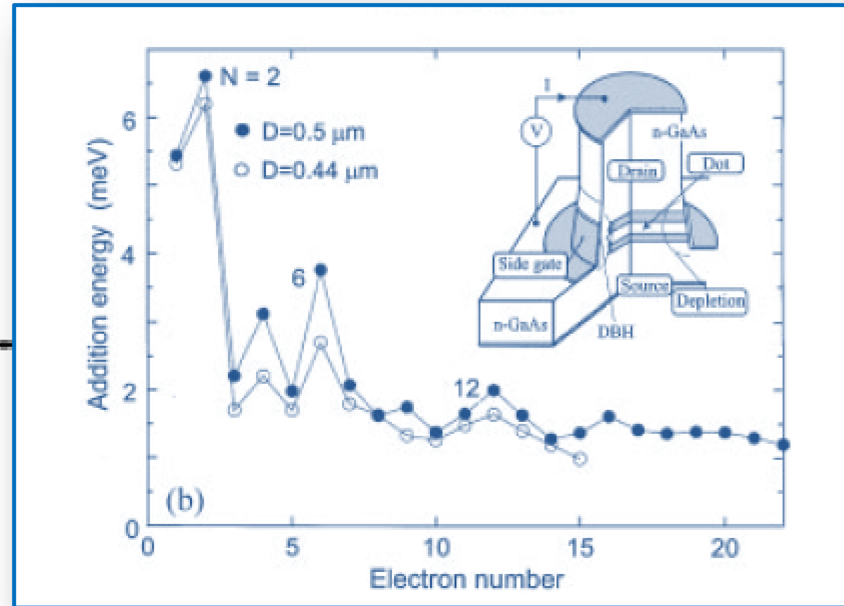


Electron tunneling through a QD

Coulomb blockade

Fine structure of Coulomb oscillations provides information about shell structure





Tarucha PRL 96

L. P. Kouwenhoven et al., Z. Phys. B 85, 367 (1991).

Coulomb blockade

Charge fluctuations to dot should be sufficiently small

$$\left(N - \langle N \rangle\right)^2 \ll 1$$

Temperature should be sufficiently low

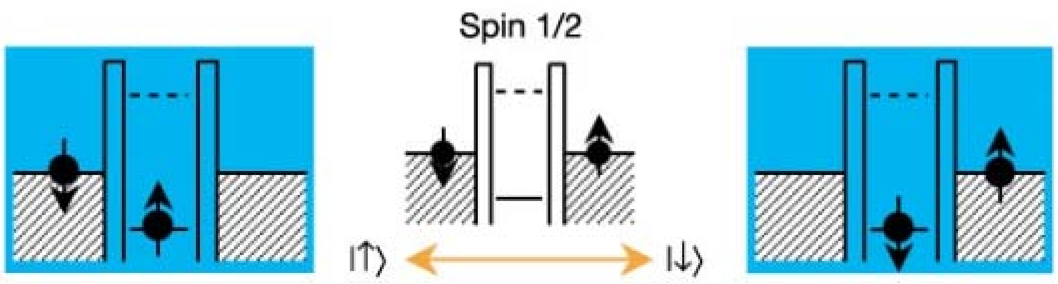
$$\frac{e^2}{2C} \gg k_B T$$

Tunnel couping should be sufficiently small – high tunnel resistance

$$\Delta E \Delta t \approx \left(\frac{e^2}{2C}\right) \times \left(R_T C\right) > \frac{\hbar}{2}$$

$$R_T > \frac{\hbar}{e^2} \sim 25\,\mathrm{k}\Omega$$

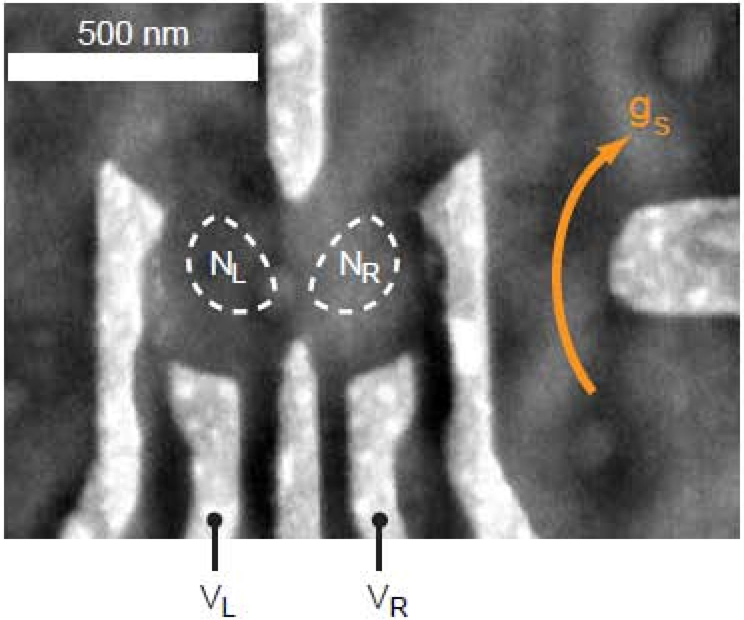
Other effects become important at low temperartrures (e.g. Kondo)

