Scanning Tunneling Microscopy

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6. Scanning Tunneling Spectroscopy
7. Surface States
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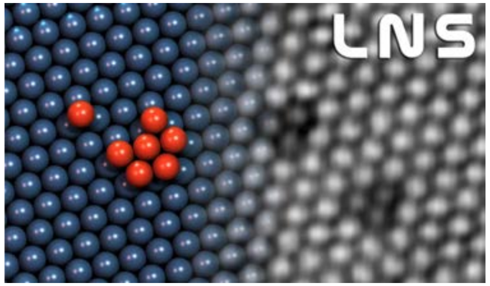
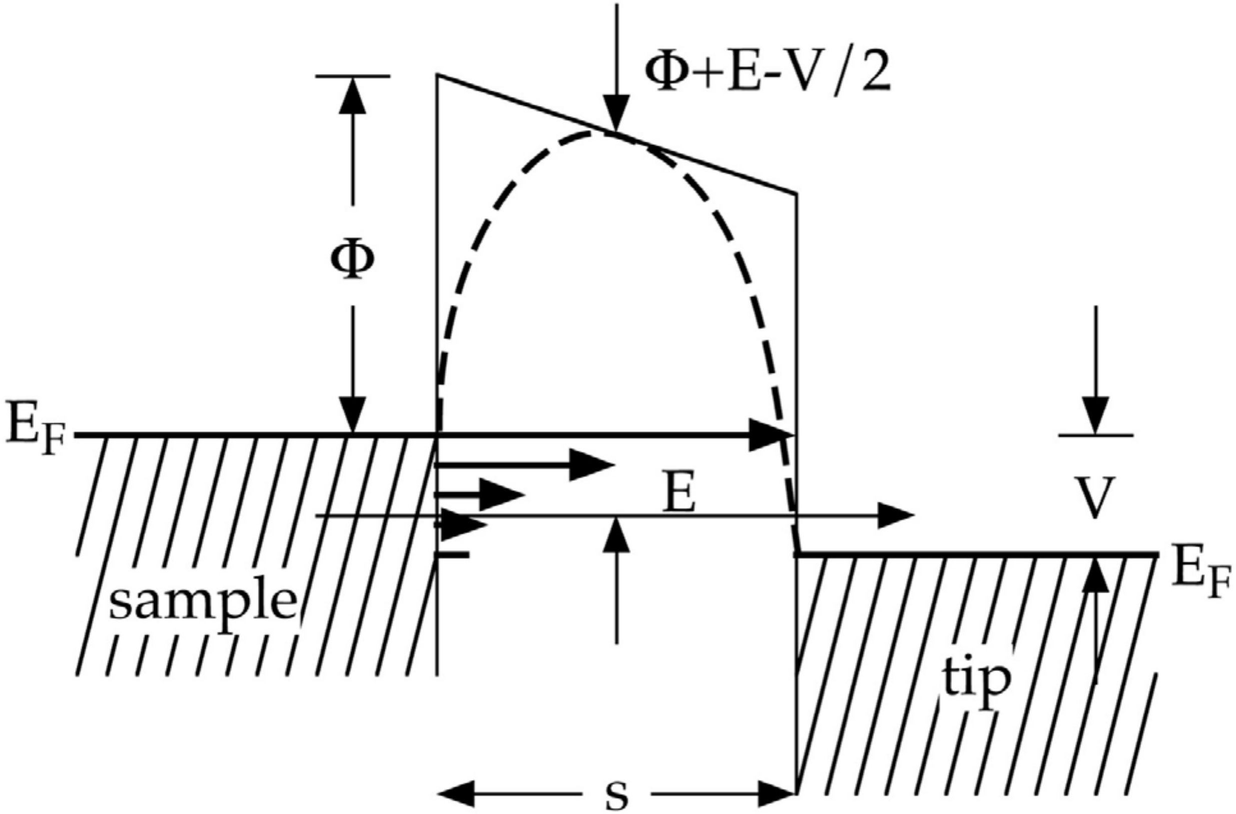
9. Electron Spin Resonance with the STM

EPFL



Vacuum Tunneling



Tunnel Current in transfer Hamiltonian:

$$I = \frac{2\pi e}{\hbar} \sum_{\mu,\nu} f\left(E_\mu\right)\left(1 - f\left(E_\nu + eV\right)\right)\left|M_{\mu\nu}\right|^2 \delta\left(E_\mu - E_\nu\right)$$

$$M_{\mu\nu} = \frac{\hbar^2}{2m} \int \left(\psi_\mu^* \nabla \psi_\nu - \psi_\nu \nabla \psi_\mu^*\right) dS$$

J. Bardeen, Phys. Rev. Lett. 6, 57 (1961).

Calculating the Tunnel Current

Application of Transfer Hamiltonian to STM geometry :

$$I = \rho\left(\mathbf{r}_0, E_F\right) e^{-2ks}$$

s tip-sample distance

With decay length $k = \sqrt{2m/\hbar^2\left(\Phi + E - eV/2\right)}$

Φ workfunction

where $\sqrt{2m/\hbar^2} = 0.51 \mathring{A}^{-1} \sqrt{eV}^{-1}$

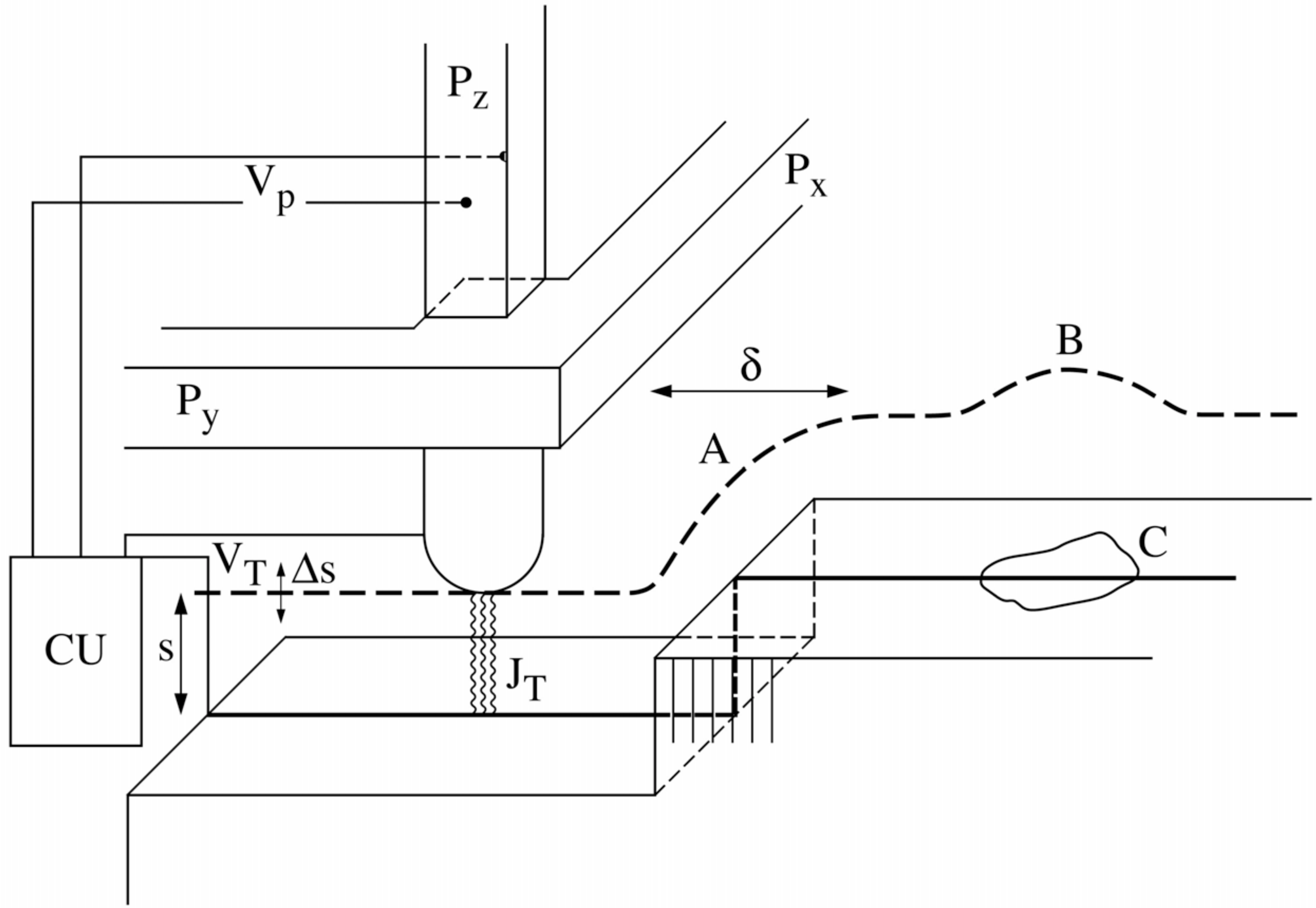
$$\Phi = 4eV \Rightarrow 2k = 2/\mathring{A}$$

Tunnel current decays by 1 order of magnitude per Å change in tip-sample distance

