Scanning Tunnelling Microscopy (STM)

An introduction to the principles with research example

Steven R. Schofield

Professor of Physics

London Centre for Nanotechnology
Department of Physics and Astronomy
s.schofield@ucl.ac.uk

Nanosciences@Surfaces – Summer School
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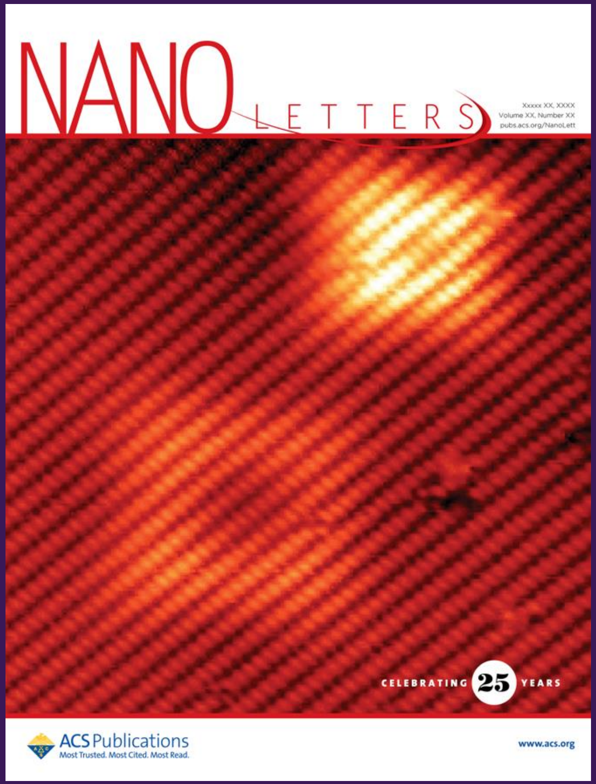
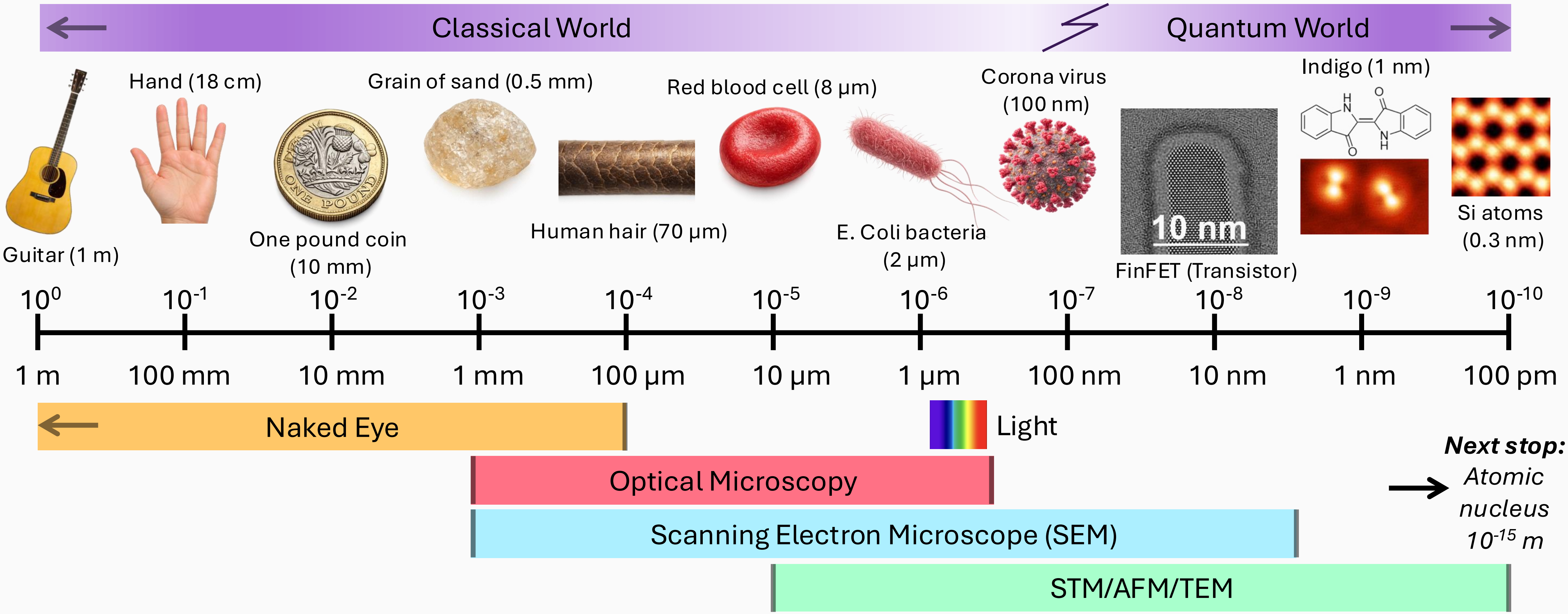


Acceptor states on a Si(001) surface

Siegl *et al.*, Nano Lett. **25**, 13996 (2025)

schofield-lab.github.io

How does the world look when you zoom in a billion times?

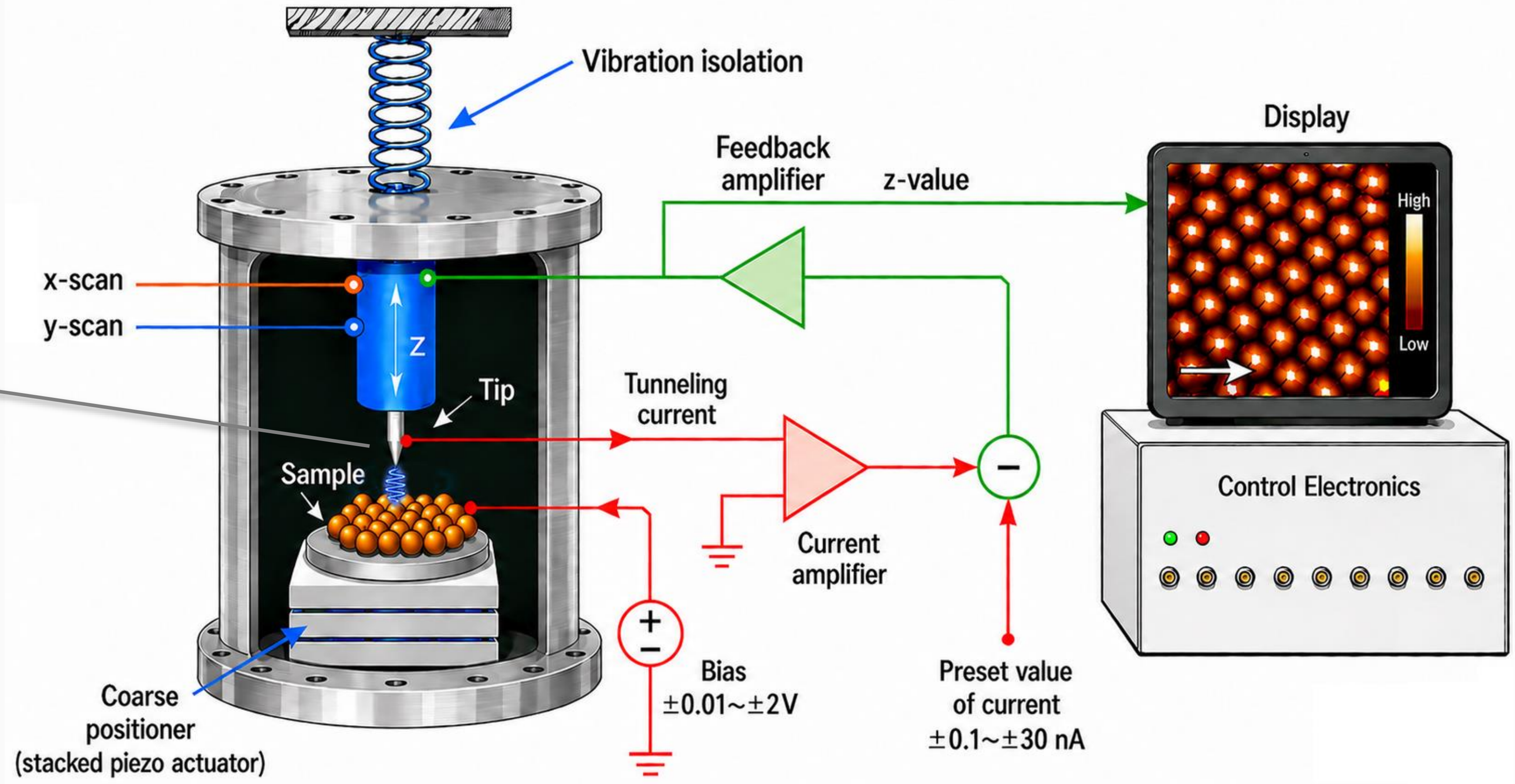


Scanning Tunnelling Microscopy

Sub-Angstrom sensitivity to tip height enables atomic-resolution imaging via a feedback loop.