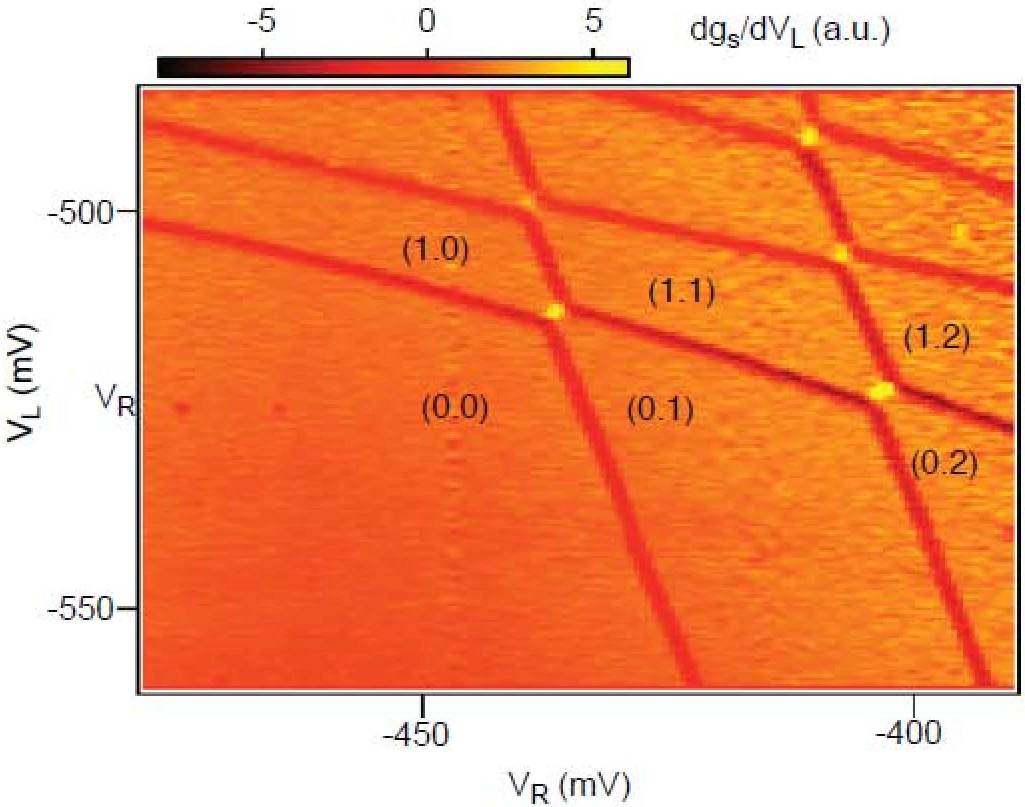


Coulomb blockade diamond

Variation of different voltages allows control and spectroscopy of states

Marcus lab, Harvard

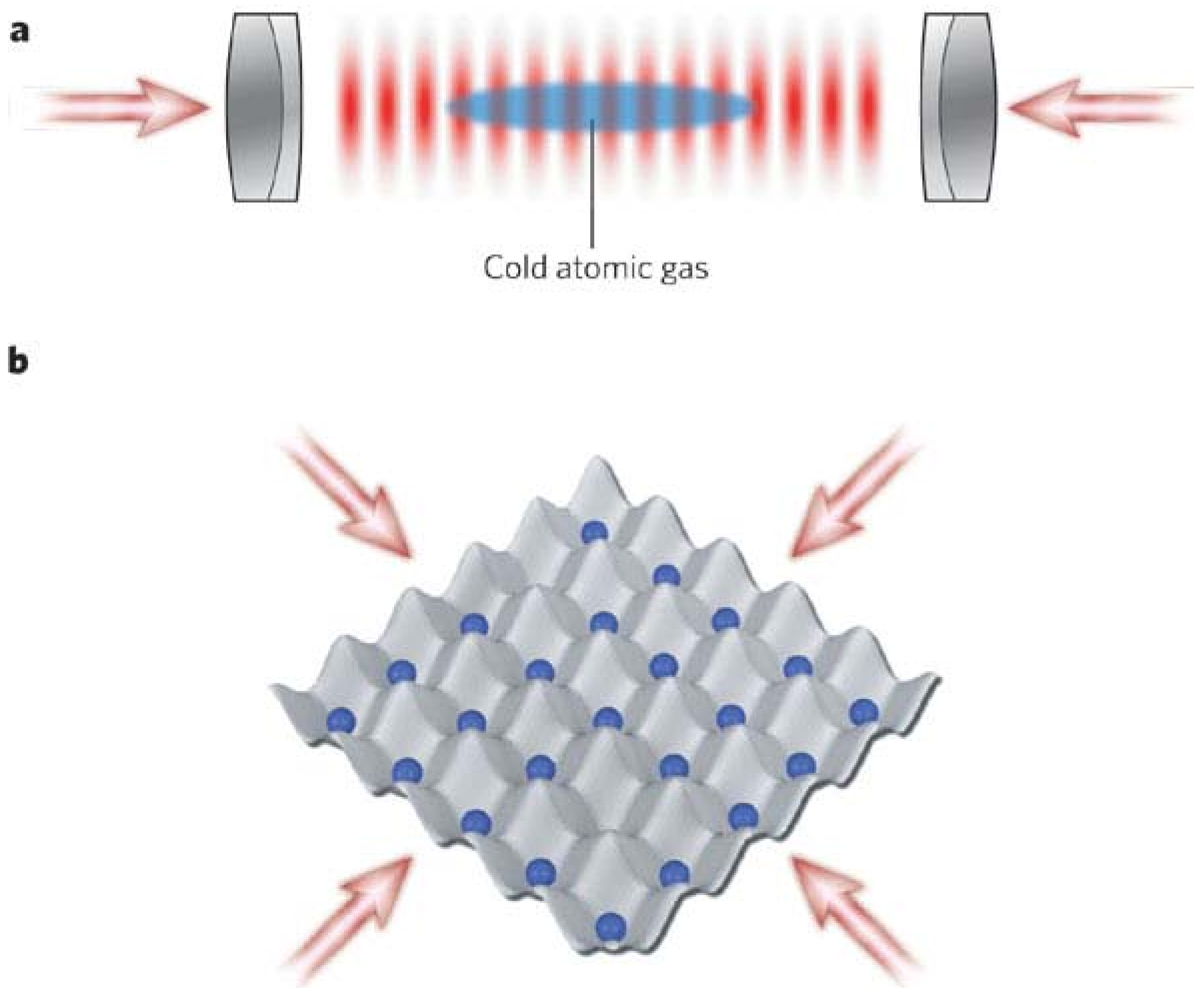




Double quantum dot states: competition between tunneling and Coulomb repulsion U

$t \gg U$ … electrons delocalized over structure

$U \gg t$ … electrons localized in separate wells

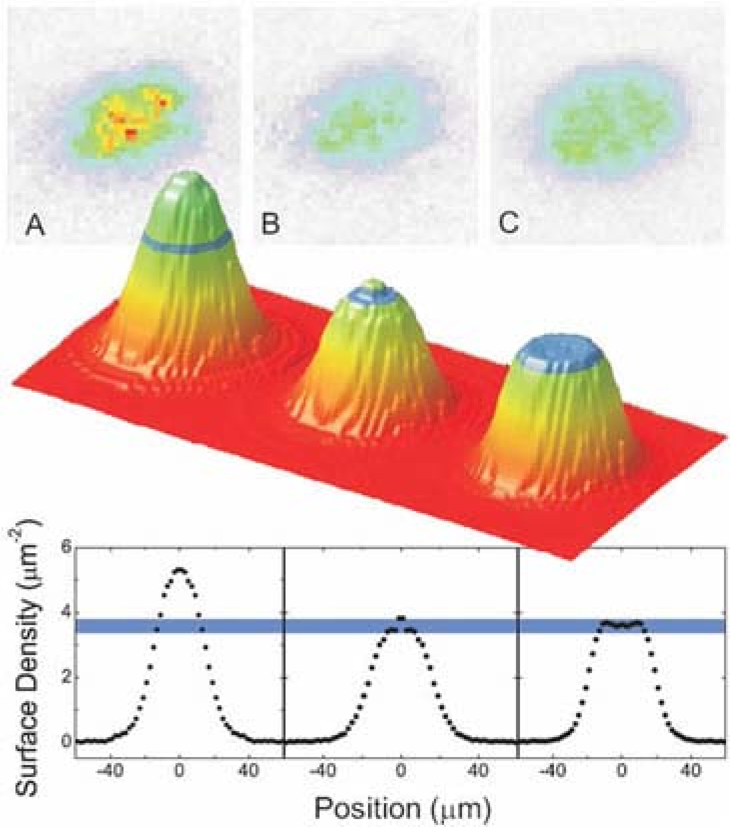


Atomic lattice:
control of tunneling and repulsive interaction

Delocalization vs. localization

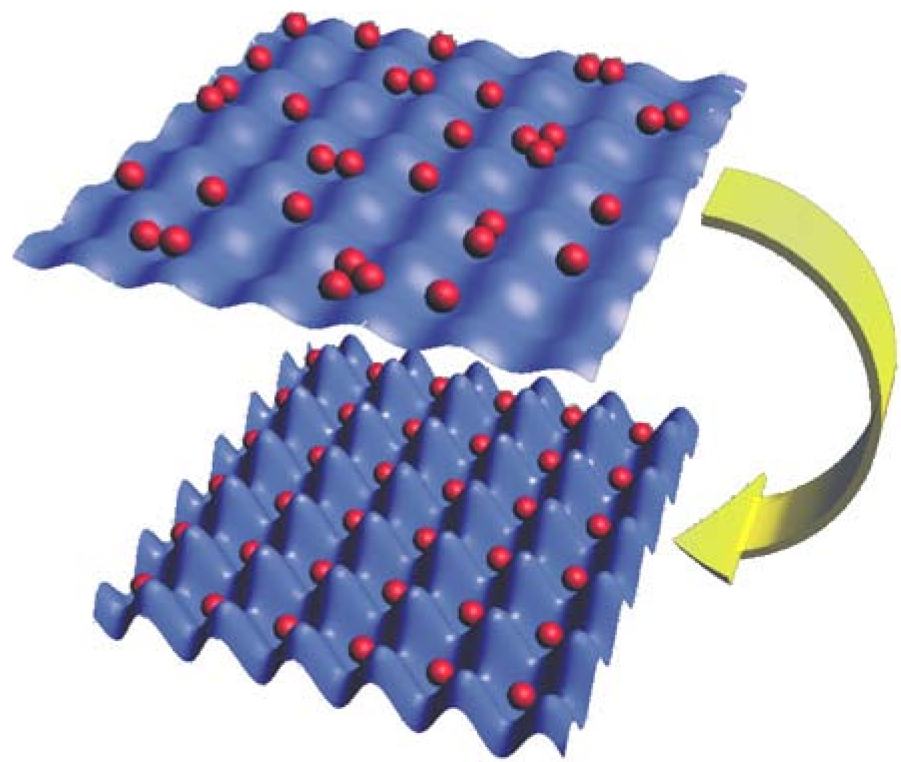