J. Tersoff and D. R. Hamann, Phys. Rev. Lett. **50**, 1998 (1983).

History

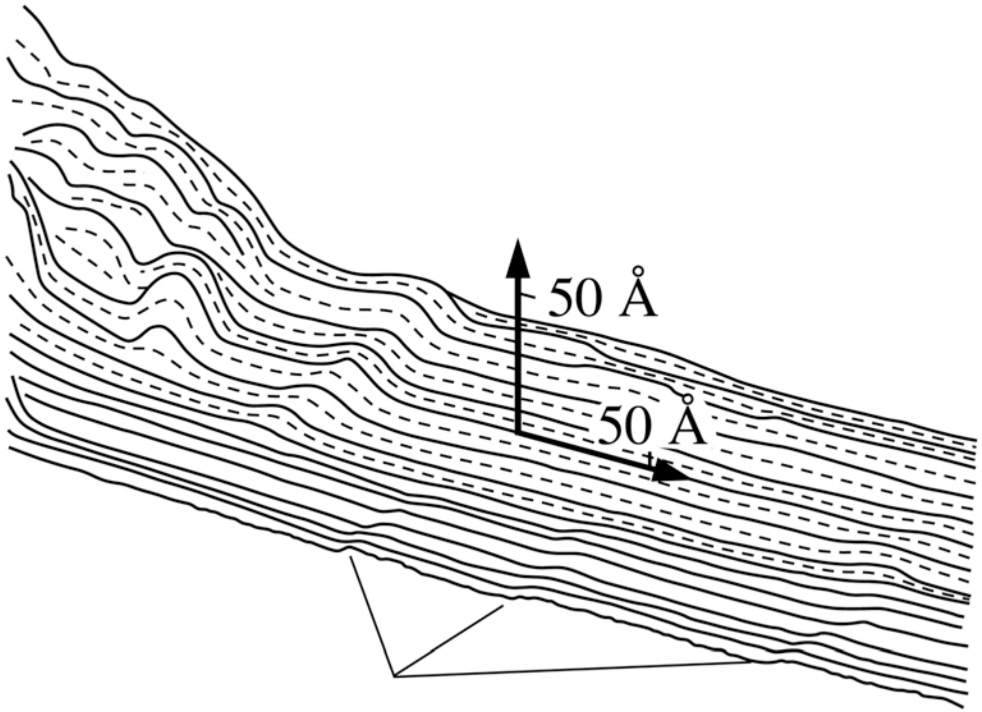
First STM by Binnig & Rohrer



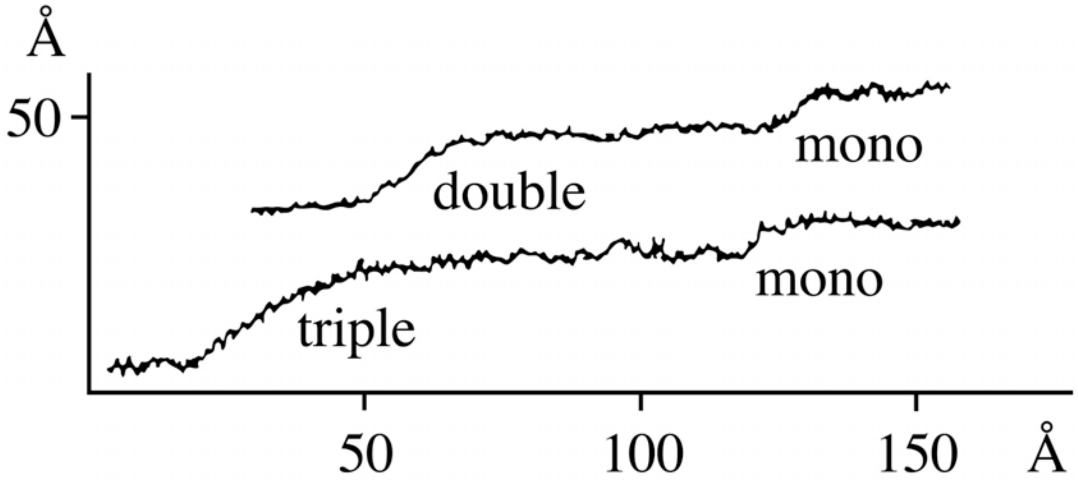
G. Binnig and H. Rohrer, Helv. Phys. Acta **55**, 726 (1982).