$$I \propto e^{-2\kappa d}$$

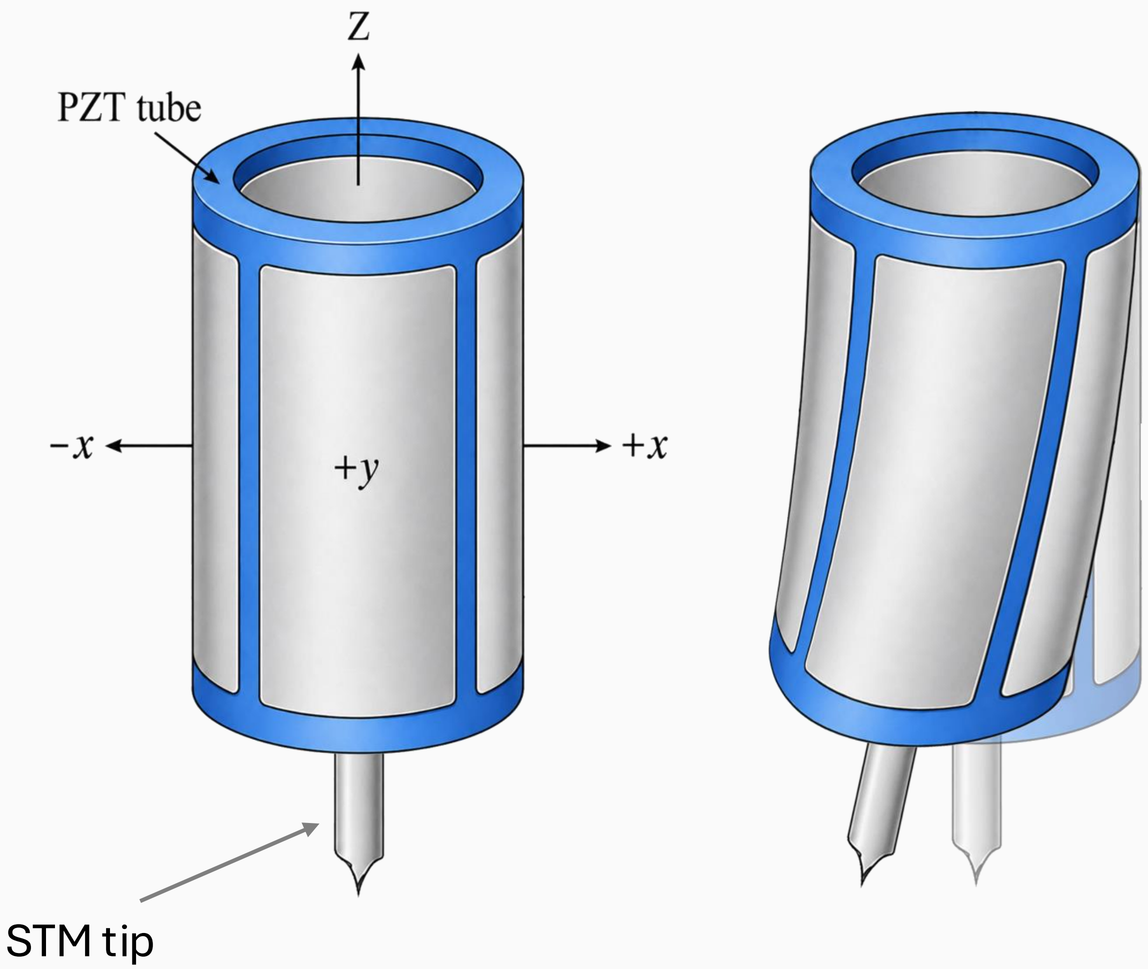
$\sim \times 10$ per 0.1 nm



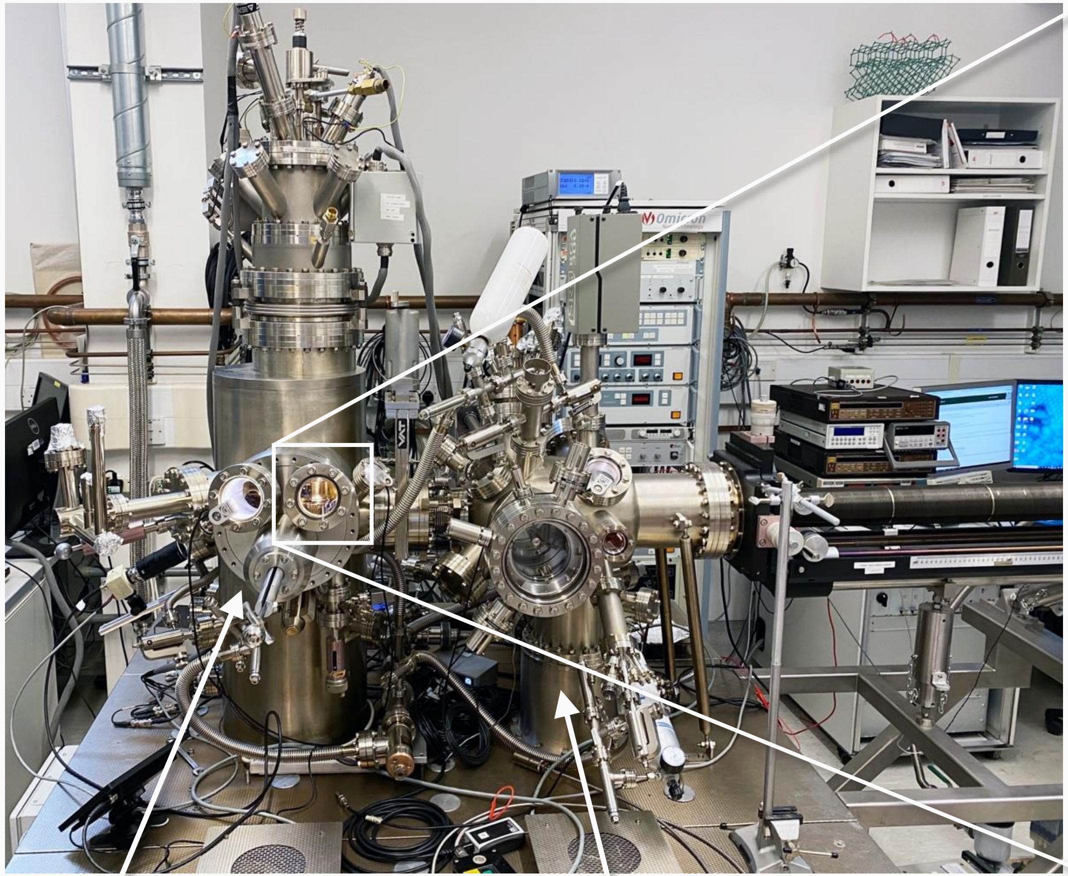
STM scanner tube

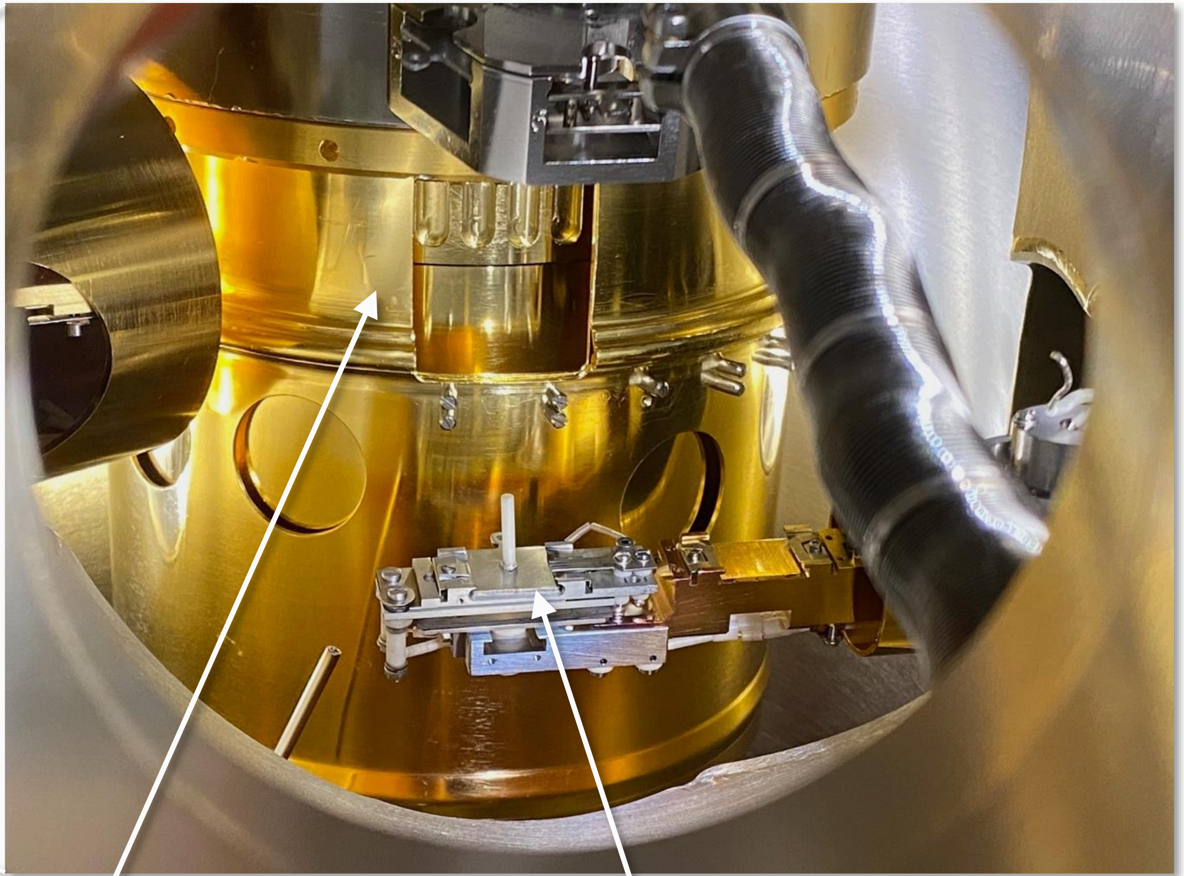
- Scanner: hollow piezoelectric tube
- Outer electrode split into four quadrants (±x, ±y); single inner electrode
- z extension/retraction: voltage between inner and outer electrodes
- x-y scanning: differential voltage across opposing quadrants causes tube to bend.
- Typical piezo constant: ~50 Å/V (200 V gives 1 µm extension)
- Tube geometry is compact, stiff, and has a high resonance frequency, making it the standard scanner in modern STMs

STM Piezo Scanner Tube



Ultra-high Vacuum Cryogenic STM





STM chamber

Preparation chamber

Thermal shielding
(STM is inside)

Sample and cleave post
on manipulator arm

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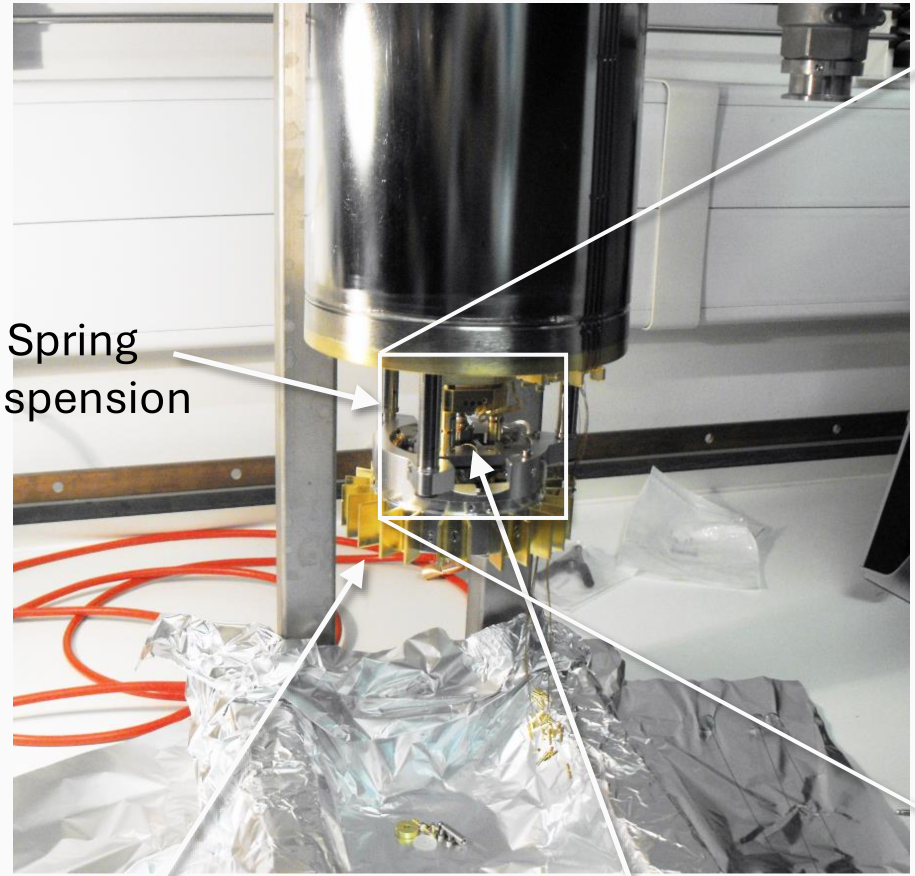
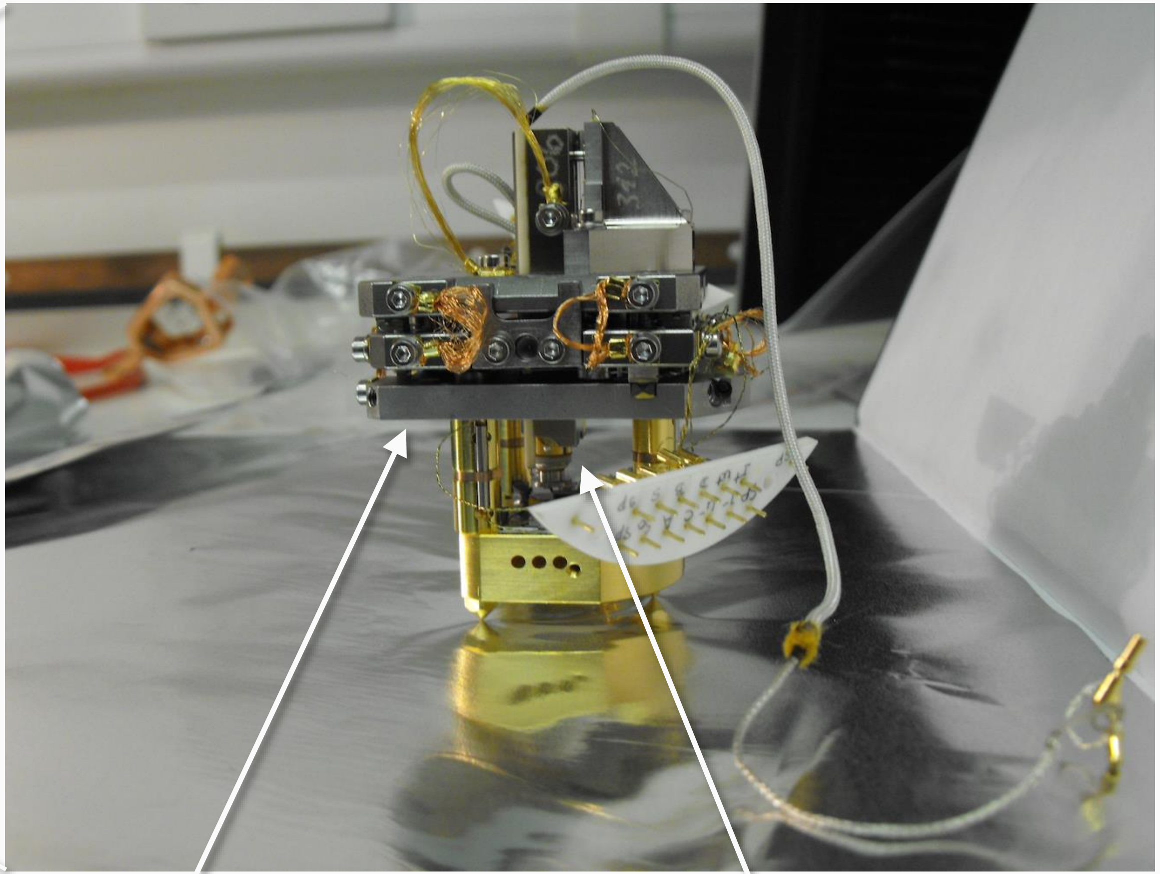
Ultra-high Vacuum Cryogenic STM