Variation of t and U: transition between superfluid and Mott insulator phase

Density at one lattice site

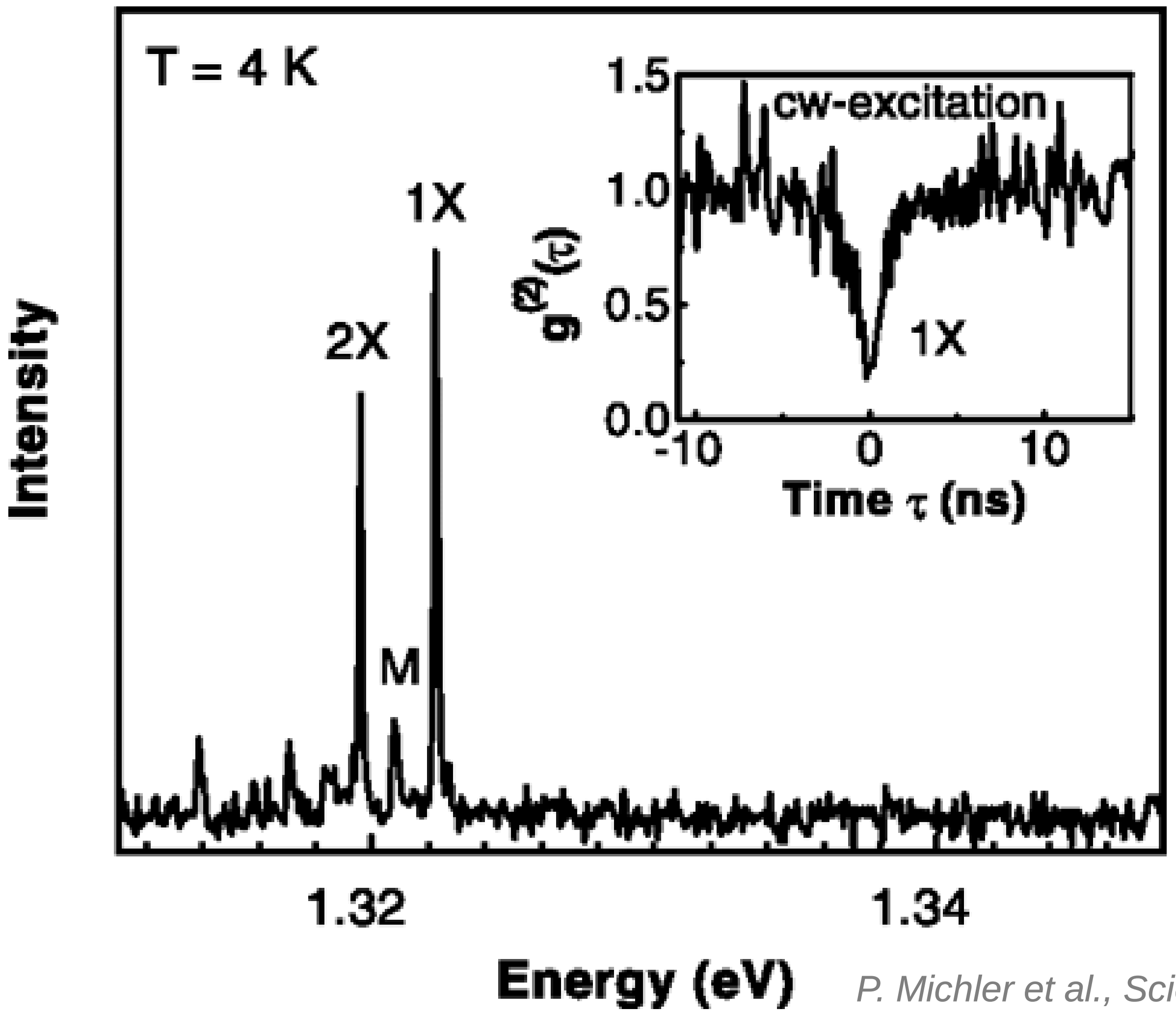


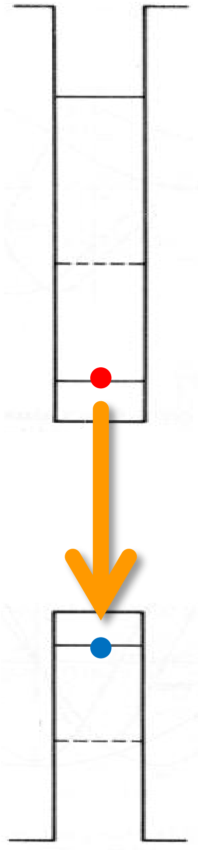
*Nathan Gemelke et al., Nature **460**, 995 (2009).*

Transition from t >> U to U >> t



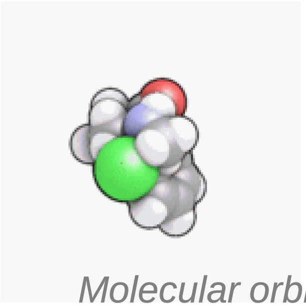
Excitons





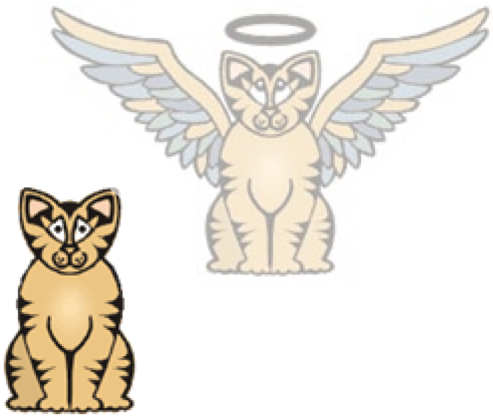
*P. Michler et al., Science **290**, 2282 (2000).*

Exciton = Electron-hole pair + Coulomb attraction



Molecular orbitals

How quantum is the nanoworld ?