First Results on $CaIrSn_4(110)$

Growth Spiral

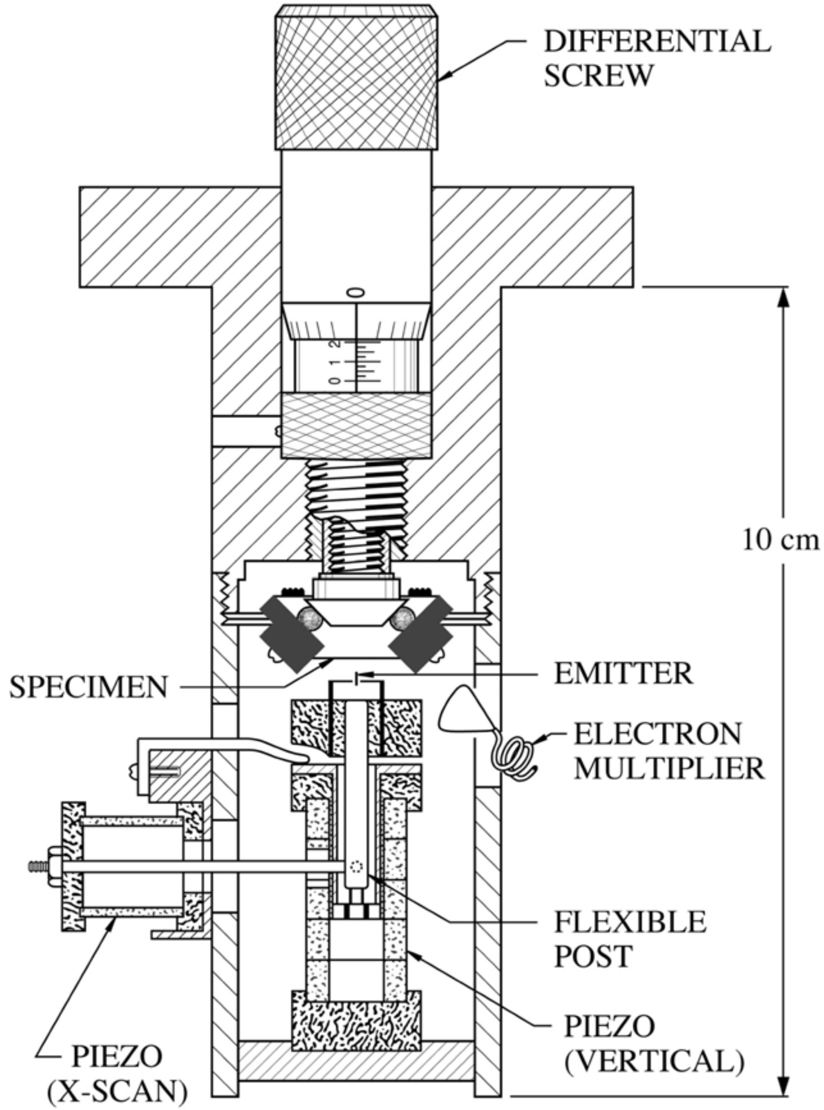


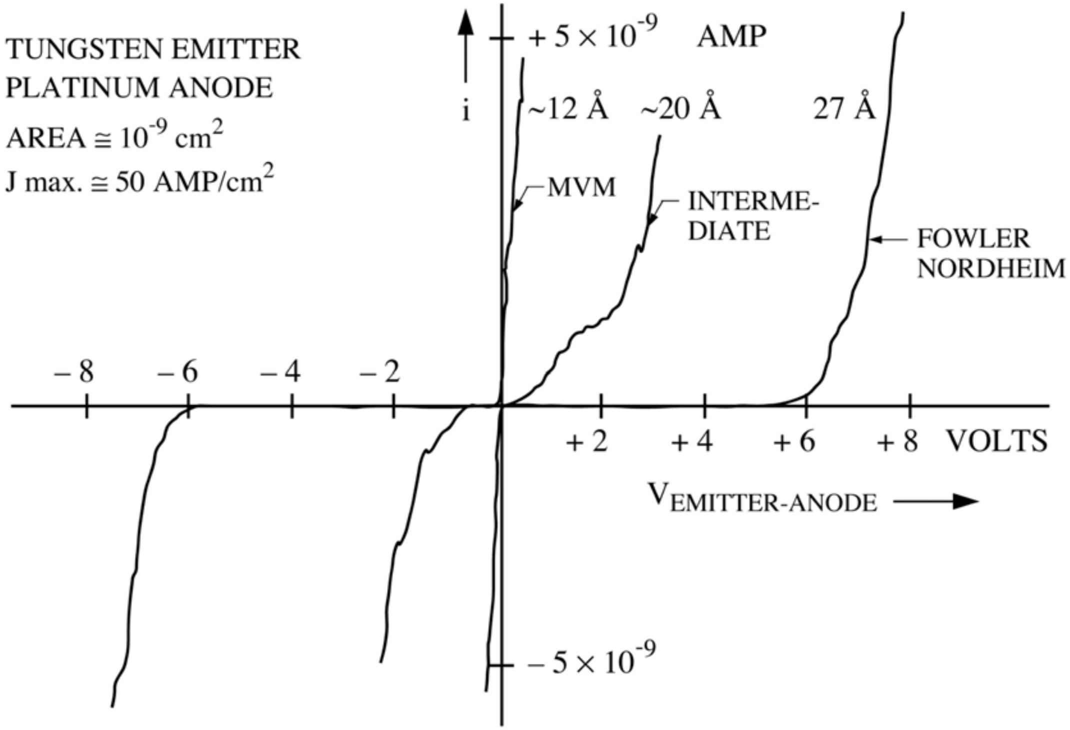
Atomic Steps



G. Binning *et al*., Phys. Rev. Lett. **49**, 57 (1982).

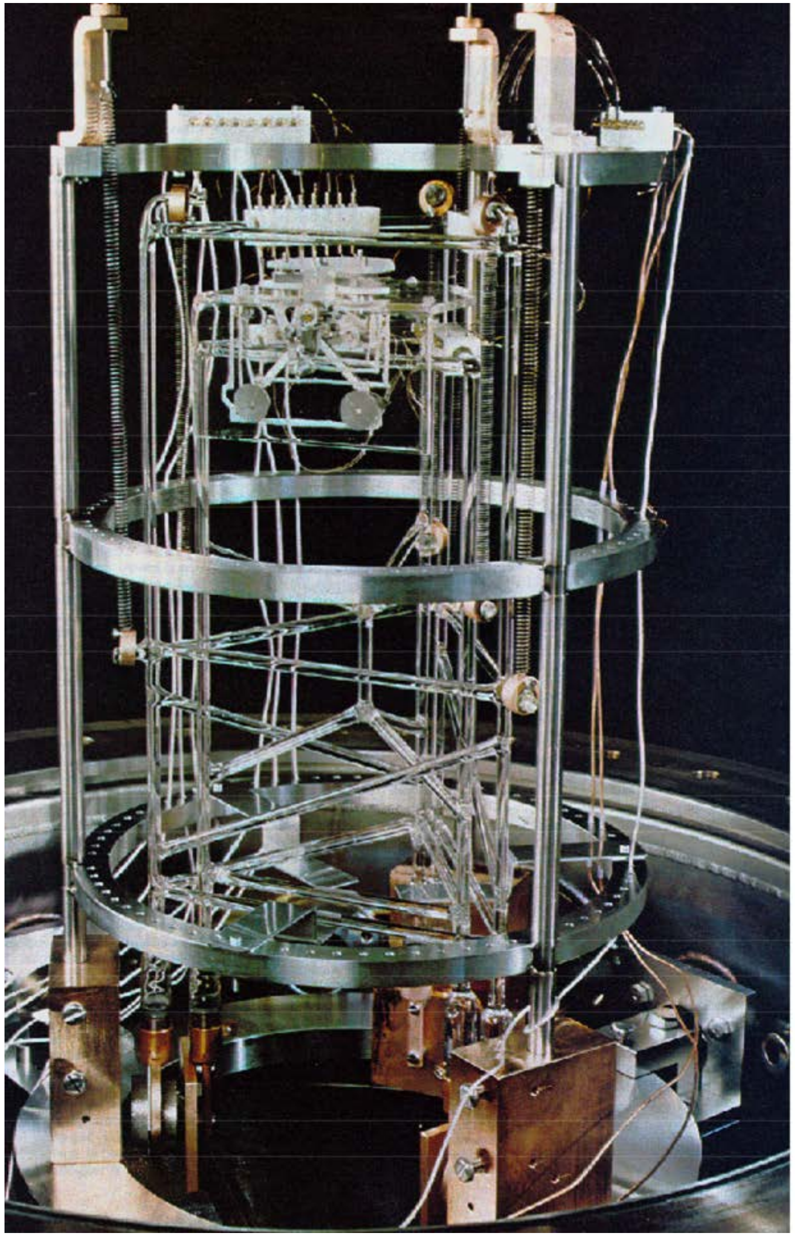
Topografiner – the Predecessor of the STM

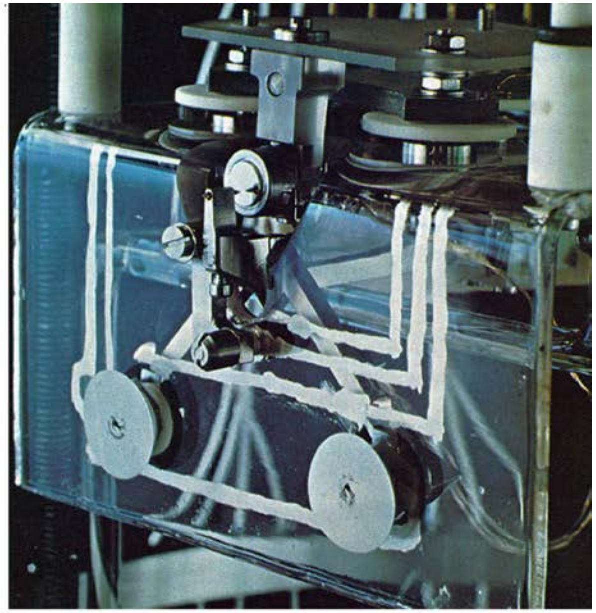


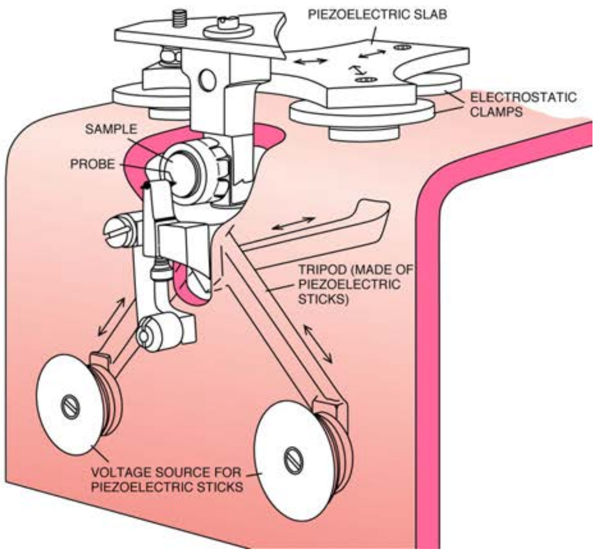


R. Young *et al*., Rev. Sci. Instrum. **43**, 999 (1972);
See also: I. Amato, Science **276**, 1982 (1997).

Realization of Coarse Approach and Vibration Damping



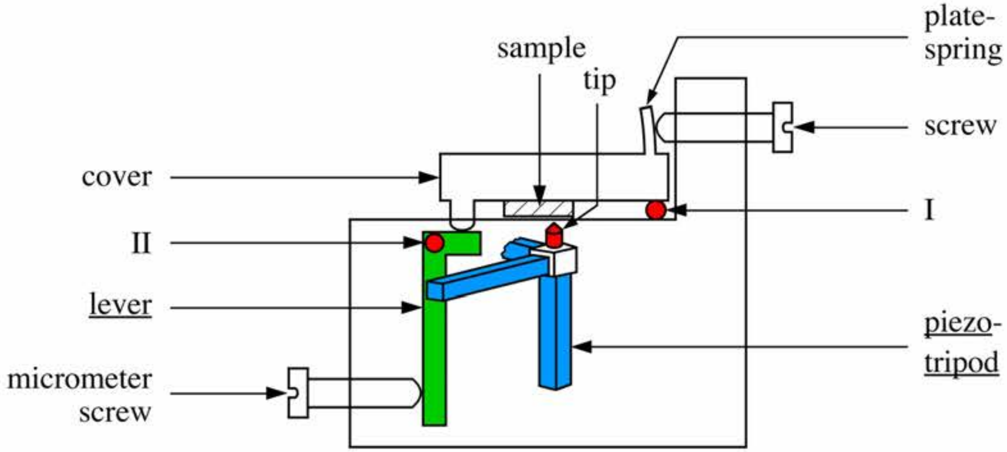




Pocket-size STM and viton stack for vibration damping

Mechanical properties

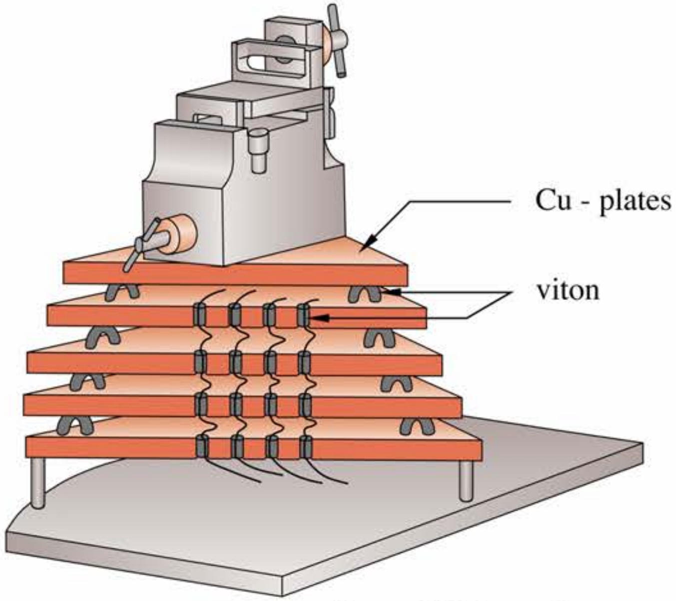
- sample – tip approarch:



microscope : $f_0 = 2$ kHz

piezo – tripod : $f_0 = 7$ kHz

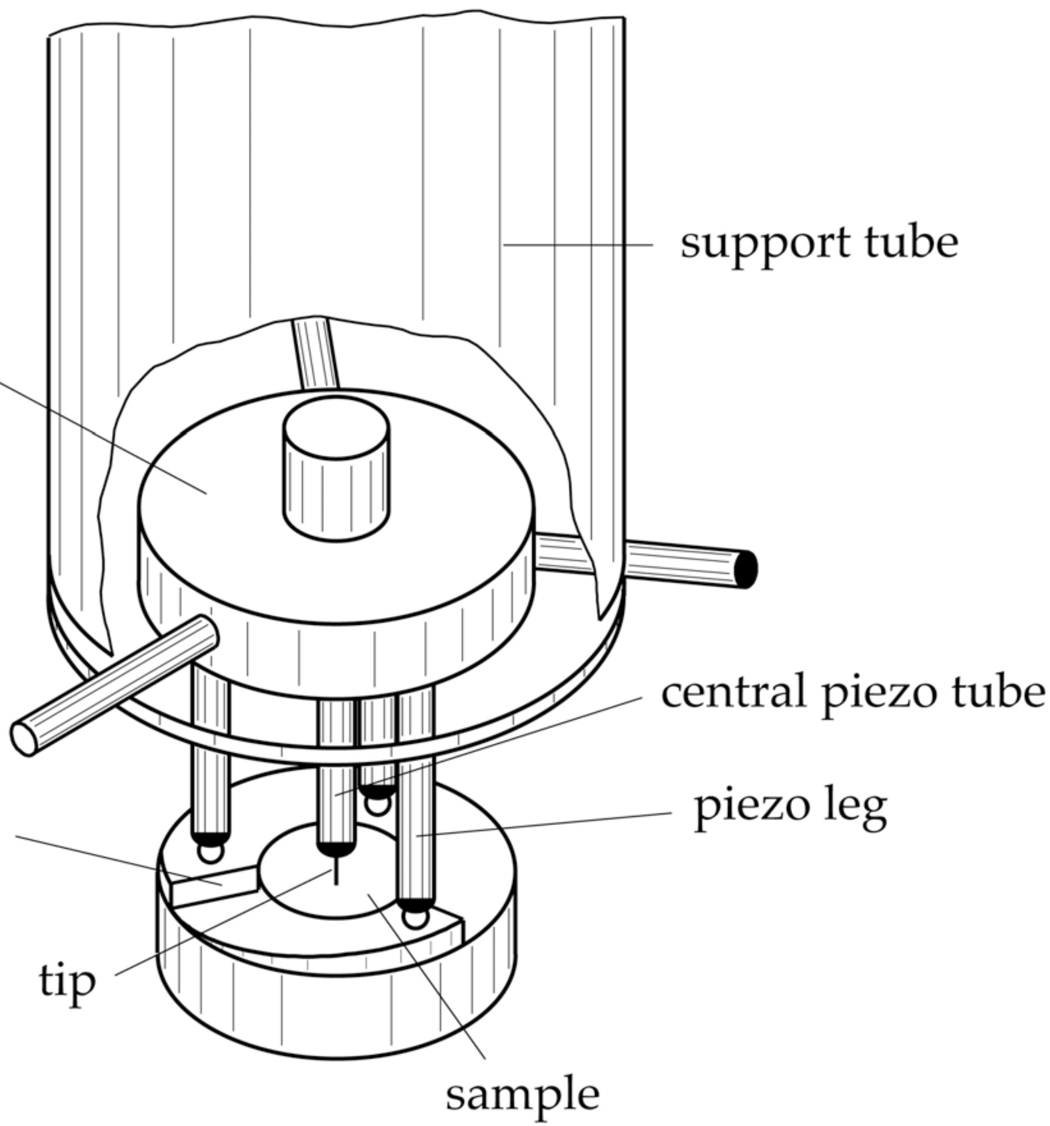
- viton – damped stack:



$f_0 = 25$ Hz , slope : $-\frac{24\ \text{dB}}{\text{octave}}$

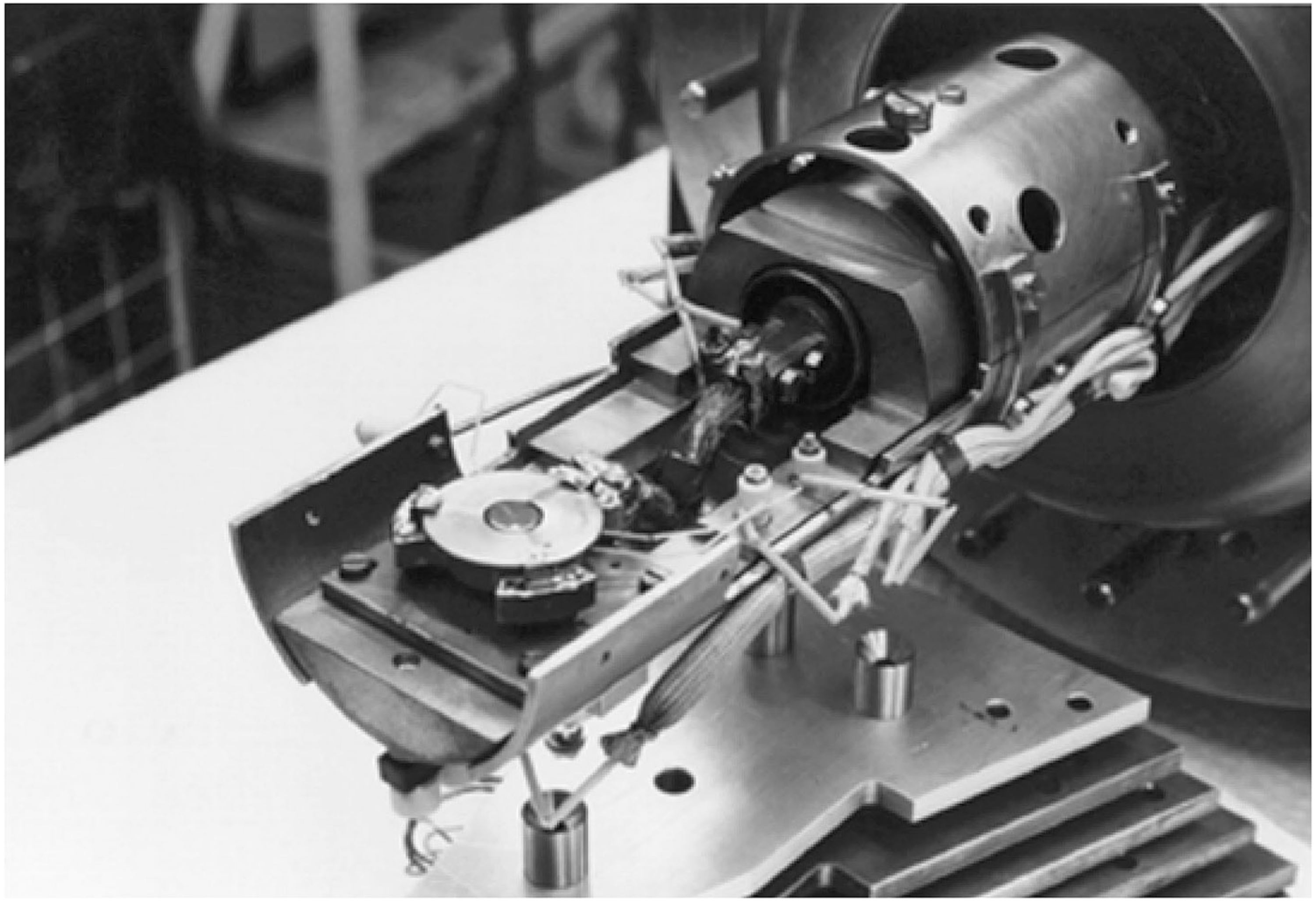
Beetle Type STM Compensating Thermal Drifts

Beetle-STM Principle



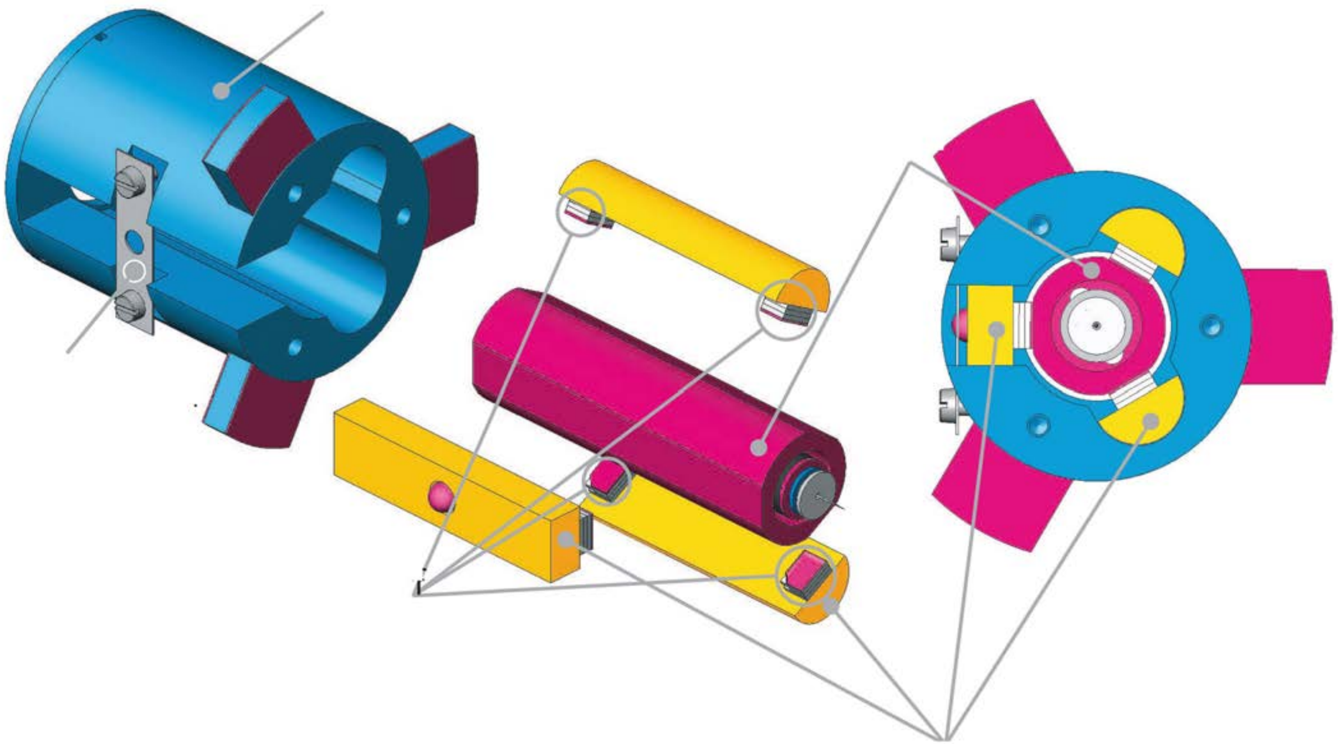
J. Frohn *et al*. Rev. Sci. Instrum. **60**, 1200 (1989).