Coarse positioner and STM scanner – its upside down compared to the left image



Spring suspension



Copper fins for eddy current damping

STM scanner tube

Coarse positioner (stacker piezo actuator)

STM scanner tube

Quantum tunnelling through a barrier

- The one-dimensional Schrödinger equation

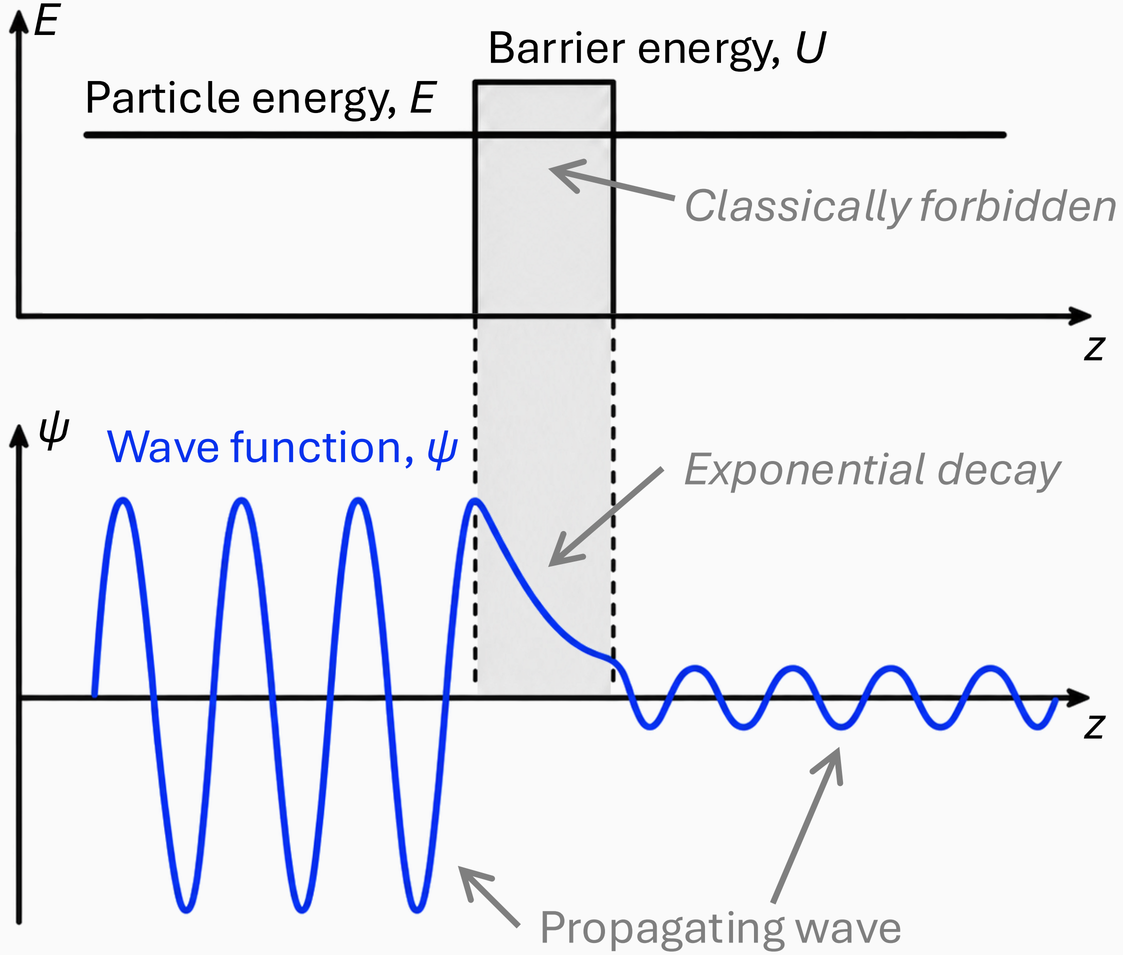
$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dz^2}+U(z)\right)\psi(z)=E\psi(z)$$

- Classically-allowed region: propagating wave

$$\boxed{\psi(z)=Ae^{\pm ikz}} \qquad k=\sqrt{2m(E-U)}/\hbar$$

- Classically-forbidden region: evanescent decay

$$\boxed{\psi(z)=Be^{\pm\kappa z}} \qquad \kappa=\sqrt{2m(U-E)}/\hbar$$

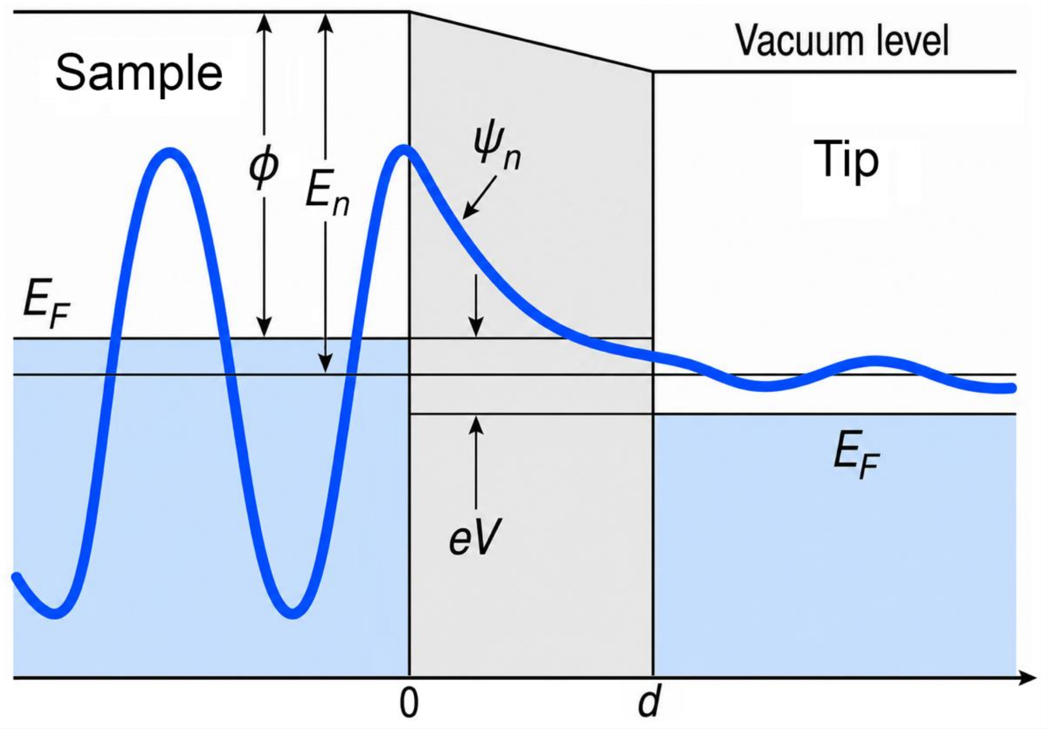


Quantum tunnelling through a barrier

- This 1D barrier model maps directly to the STM.
- For electrons close to E_F the barrier height is approximately the work function ϕ, so that the decay constant is:

$$\kappa = \frac{\sqrt{2m(U - E_n)}}{\hbar} \simeq \frac{\sqrt{2m\phi}}{\hbar}$$

- A small applied bias voltage offsets the Fermi levels, enabling a tunnelling current.



Quantum tunnelling through a barrier

- In the barrier, the wave function is dominated by

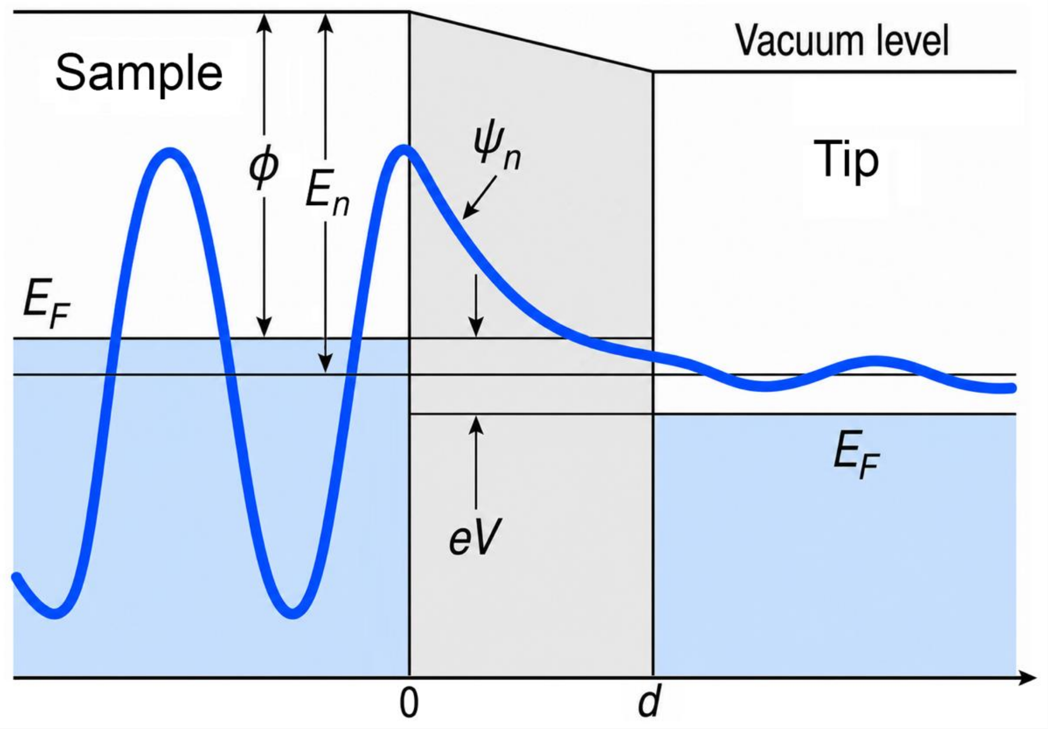
$$\psi(z) = \psi(0)e^{-\kappa z} \qquad \kappa = \sqrt{2m\phi}/\hbar$$

- The transmission probability is set by the ratio of probability density at the far side (z=d) to the near side (z=0):

$$T \propto \frac{|\psi(d)|^2}{|\psi(0)|^2} = e^{-2\kappa d}$$

- Thus the tunnelling current varies exponentially with tip-sample separation, d:

$$I \propto e^{-2\kappa d}$$



The Origin of Atomic Resolution: *z*-sensitivity

- Tunneling current decays as: $$I \propto e^{-2\kappa d}$$
- The exponential decay rate: $$\kappa = \frac{\sqrt{2m\phi}}{\hbar} = 5.123\sqrt{\phi(\mathrm{eV})}$$
- Work functions of common tip/sample materials are ~5 eV.