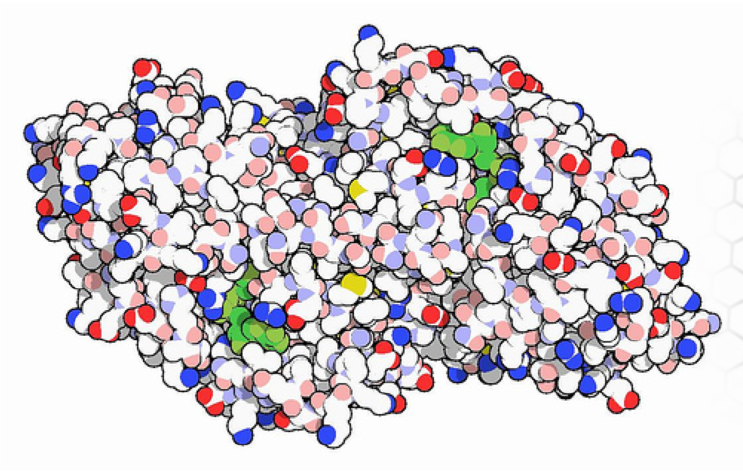
Superposition

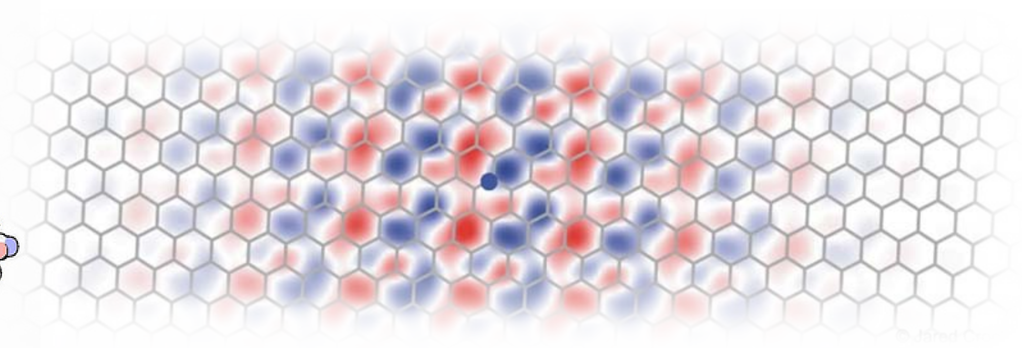
Eigenstates

System in contact with its environment

$$H = H_S + H_{\text{env}} + H_{\text{int}}$$

Eigenenergies and eigenstates E_i, ϕ_i





Wavefunctions can be complicated – this does not matter …

Superposition of eigenstates

Tunnel – coupled quantum dots

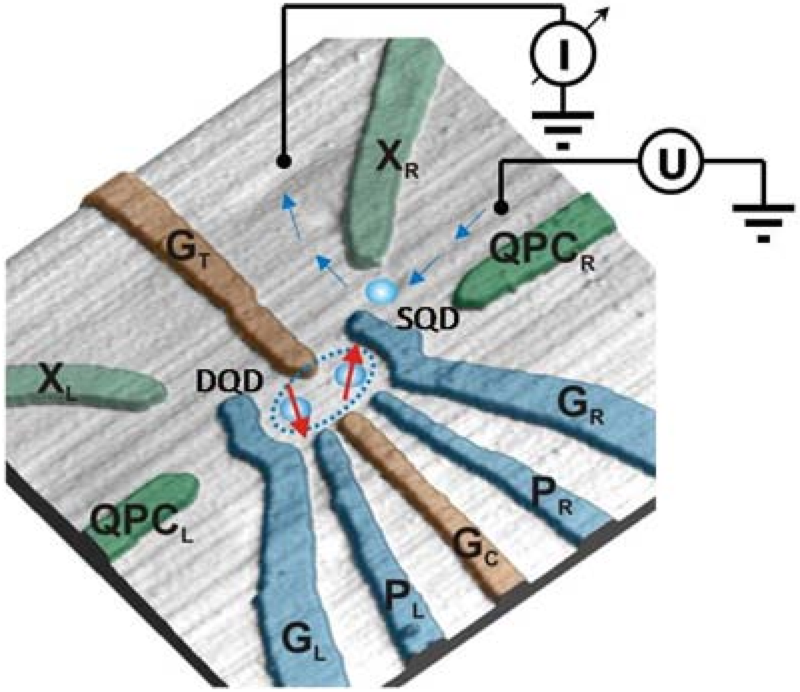
Hamiltonian of QDs

$$H_S = \begin{pmatrix} \epsilon_0 & t \\ t & \epsilon_0 \end{pmatrix}$$

Eigenstates

$$E_\pm = \epsilon_0 \pm |t|$$

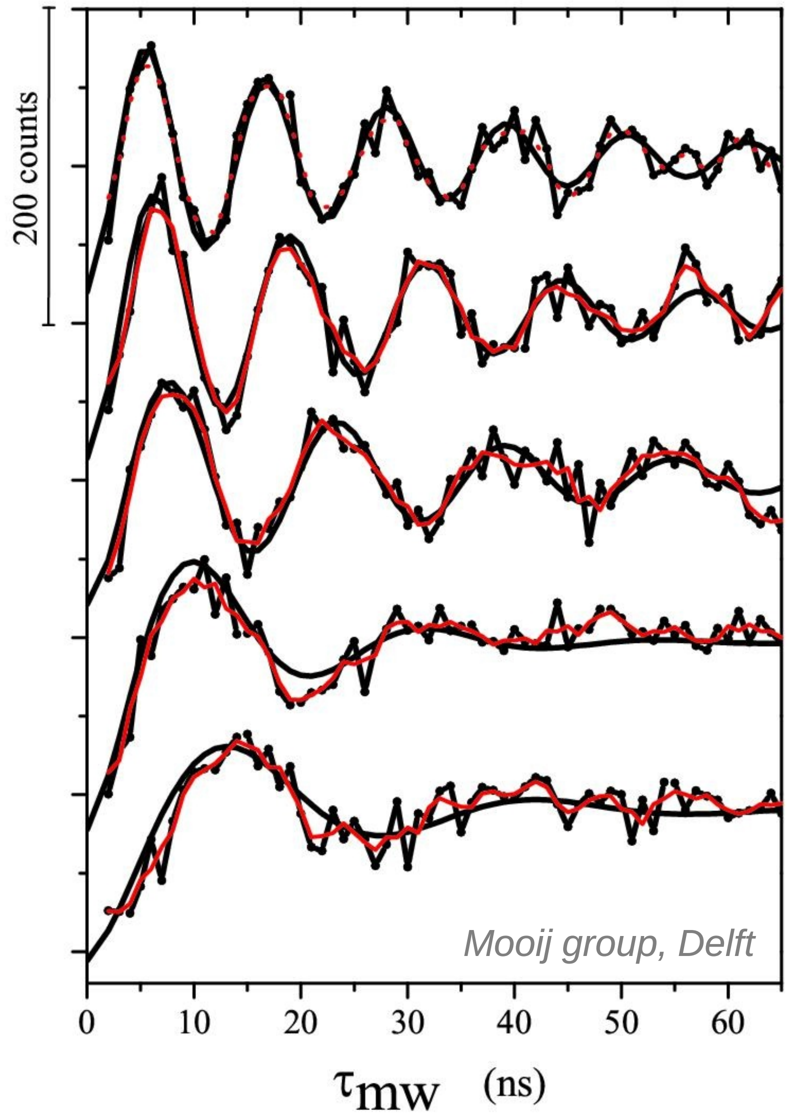
$$\phi_\pm = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \pm 1 \end{pmatrix}$$