Sample Holder for Variable-Temperature STM 30 - 600 K

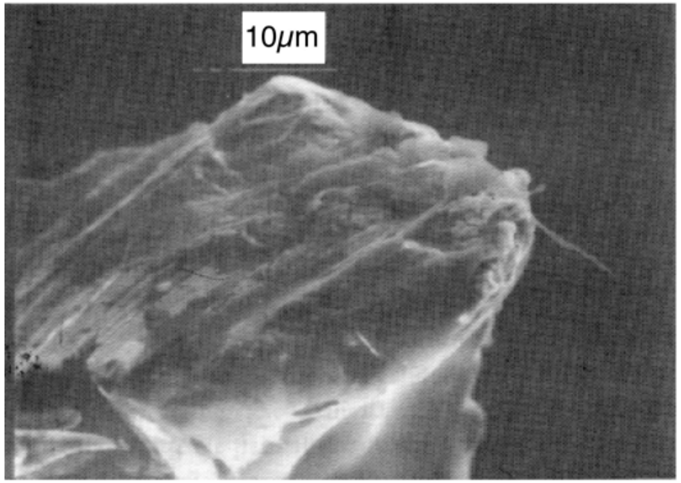


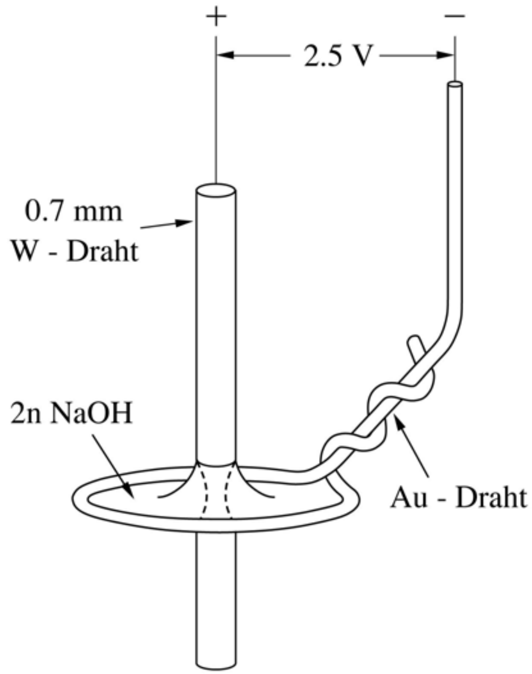
H. Brune *et al*., Thin Solid Films **264**, 230 (1995).

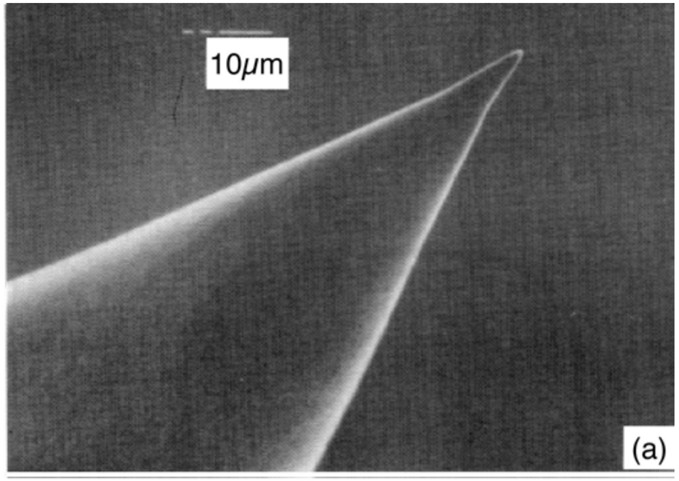
Stick-and-Slip Linear Motor for Coarse Approach