Element	Al	Au	Cu	Ir	Ni	Pt	Si	W
ϕ (eV)	4.1	5.4	4.6	5.6	5.2	5.7	4.8	4.8
κ (nm^{-1})	10.3	11.9	10.9	12.1	11.6	12.2	11.2	11.2

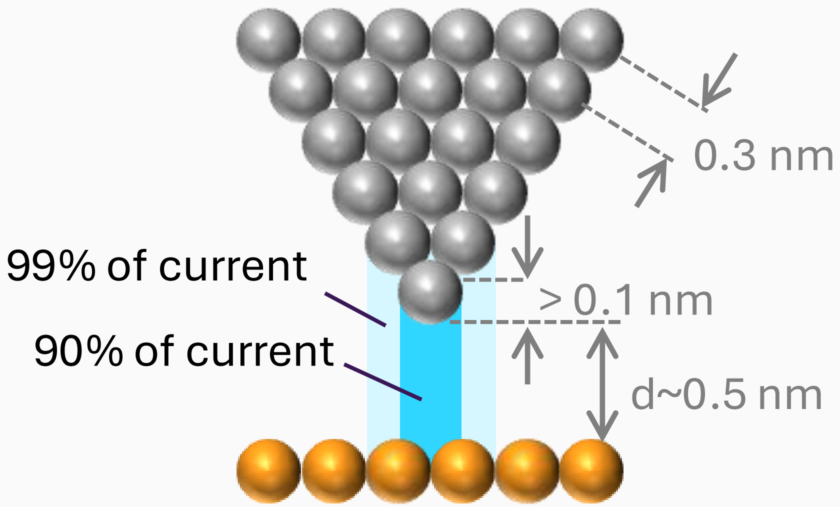
- **Rule of thumb: current drops by 10× for every 0.1 nm increase in tip-sample separation**
- *This exceptional sensitivity to distance is the physical origin of atomic resolution in STM*

UCL

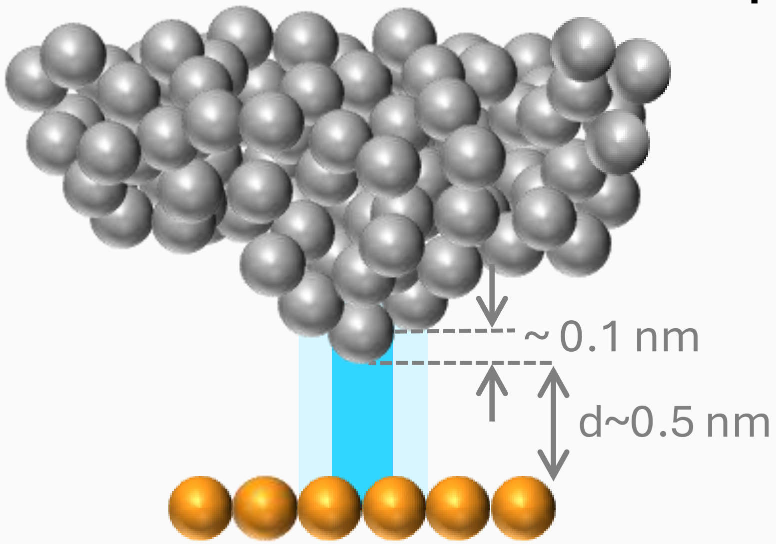
The Origin of Atomic Resolution: *xy*-sensitivity

- The order of magnitude decrease in tunnelling current per Angstrom is also responsible for the spatial resolution of STM
- With interatomic distances ~ 3 Ang., one atom of the tip is very often at least 1 Ang. Closer to the surface, such that 90% of the tunnelling current passes through this one atom.

"Ideal crystalline tip"



Remains true even for disordered tips

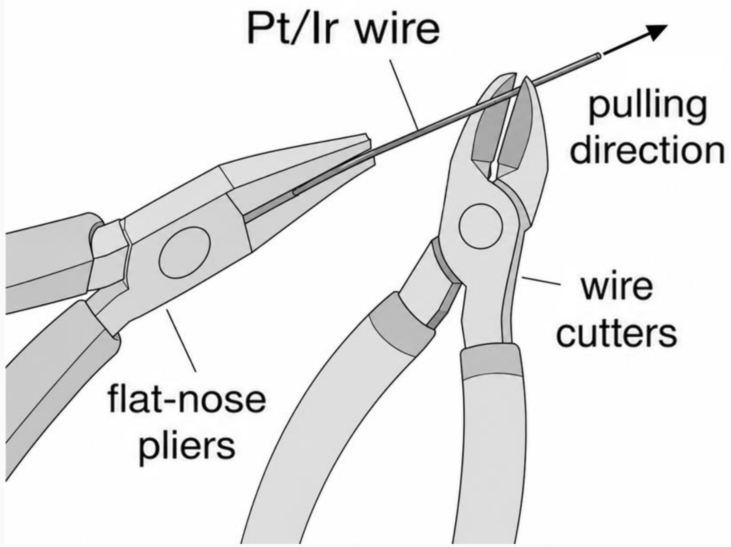


STM tips and how they are made

Platinum-iridium and tungsten are the two most common tip materials

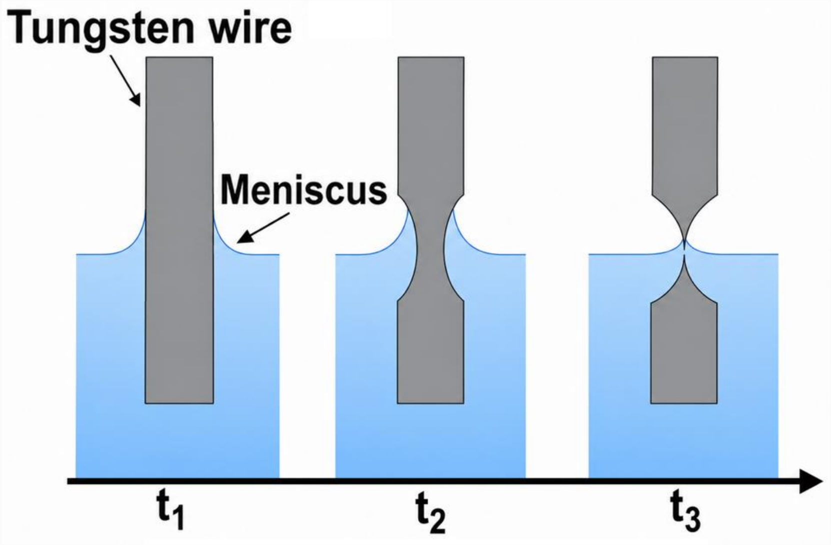
Platinum-iridium (Pt/Ir)

- Made by simply by cutting.
- Used in air or vacuum
- Used as cut

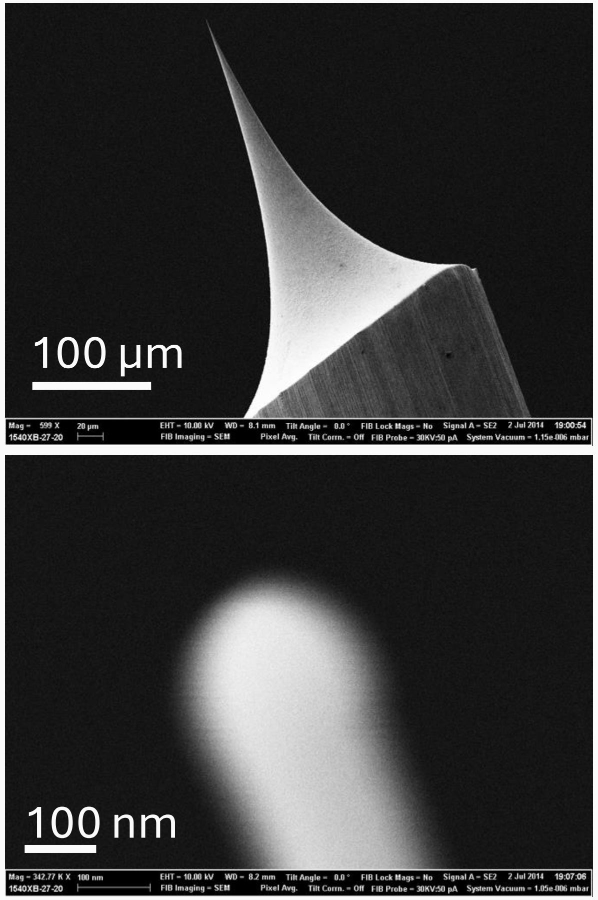


Tungsten:

- Electrochemically etched in KOH
- Mainly used in ultrahigh vacuum (UHV)
- Best when oxide removed in UHV



SEM images



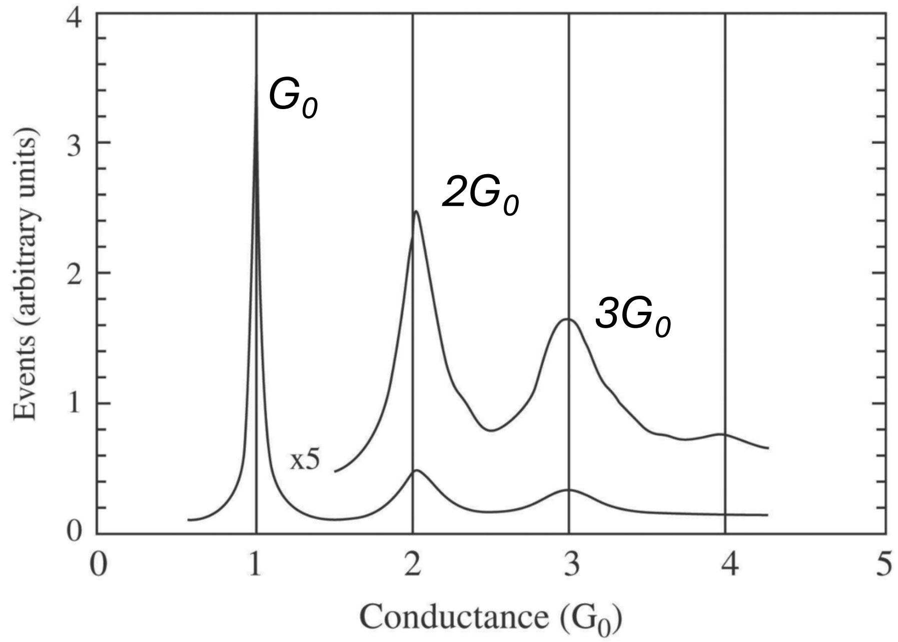
Setting the current scale: the quantum of conductance

- Landauer's model of transmission through a single channel, gives the natural unit of conductance in quantum systems: the quantum of conductance (or resistance):

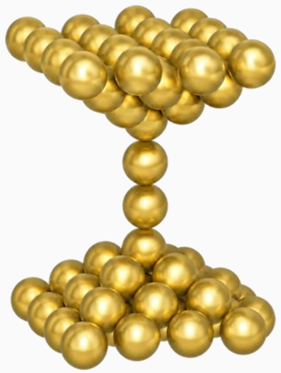
$$G_0 = \frac{2e^2}{h} \approx 77.48\,\mu\mathrm{S} \quad \left(R_0 = \frac{1}{G_0} \approx 12.9\,\mathrm{k}\Omega\right)$$

- For example, stretching a gold contact forms atomically thin bridges, down to a single-atom wire.
- A histogram over many break events peaks at integer multiples, the first at G_0