Time evolution of superposition state

System tunnels between left and right well

$$\Psi(\tau) = \frac{1}{2} \left[\begin{pmatrix} 1 \\ 1 \end{pmatrix} e^{it\tau} + \begin{pmatrix} 1 \\ -1 \end{pmatrix} e^{-it\tau} \right] = \begin{pmatrix} \cos t\tau \\ i \sin t\tau \end{pmatrix}$$



Population oscillations are damped

Decoherence

von – Neumann measurement principle

Eigenstates of measurement apparatus

$$A\,\phi_i = \lambda_i \phi_i$$

Wavefunction collapse

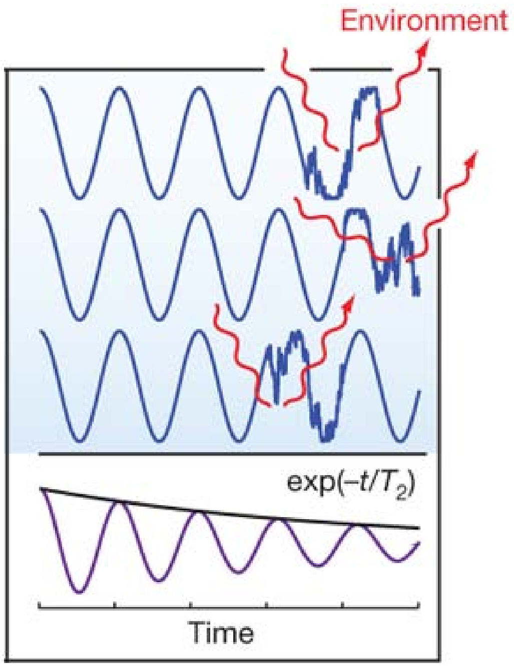
$$\Psi = \sum_i C_i\,\phi_i \longrightarrow (\lambda_k \text{ with probability } |C_k|^2) \longrightarrow \Psi = \phi_k$$

Environment

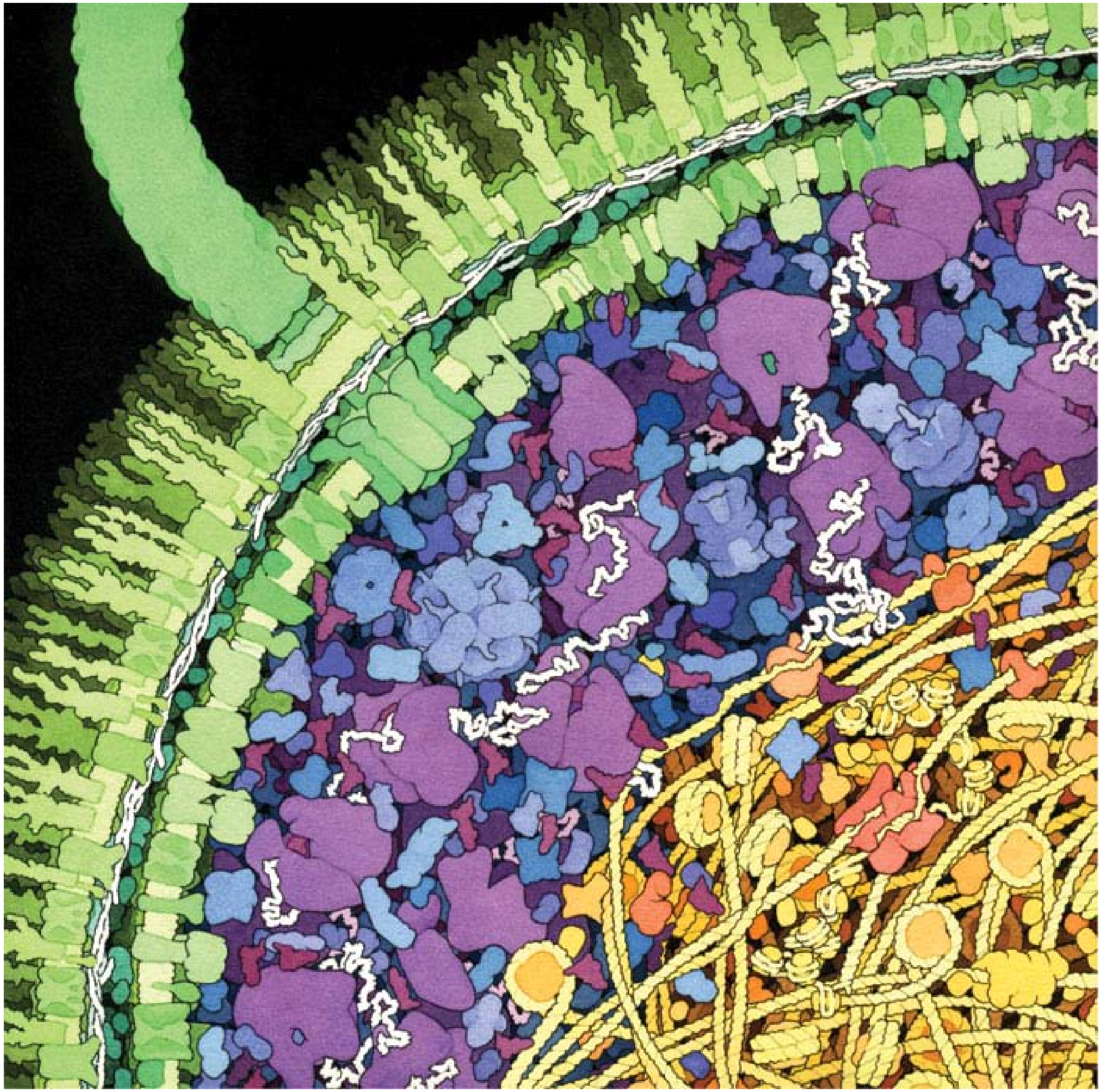
Also coupling to phonons, light, molecules etc. leads to decoherence