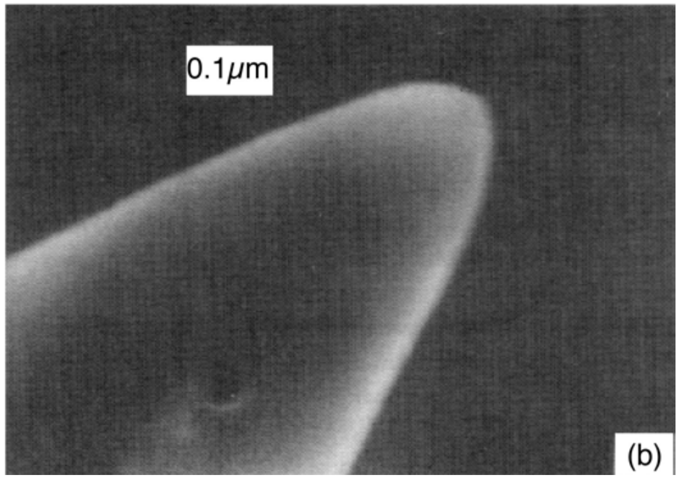


Electrochemical Etching of W-tips

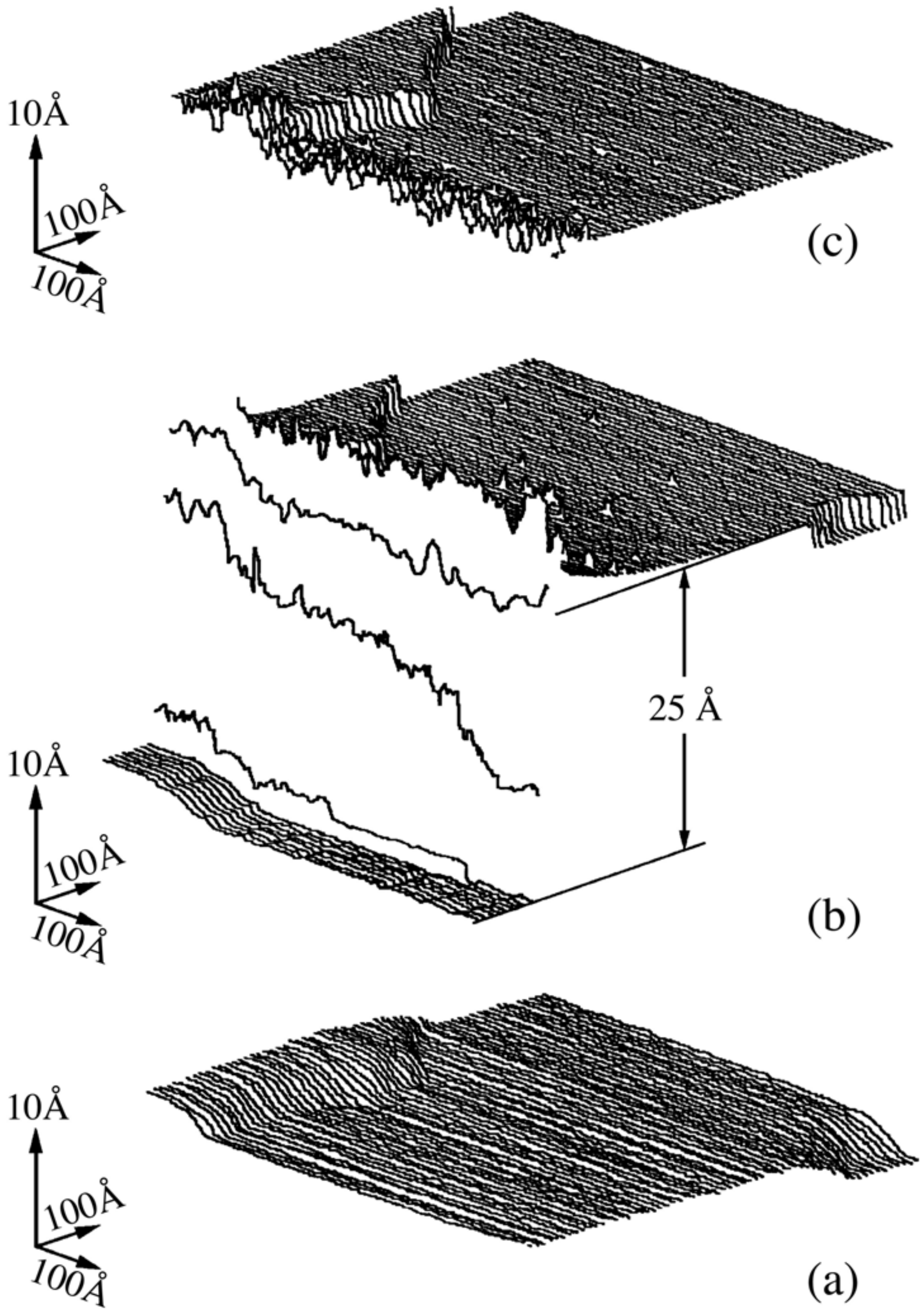


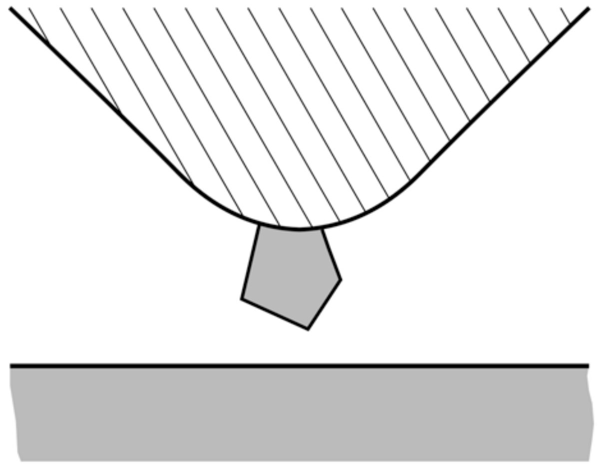






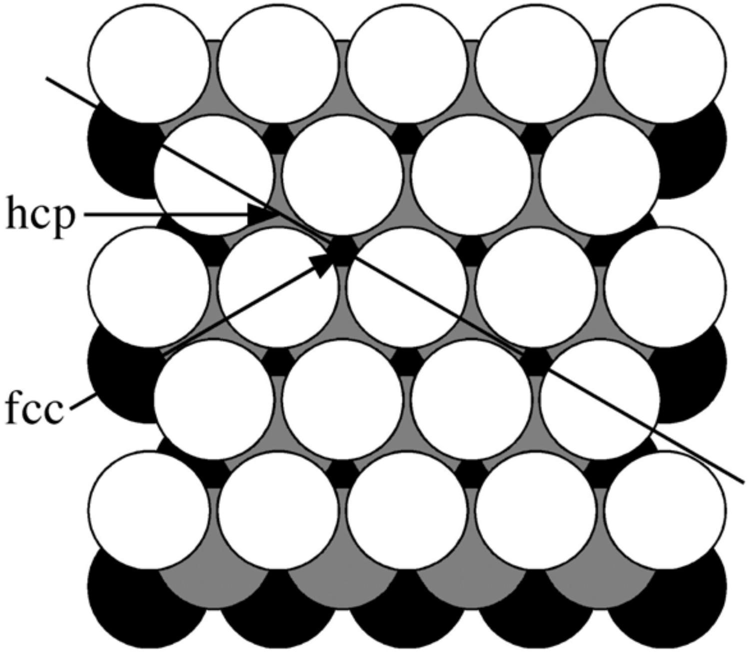
Tip preparation by Voltage Pulses during STM Operation