Histogram of conductance measurements

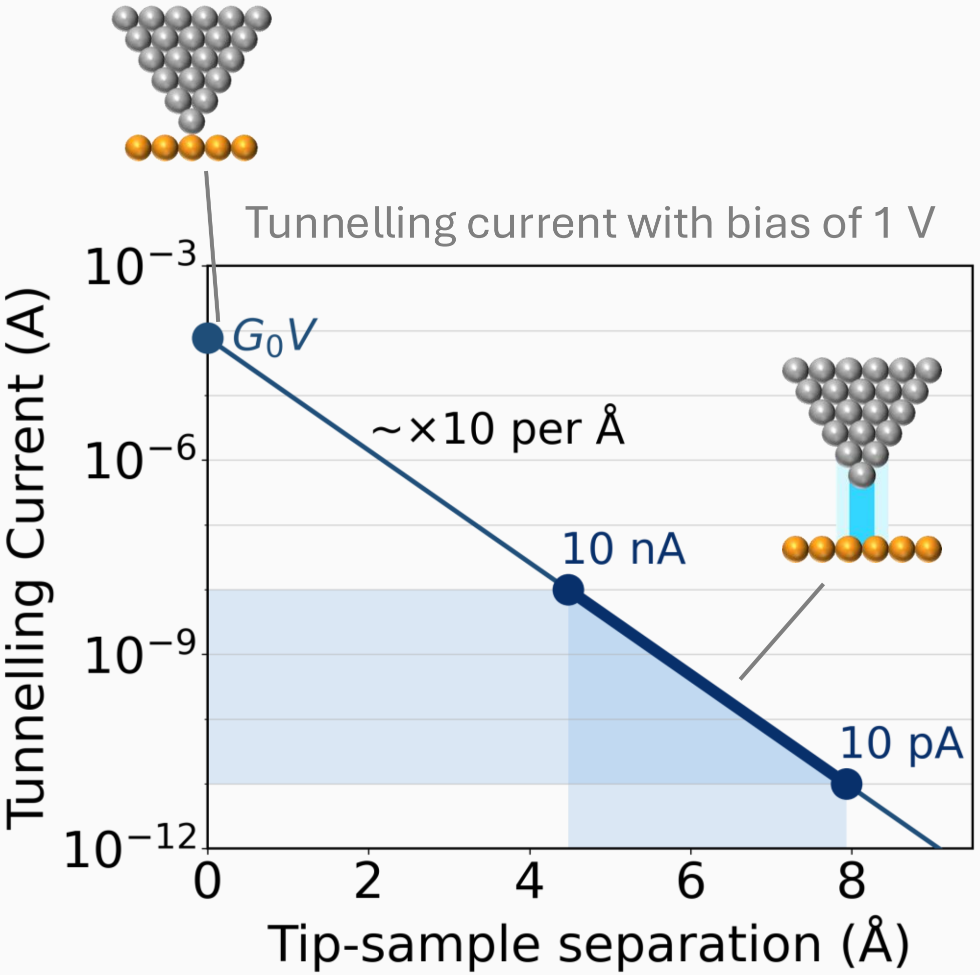


Single-atom gold wire



Absolute Current in STM

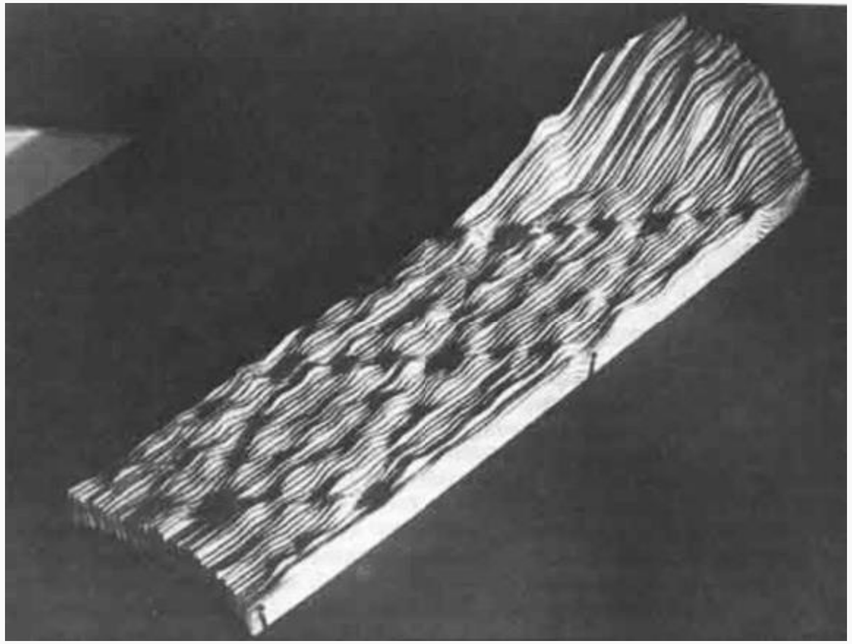
- This sets the current scale for STM: a single-atom contact sits near G_0, and the current falls as $e^{-2\kappa d}$ as the tip retracts: $$G(d) = G_0 e^{-2\kappa d}$$
- Current follows from Ohm's law: $$I = G(d)V$$
- At $d = 0$, this recovers the contact value, $G_0 V$
- With $\kappa \approx 1$ Å^{-1}, each extra Å of separation suppresses the current by ~e^2, roughly an order of magnitude
- Typical STM currents, 10 pA to 10 nA, correspond to $d \approx 4.5$ to 8 Å
- Because d depends on the log of the current, even a large error in bias or tip transmission shifts the inferred separation by less than an Å.



STM's first triumph: solving Si(111)-7×7

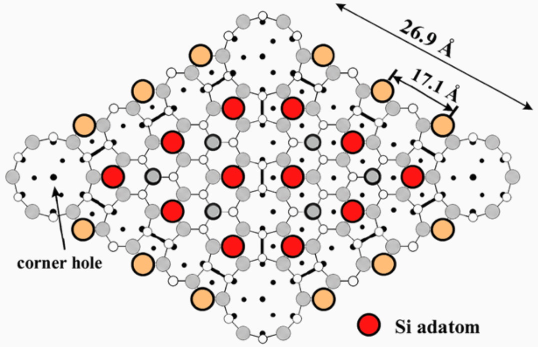
- Competing theoretical models of the Si(111) surface existed and could not be distinguished by diffraction.
- One STM image in 1983 settled it.
- The surface reconstructs into complex 3-layer rearrangement of surface atoms, forming a 7×7 super-cell with 12 ad-atoms.
- This established STM as a transformation surface science technique.
- The STM inventors, Binnig and Rohrer won the 1986 Nobel Prize.

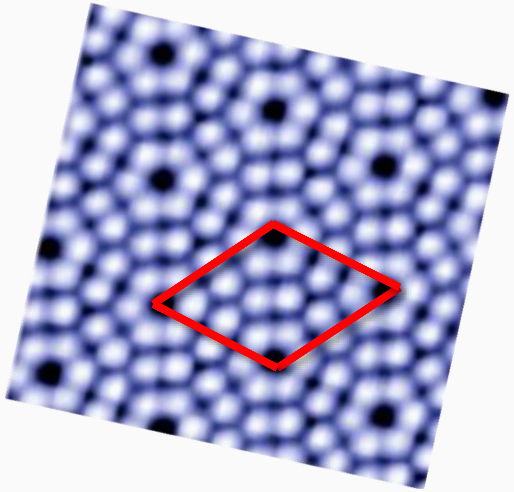
Original STM image of Si(111)7x7



Binnig et al., PRL, 50 120 (1983)

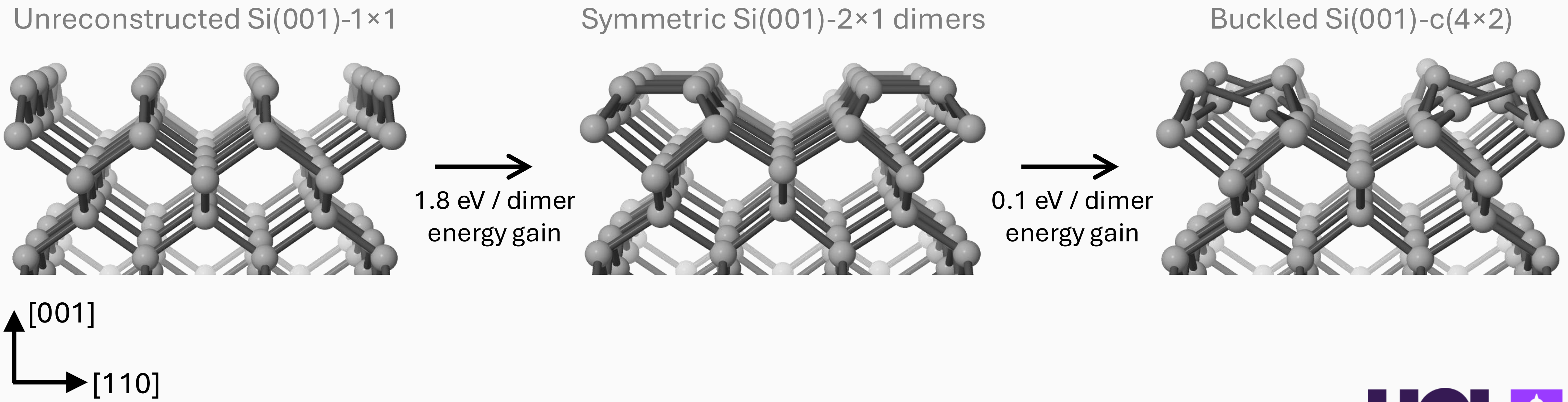
Schematic and modern image





Silicon (001) surface reconstruction

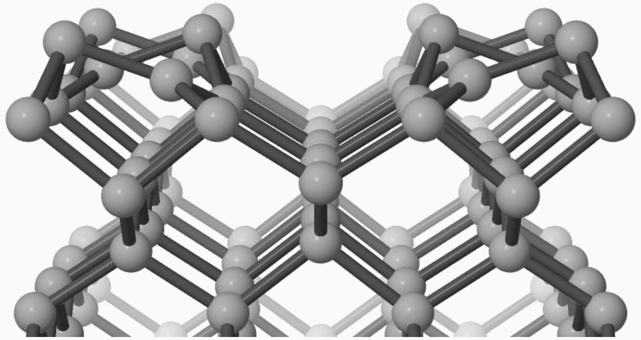
- The (001) surface of silicon reconstructs into rows of paired atoms, called *dimers*
- Dimerisation reduces the dangling bonds at the surface and is more stable than the ideal surface
- A further energy gain comes from buckling the dimers alternately along and across rows – c(4x2)



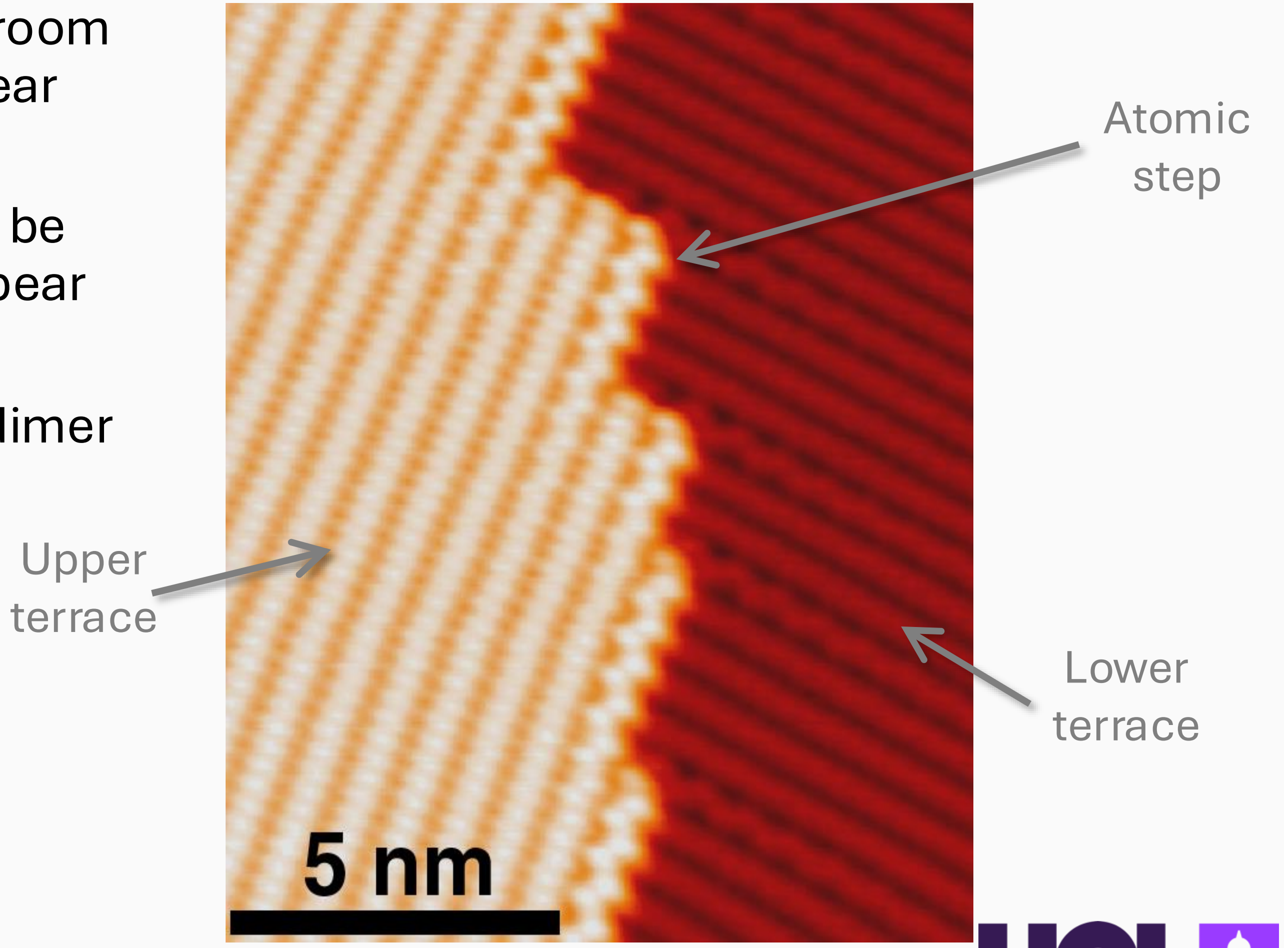
Valence and conduction bands states

- While buckled dimers are the ground state, at room temperature thermal motion makes them appear symmetric in STM images
- Near defects and step edges, the buckling can be *pinned* into one orientation and the dimers appear zig-zagged
- Because of the tetrahedral crystal lattice, the dimer rows rotate 90° across a single atomic step