Good qubits are well proteced from the environment

Photon, electron spin, nuclear spin,
NV centers in (nano)diamand,
flux or phase qubits in superconductors, …



*T. D. Ladd et al., Nature **464**, 45 (2010).*



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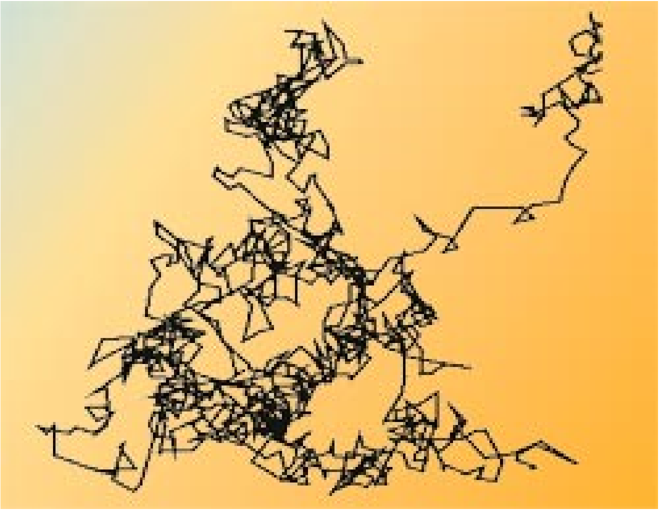
Bio machines are not very quantum …

Life needs temperature

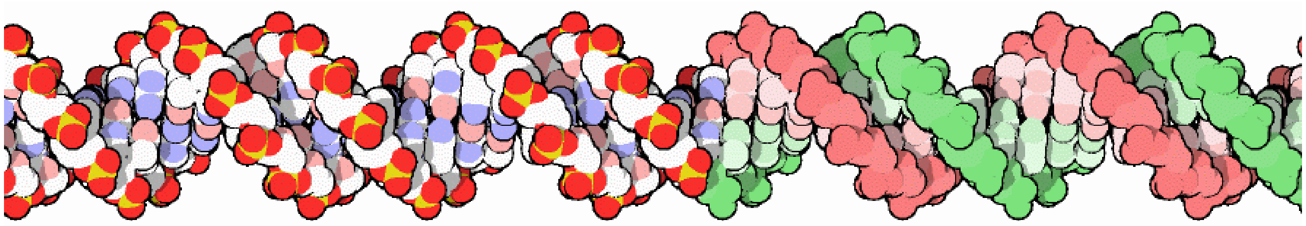
Brownian motion

Molecules, proteins in cells propagate through Brownian motion
If the cell is small enough, two molecules will find each other on a timescale of seconds

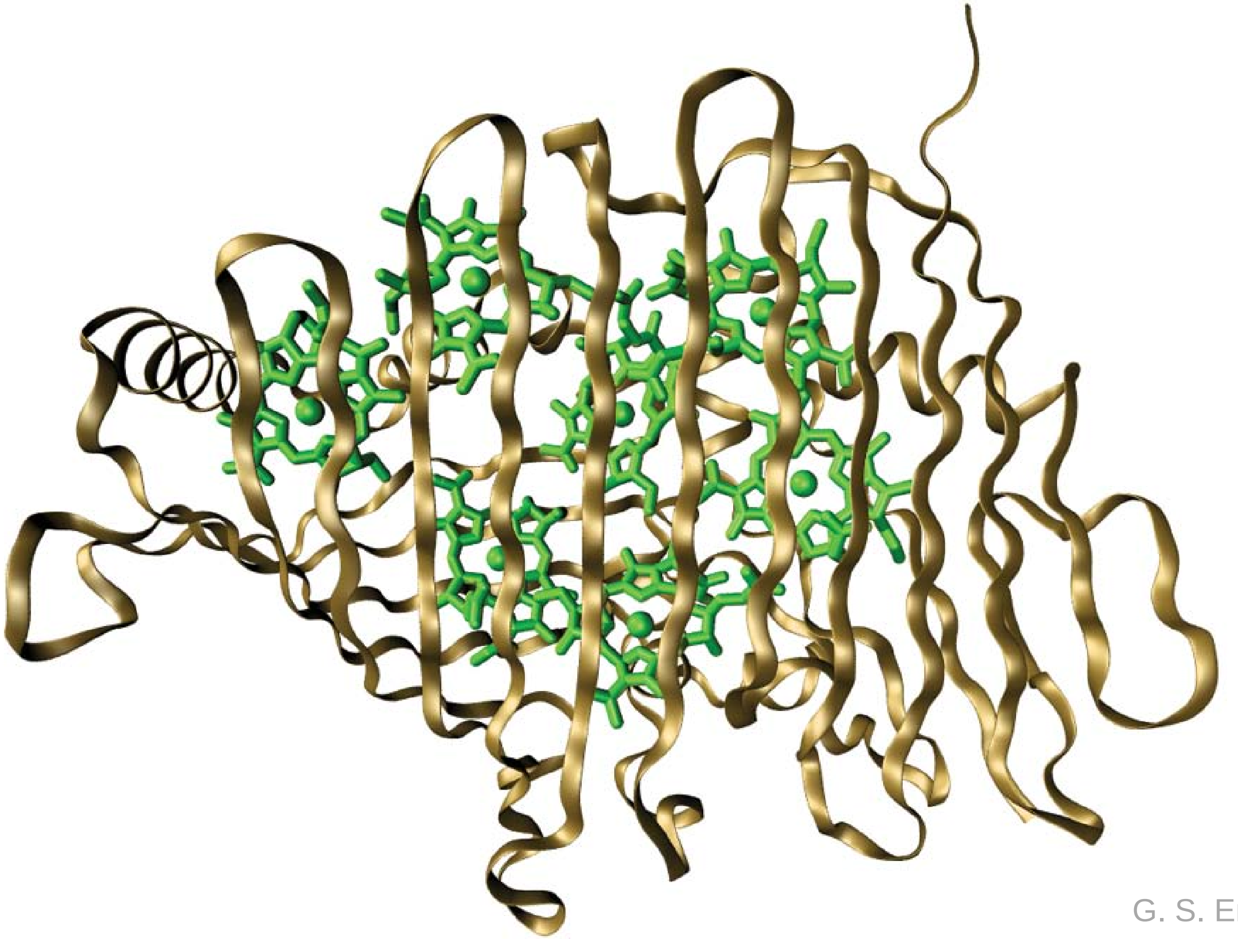


Thermal activation

Many processes in a cell require temperature,
e.g., DNA is usually close to the melting point



Quantum coherence in photosynthesis



G. S. Engel et al., Nature 446, 782 (2007).

The Fenna–Matthews–Olson complex helps green sulphur bacteria to perform photosynthesis. A quantum algorithm known as 'quantum walk' might be behind the remarkably efficient energy transfer between the light-collecting antennae and the reaction centre, where, ultimately, the photon energy is transformed into chemical energy.