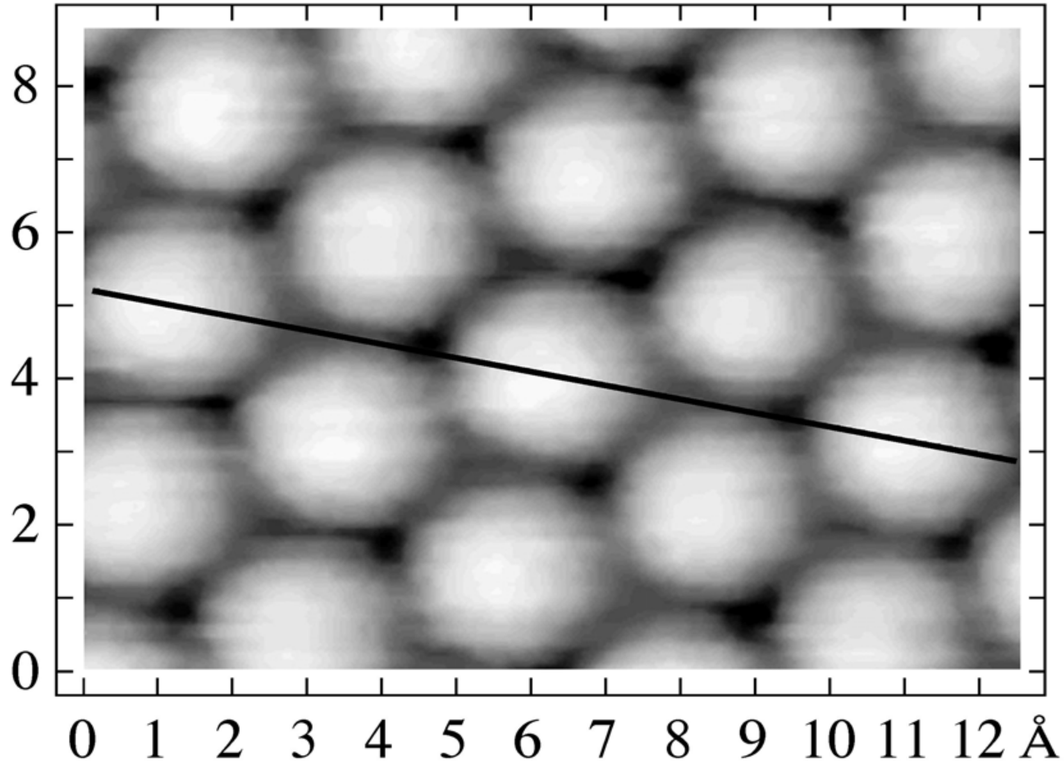


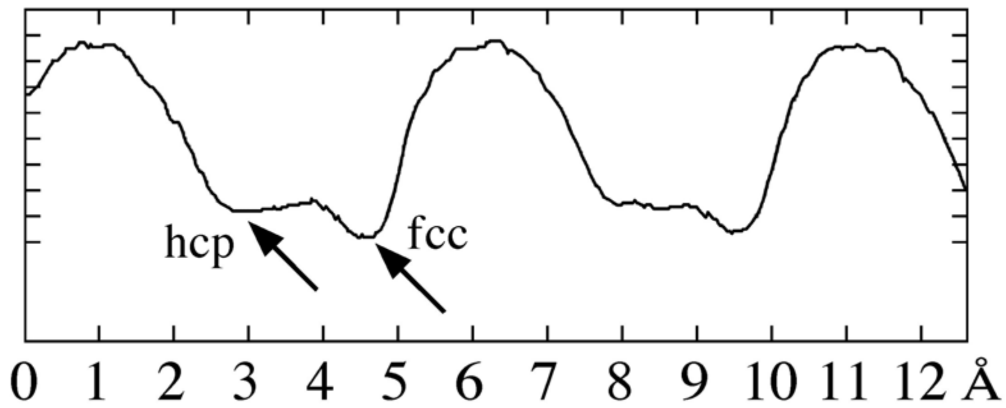


What 'sees' the STM

Al(111) – seeing atoms and below – fcc vs hcp hollows

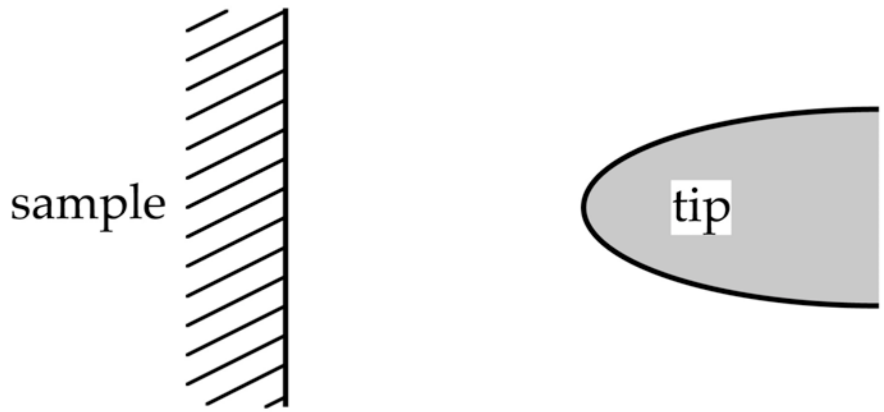


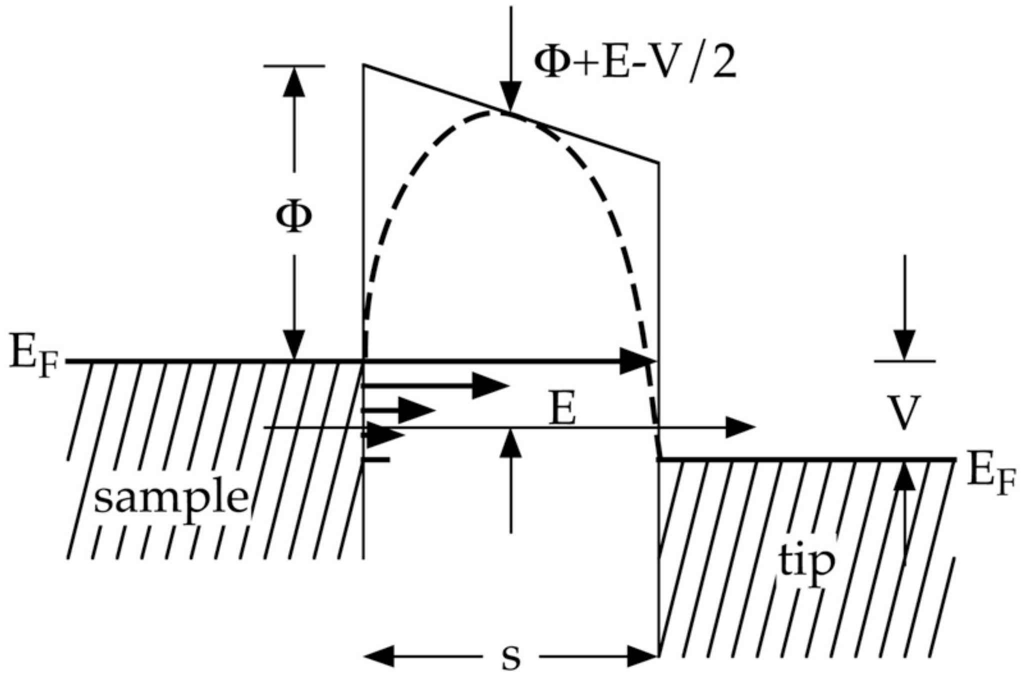




H. Brune *et al*., Europhys. Lett. **13**, 123 (1990);
W. A. Hofer *et al*., Chem. Phys. Lett. **397**, 354 (2004).

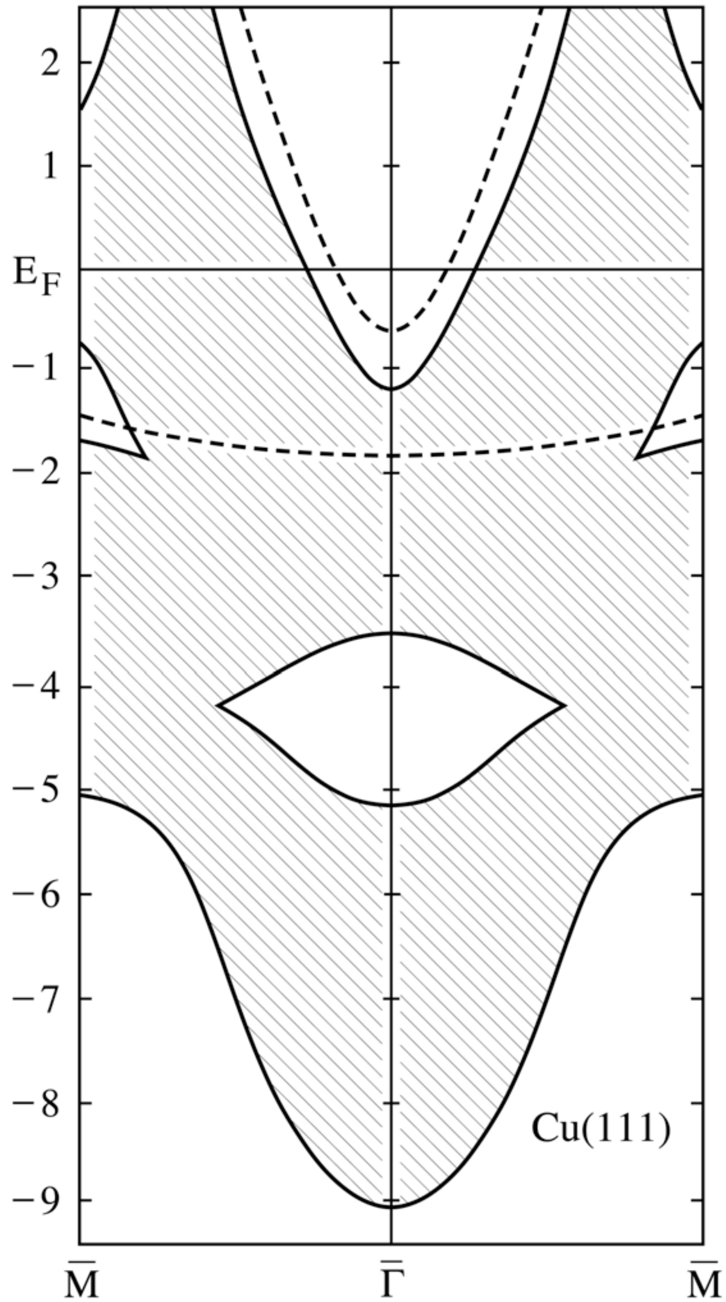
Scanning Tunneling Spectroscopy - STS





$$I \propto \int_0^{eV} dE \rho_{sample}(E,x,y)\rho_{tip}(E-eV) \longrightarrow dI/dV(V,x,y) \approx \rho_{sample}(eV,x,y)$$

Surface States – Cu(111)

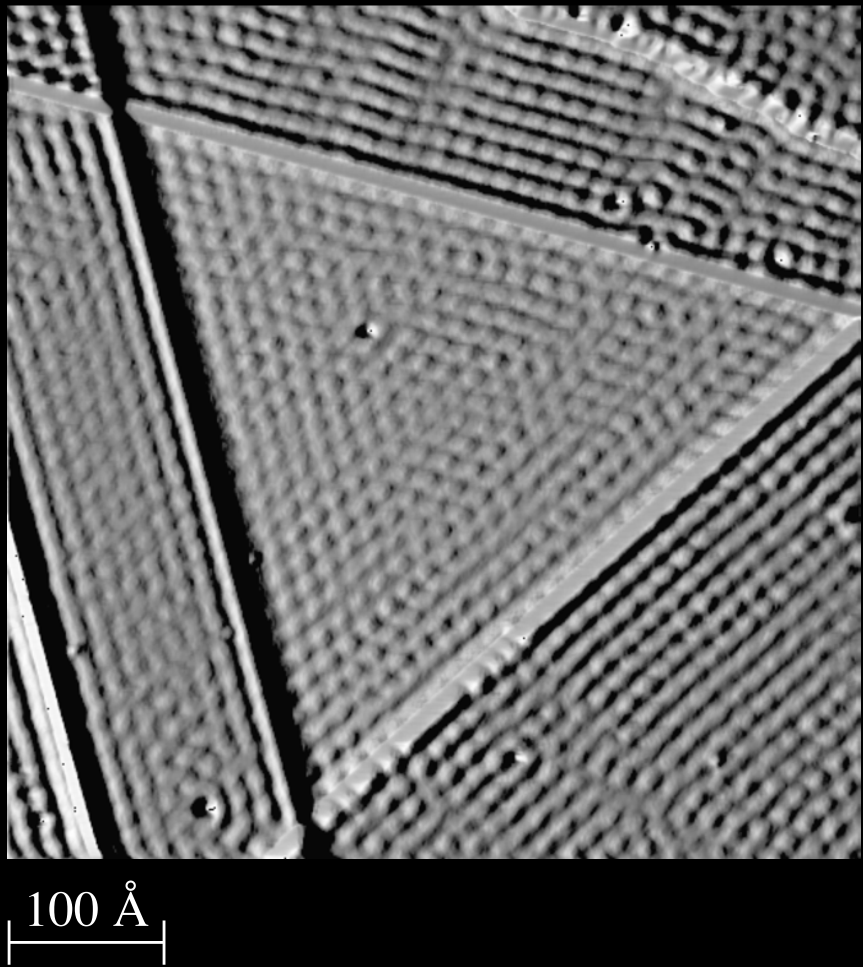


(111)-projected bulk bandstructure of Cu

Bylander & Kleinman (1983).

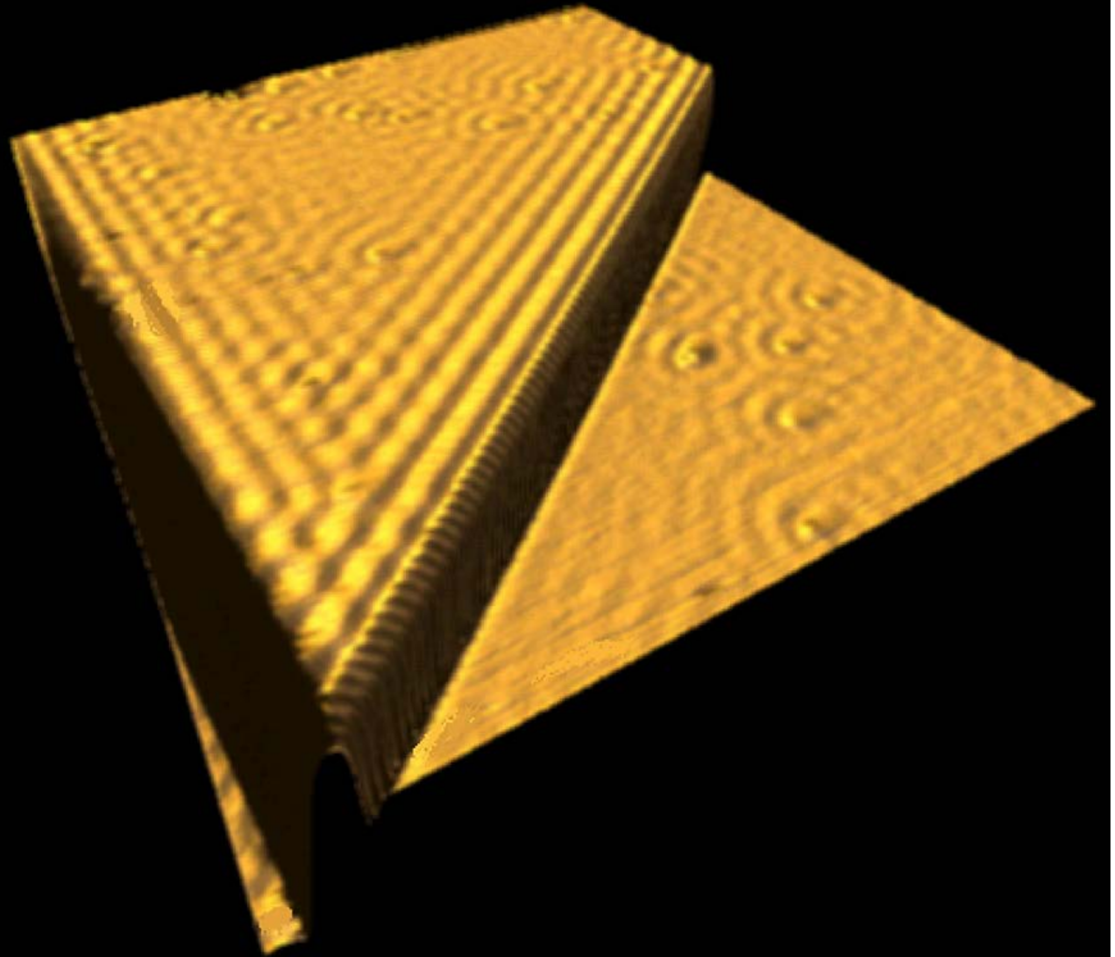
Electron scattering at atomic steps

Cu(111)