c(4x2) – the Si(001) ground state



Room temperature STM image



S. R. Schofield, PhD Thesis (UNSW; 2004)

Bardeen approach: overlap integral of wave functions

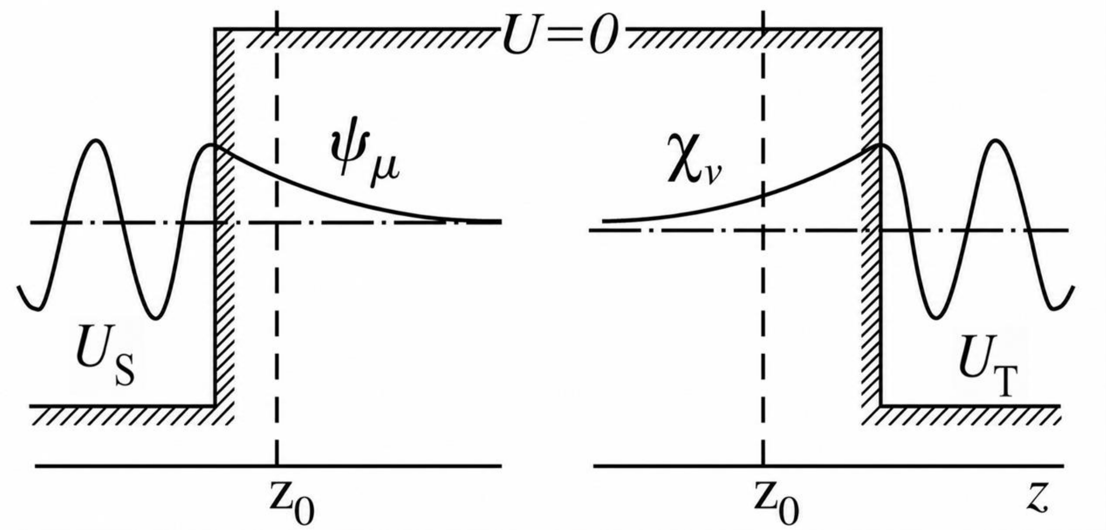
- The wave functions of an electron in the tip and sample (χ, ψ) are calculated separately (can be done accurately)
- The amplitude of transmission is a flux-like surface integral calculated over an arbitrary surface plane in the barrier region at $z = z_0$

$$M = \frac{\hbar}{2m} \int_{z=z_0} \left(\chi^* \frac{\partial \psi}{\partial z} - \psi \frac{\partial \chi^*}{\partial z} \right)$$

- The rate of electron transfer is determined by first order perturbation theory (Fermi's Golden Rule)

$$w = \frac{2\pi}{\hbar} |M|^2 \, \delta(E_\psi - E_\chi)$$

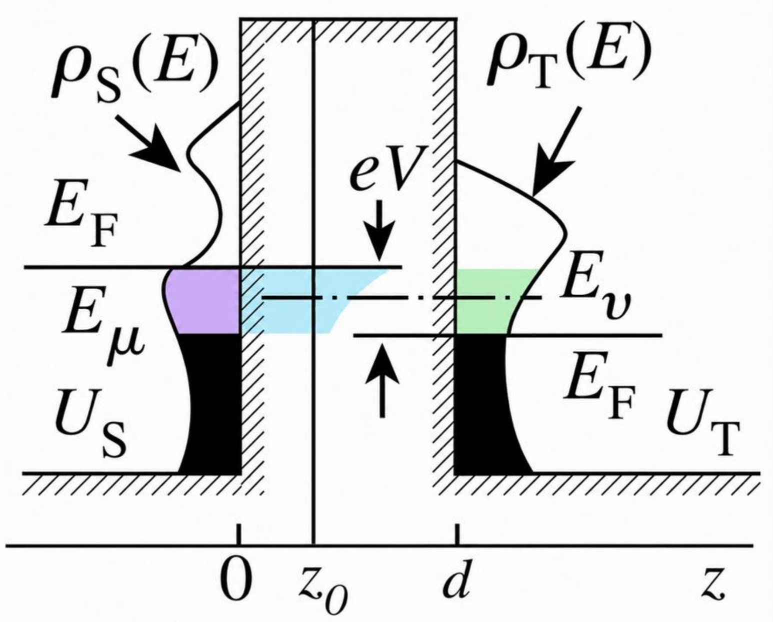
where the delta function restricts tunnelling to states with the same energy



Bardeen approach: tunnelling current maps the sample DOS

- The tunnelling current is the integral over all such transfer rates, modulated by the Fermi-Dirac distribution and the density of states in the tip and sample.

$$I = \frac{4\pi e}{\hbar} \int_{-\infty}^{\infty} \left(f(E_\mathrm{F} - eV + \epsilon) - f(E_\mathrm{F} + \epsilon)\right) \rho_\mathrm{S}(E_\mathrm{F} - eV + \epsilon) \rho_\mathrm{T}(E_\mathrm{F} + \epsilon) \left|M\right|^2 \, d\epsilon$$



- If $k_B T$ << energy resolution required

$$I = \frac{4\pi e}{\hbar} \int_{0}^{eV} \rho_\mathrm{S}(E_\mathrm{F} - eV + \epsilon) \rho_\mathrm{T}(E_\mathrm{F} + \epsilon) \left|M\right|^2 \, d\epsilon$$

- Assuming M and ρ_T are roughly energy independent:

$$I = \frac{4\pi e}{\hbar} \int_{0}^{eV} \rho_\mathrm{S}(E_\mathrm{F} - eV + \epsilon) \, d\epsilon$$

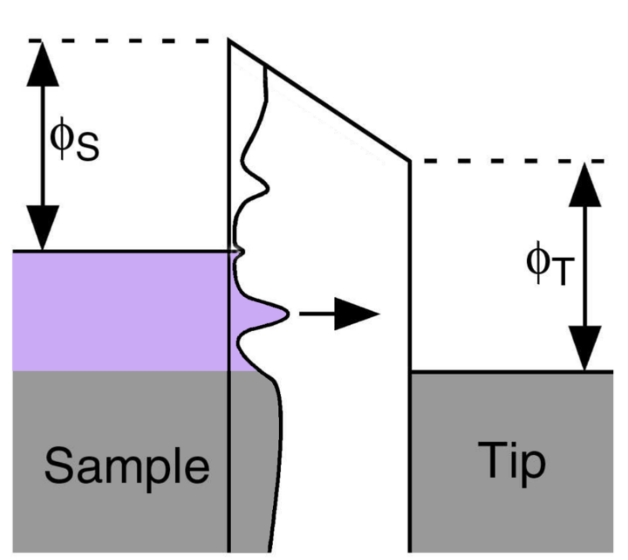
→ the tunnelling current is the integral of the density of states of the sample taken over the energy range, *eV*.

Probing the sample density of states

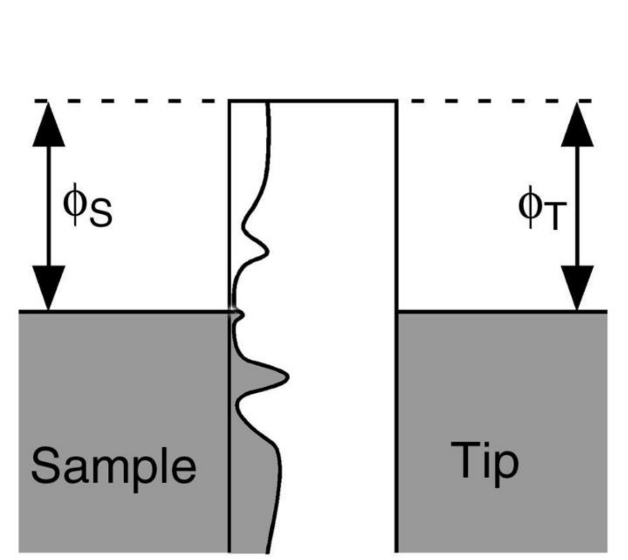
- The tunneling current is proportional to the integrated DOS:
- Can probe occupied and unoccupied DOS

$$I = \frac{4\pi e}{\hbar} \int_0^{eV} \rho_S(E_F - eV + \epsilon)\, d\epsilon$$

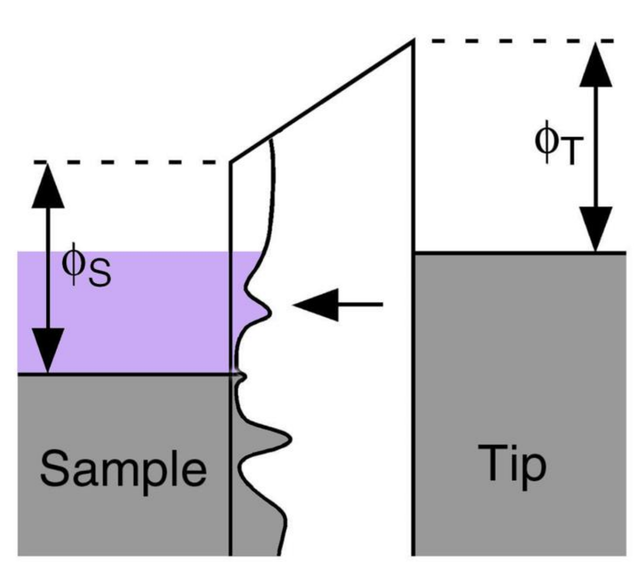
Filled-states
(negative sample bias)



Zero bias
(no tunnelling current)

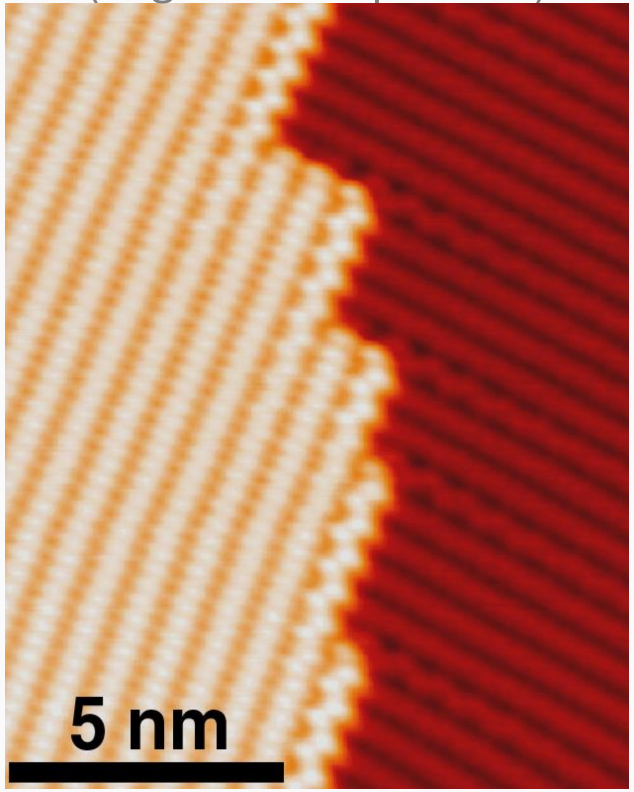


Empty-states
(positive sample bias)