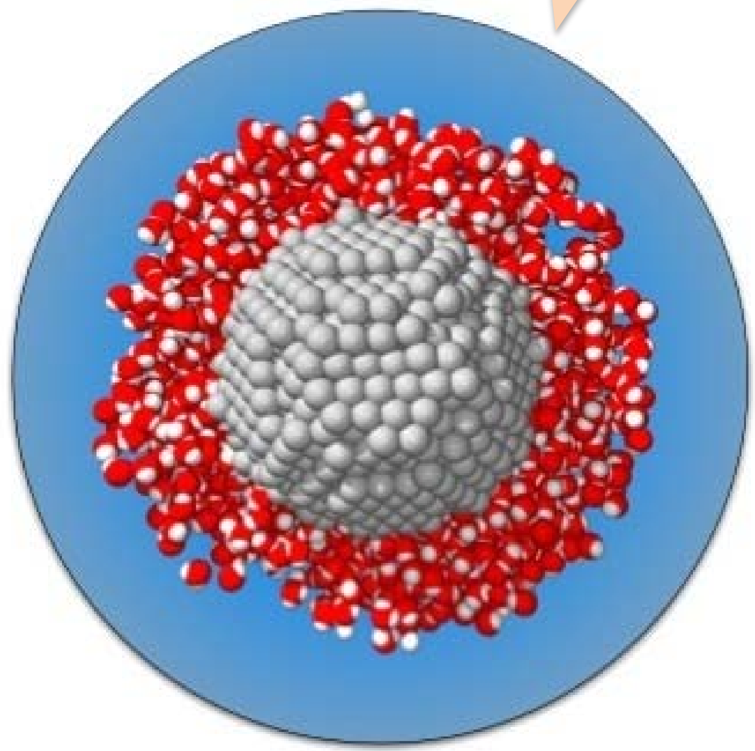
What we have done so far ...

Electrons in solids are *waves*

Confinement leads to discrete energy levels

Confinement enhances *Coulomb interactions*

Environment couplings lead to *decoherence*



Nanoscience: Fundamentals and basic properties	*Ulrich Hohenester*
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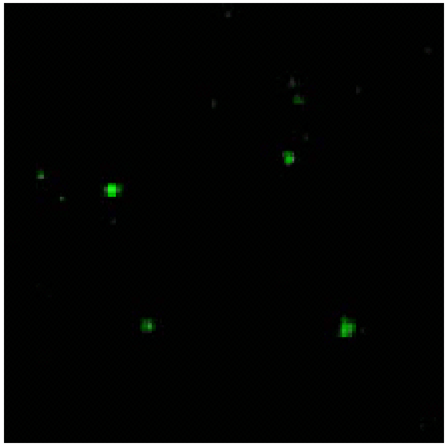
What is missing …

Single nanosystems

How do we know that we are measuring single systems ?



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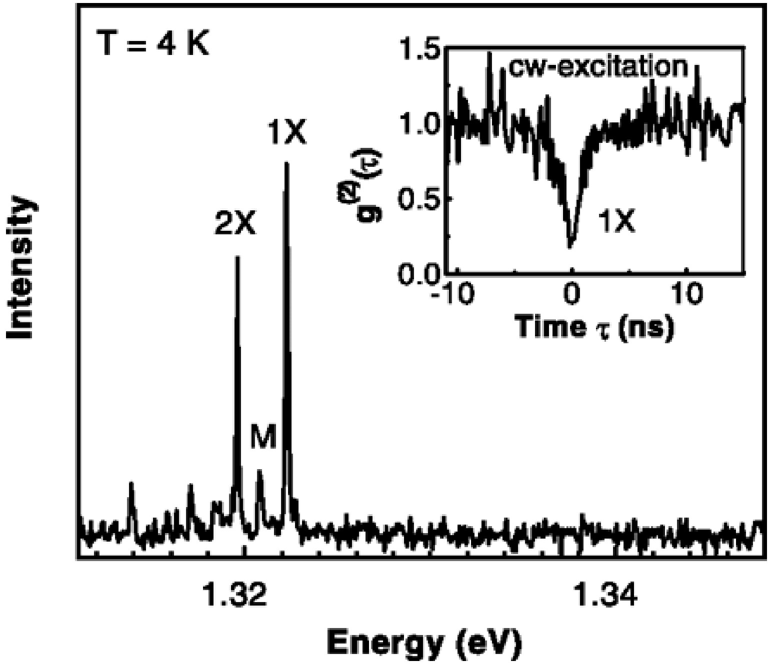
Colloidal dots exhibit „blinking“ where the dot turns between bright and dark periods on a second timescale.

This is due to charging and decharging of traps.



Photon statistics tells us whether we are investigating a single system or not:

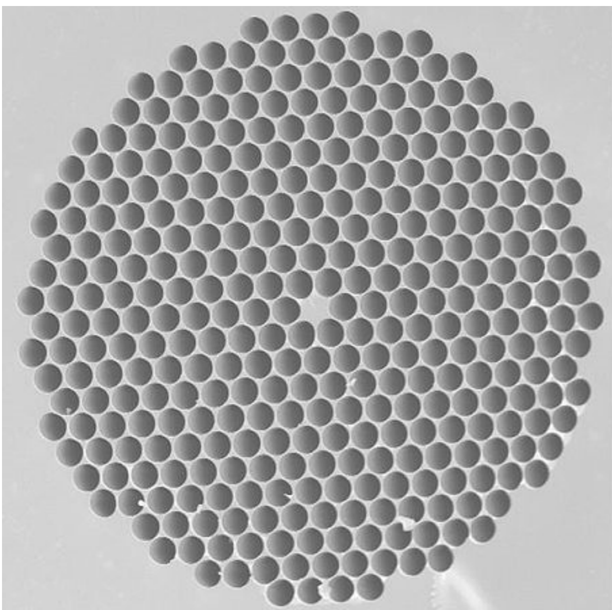
Once a photon is detected it takes a while to „reload“ the quantum emitter.

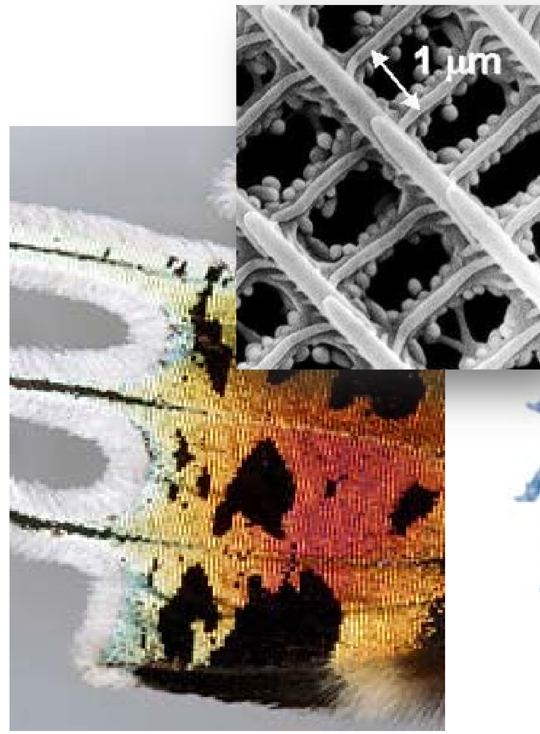
As result, two photons never arrive at the same time (photon antibunching).

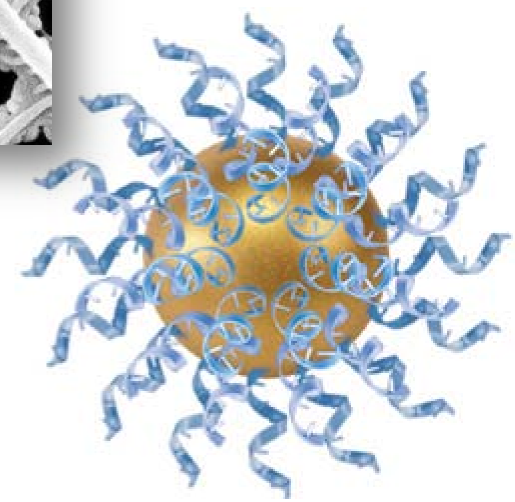
P. Michler et al., Science ***290****, 2282 (2000).*

Optics at the nanoscale

Optics ($\lambda \sim \mu$m) and nanostructures have a mismatch of dimensions





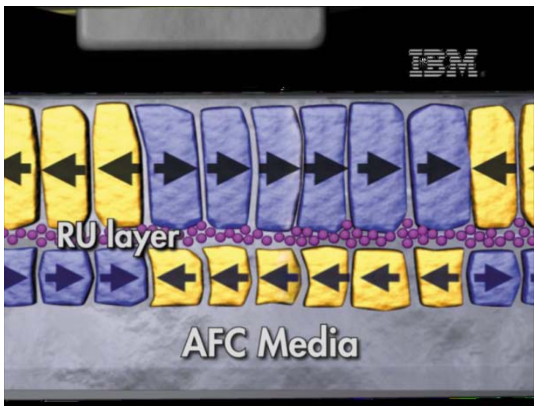


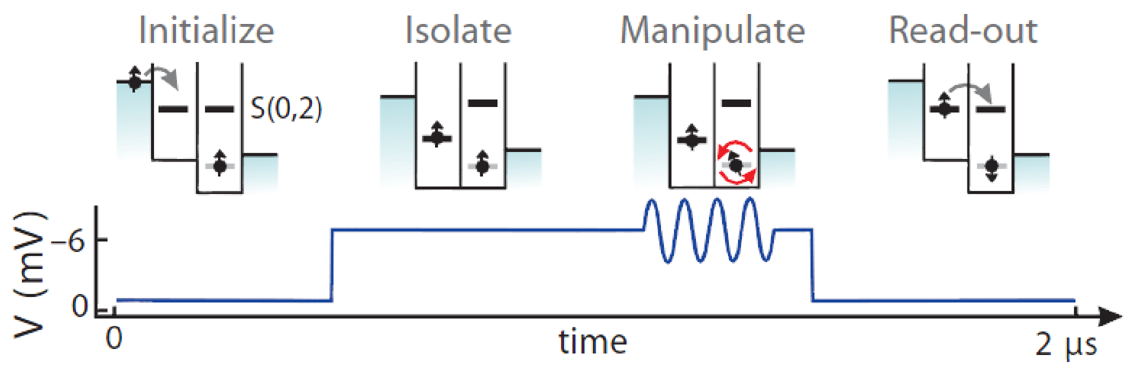
<u>Photonic crystals</u> allow the confinement of light on a micrometer length scale and to strongly enhance light matter interactions.

In <u>plasmonics</u> light is bound to metallic nanoparticles by exciting surface plasmons.

Nanomagnetism & spintronics

Spin couples only weakly to the solid state environment and thus provides an ideal means for storing (quantum) information.





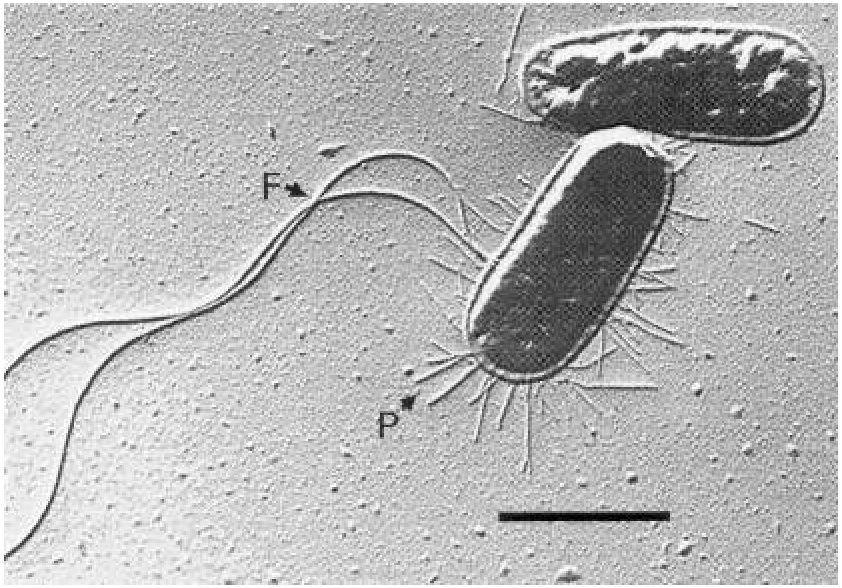
<u>(Nano)magnets</u> are used in hard disks to store information.

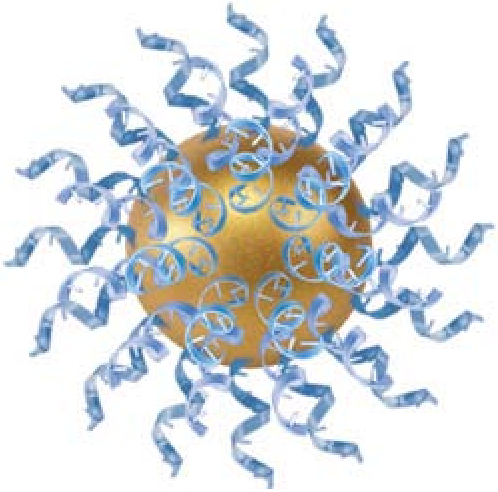
For small magnets there is a competition between bulk and surface effects, and it becomes difficult to suppress thermal flipping.

<u>Spin qubits</u> are possible candidates for building blocks of quantum computers.

Much progress has been made recently in order manipulate the spins and to suppress decoherence (due to phonons and nuclear spins).

Forces, fluids, heat at the nanoscale





Forces at the nanoscale are dominated by intermolecular and van der Waal forces. Gravity plays (usually) no role.

Nanoscale fluid mechanics has to account for the motion of single molecules. Due to the strong forces, an Escherichia coli bacterium in water comes to a complete halt on a length scale of sub-nanometers.

Heat transfer at the nanoscale is a challenge for miniaturized nanodevices and presently constitutes one of the major roadblocks of computer industry.