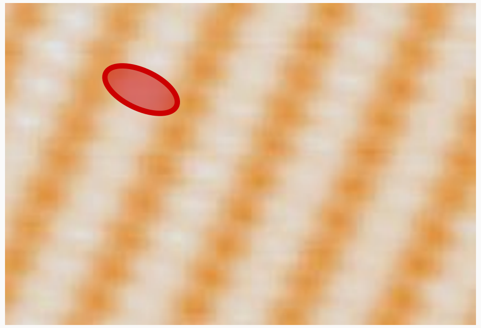


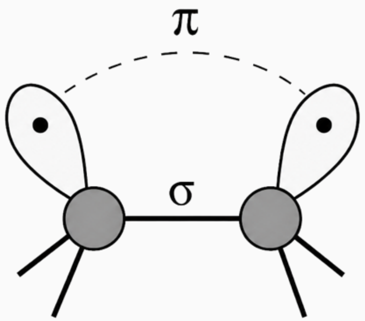
Valence and conduction bands states

Filled-states
(negative sample bias)

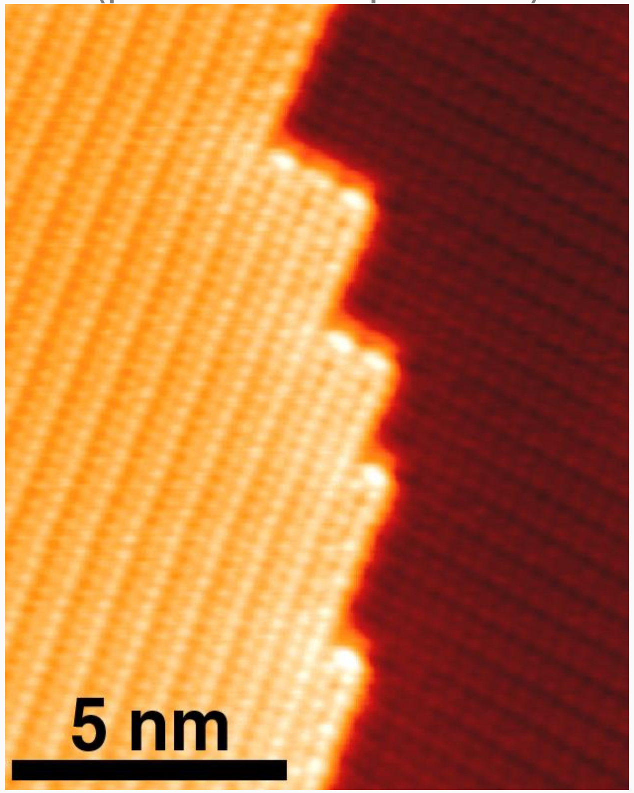


Dimer π-bonding

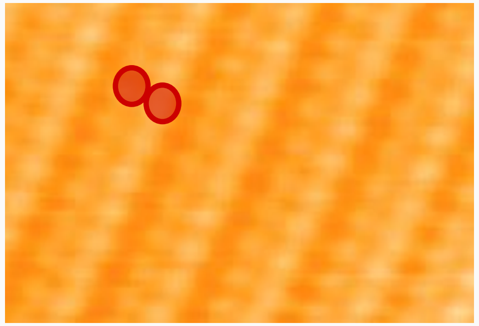


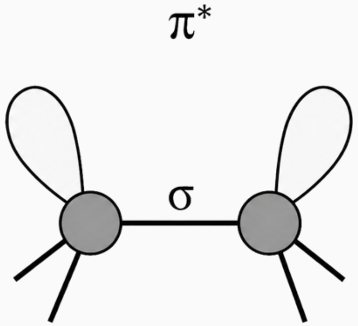


Empty-states
(positive sample bias)



Dimer π*-antibonding





dI/dV directly probes the local density of states

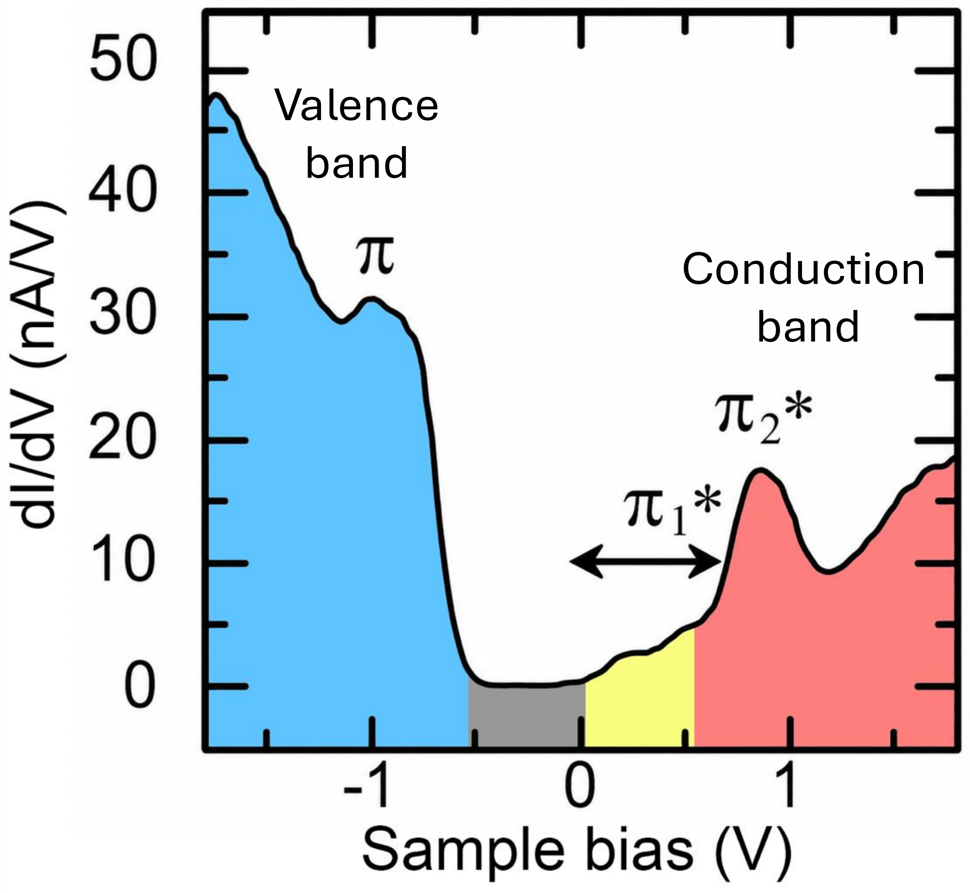
- The differential of the tunnelling current is directly proportional to the sample DOS

$$\frac{dI}{dV} \propto \rho_{\mathrm{S}}(E_{\mathrm{F}} - eV)$$

- Point spectroscopy: tip held at fixed *xy* position, feedback loop off

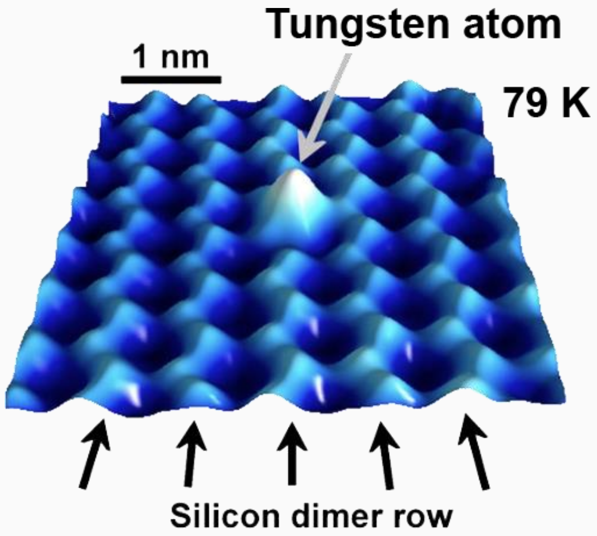
  - **Numerical differentiation:**
    Sweep bias, record I(V), differentiate numerically

  - **Lock-in detection:**
    Add small AC modulation to bias, demodulate to read dI/dV directly



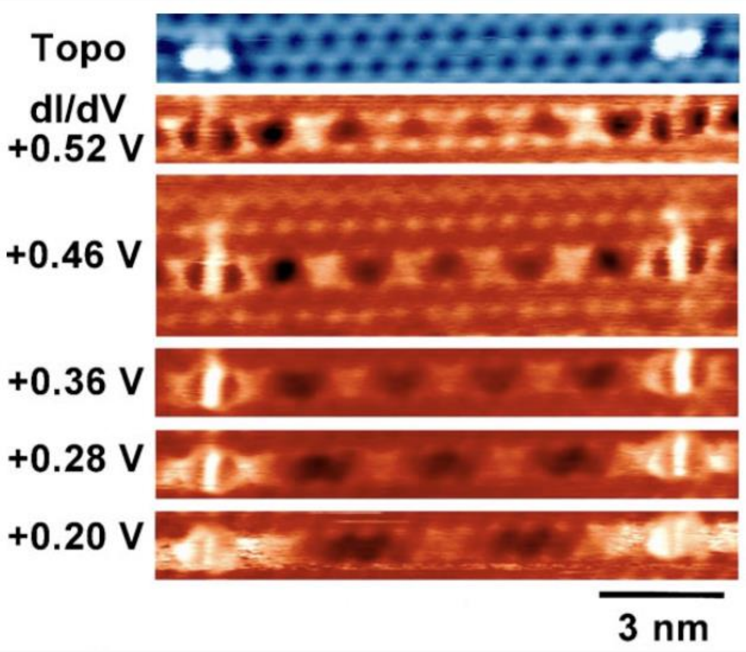
Sagisaka *et al.*, APL **88**, 203118 (2006)

Quantum confined states imaged with *dI/dV*

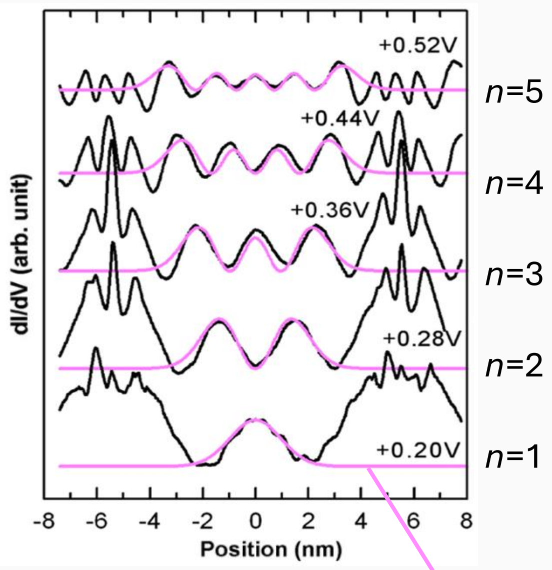


Sagisaka *et al.*, APL **88**, 203118 (2006)

Topography + dI/dV maps



dI/dV line profiles

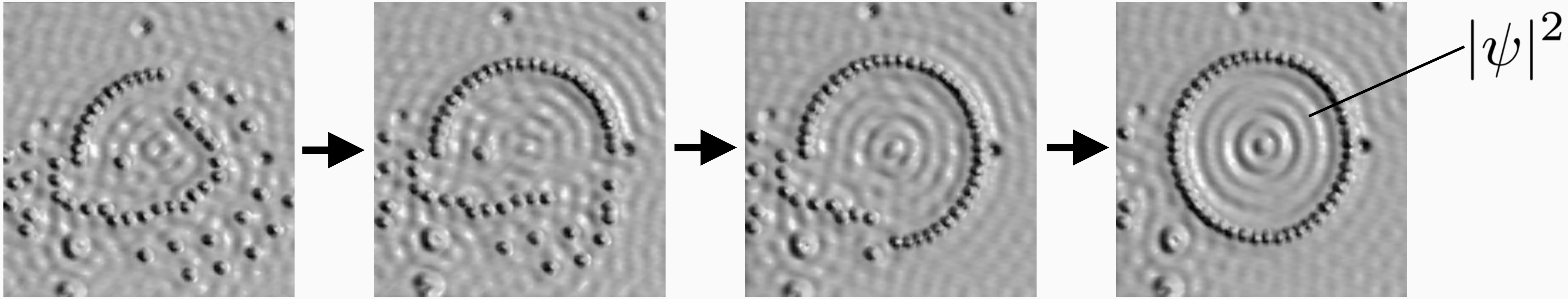


1D harmonic oscillator states

- π* state is dispersive along the dimer row and isolated within the bulk band gap
- W atoms deposited on the surface act as scatterers
- Scattering produces standing waves; spatial *dI/dV* mapping resolves quantum confinement

STM manipulation: building structures atom-by-atom

Individual Fe adatoms positioned into a ring on Cu(111) — the 'Quantum Corral'

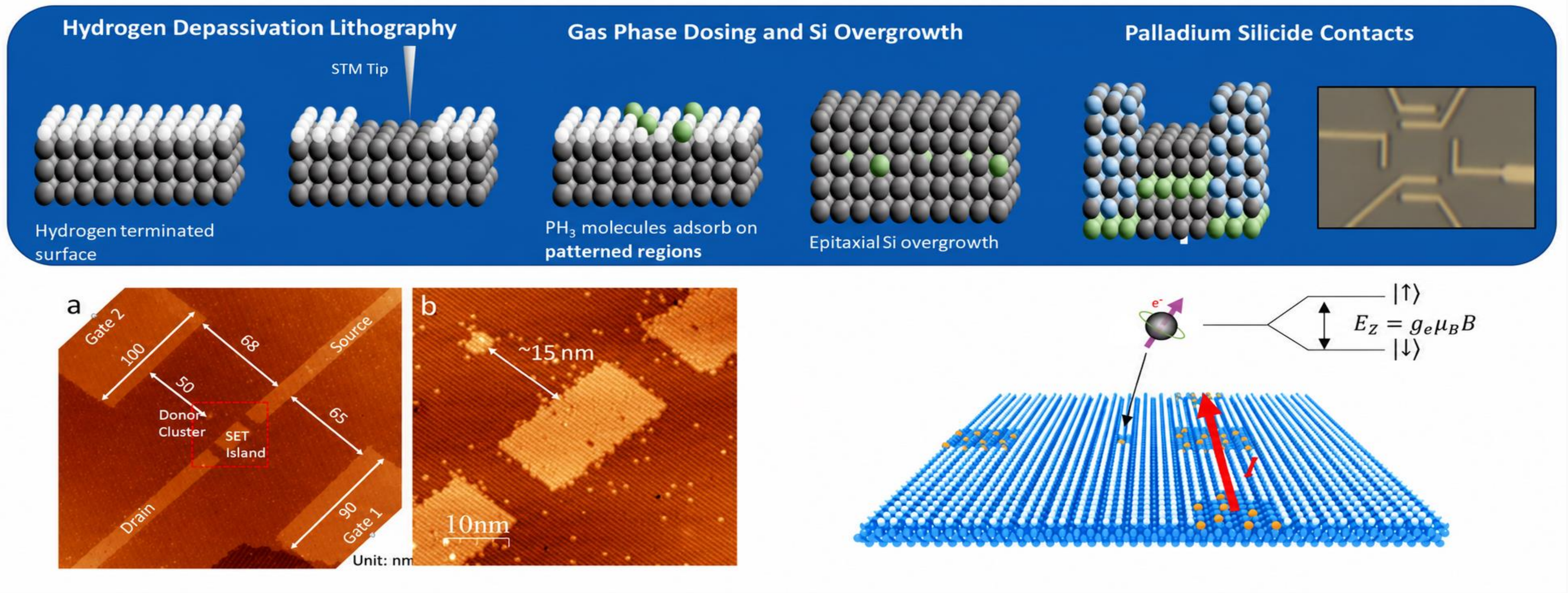


Crommie, et al., Science 262, 218 (1993)

- Fe atoms deposited on Cu(111) at 4 K
- STM tip repositions atoms individually to close the ring
- Confined surface-state electrons form a standing-wave quantum state, labelled and imaged at $|\psi|^2$

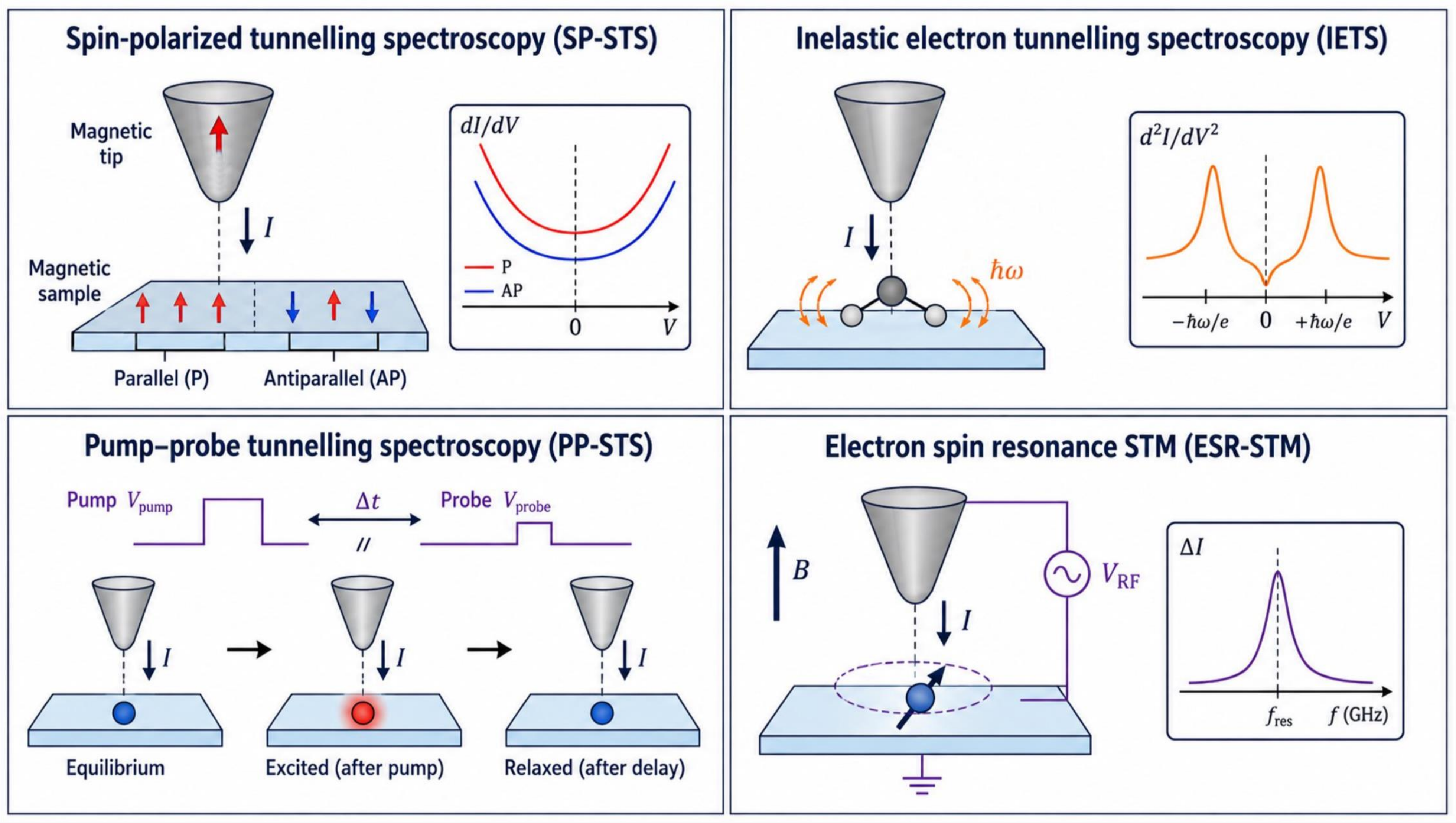
Using the STM as a tool to build at the atomic scale

Quantum devices with single atom precision can be built with STM



Silva et al. in “Roadmap on Atomic-scale Semiconductor Devices”, Nano Futures **9**, 012001 (2025)

Modern STM: spin, vibrations, dynamics...

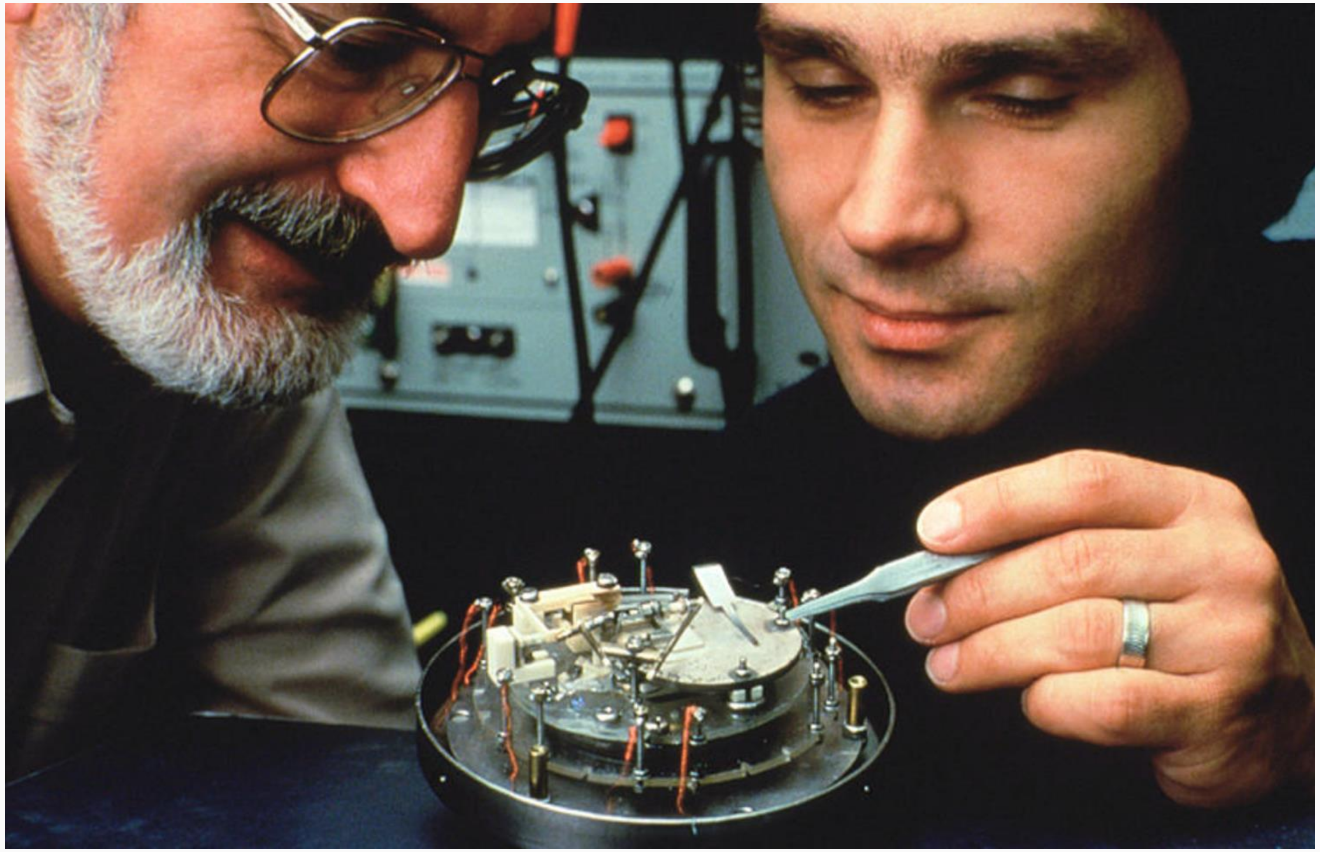


Roadmap on atomically-engineered quantum platforms, Nano Futures 9 (2025) 032001

Summary. STM: accessing the atomic world

- With a sharp tip and the quantum tunnelling effect, tunnelling, we can image and manipulate individual atoms.
- Beyond imaging, STM provides information on the surface density of states, spin, and vibrations.
- STM enables us to build as well as probe: arranging atoms one by one into new structures, including candidate quantum computers.

Heinrich Rohrer and Gerd Binnig, inventors of the STM (1982)



https://sciencephotogallery.com/featured/heinrich-rohrer-and-gerd-binnig-ibm-research.html

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