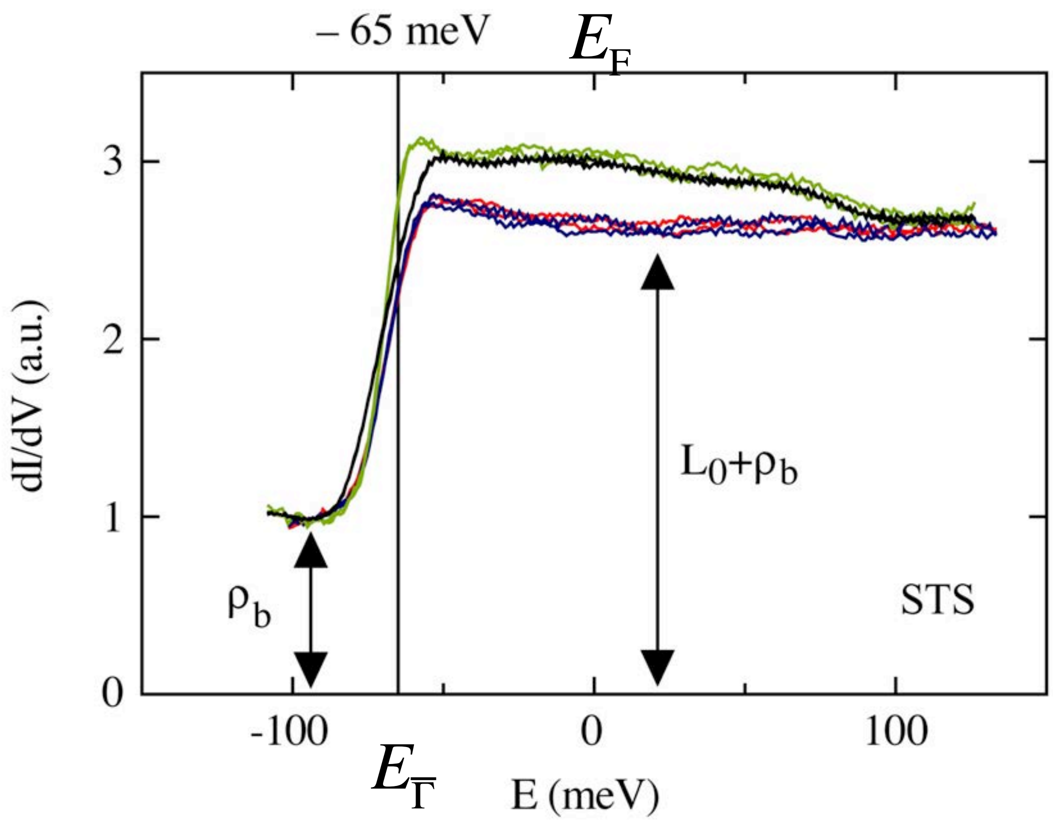
5 K, V_t = 1.0 mV, I_t = 1.1 nA

Ag(111)



5 K, V_t = 13 mV, I_t = 0.32 nA, 1000 Å x 1000 Å

Local Density of States (LDOS) of Ag(111)



2D LDOS: $$\rho_{2D}(E) = L_0\Theta(E - E_{\bar{\Gamma}}) = \frac{m^*}{\pi\hbar^2}\Theta(E - E_{\bar{\Gamma}})$$

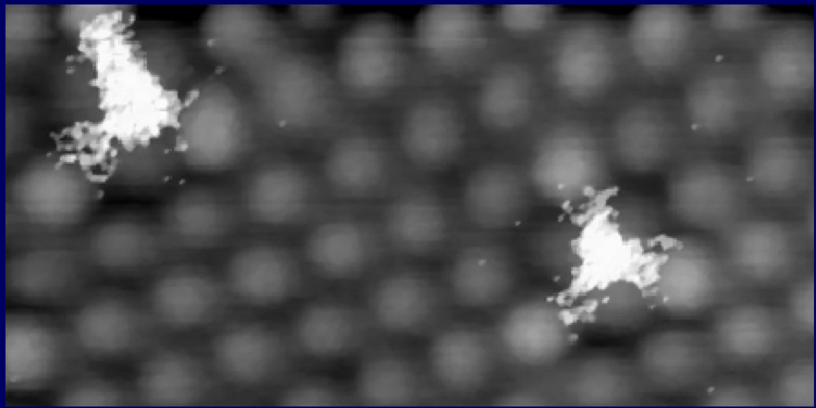
2D e^- density: $$n_{2D} = \frac{m^*}{\pi\hbar^2}\left|E_{\bar{\Gamma}}\right| \approx 10^{13}\, cm^{-2}$$

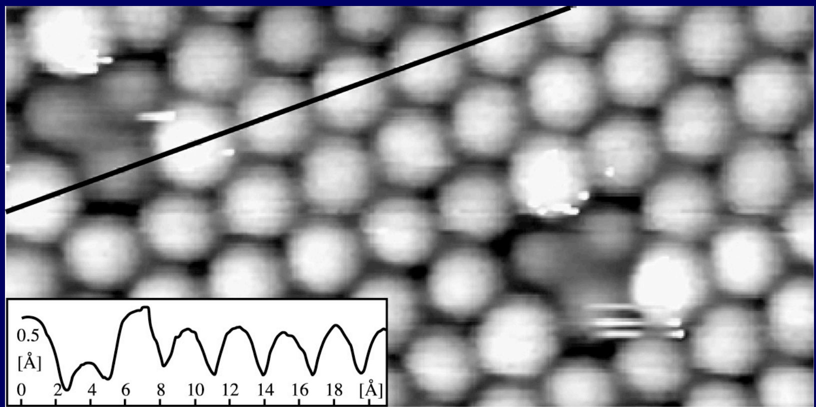
2DEG at semiconductor heterojunctions: $n_{2D} \approx 5\cdot 10^{11}\, cm^{-2}$

Friedel Oscillations

Bulk

C/Al(111)





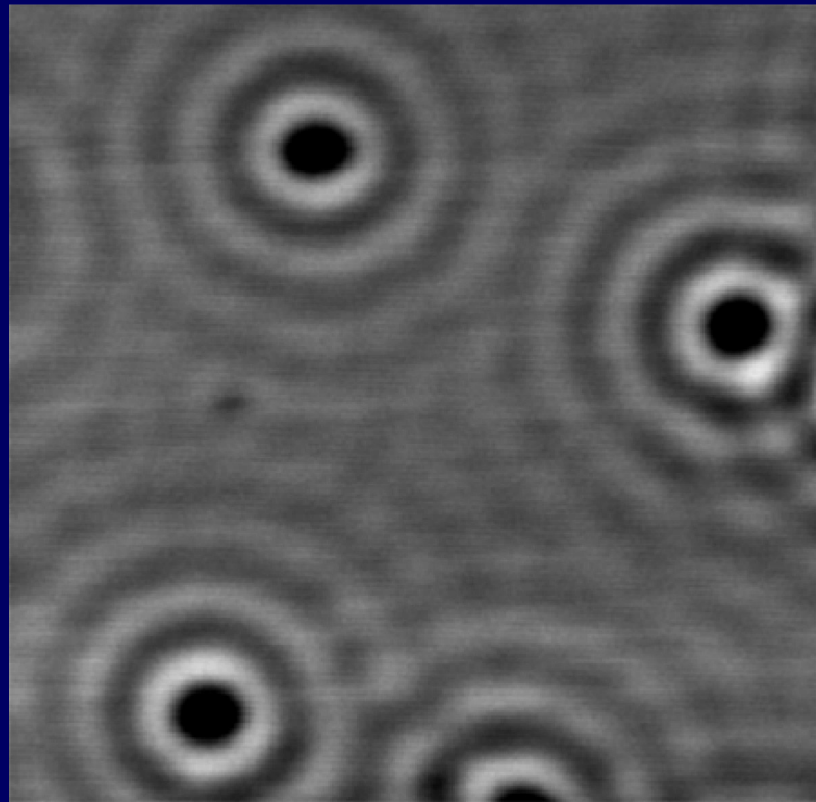
10 Å

$\lambda_F = 3$ Å

LDOS $\approx \cos(2k_F r)/r^5$

Surface State

substitutional defects on Ag(111)



100 Å

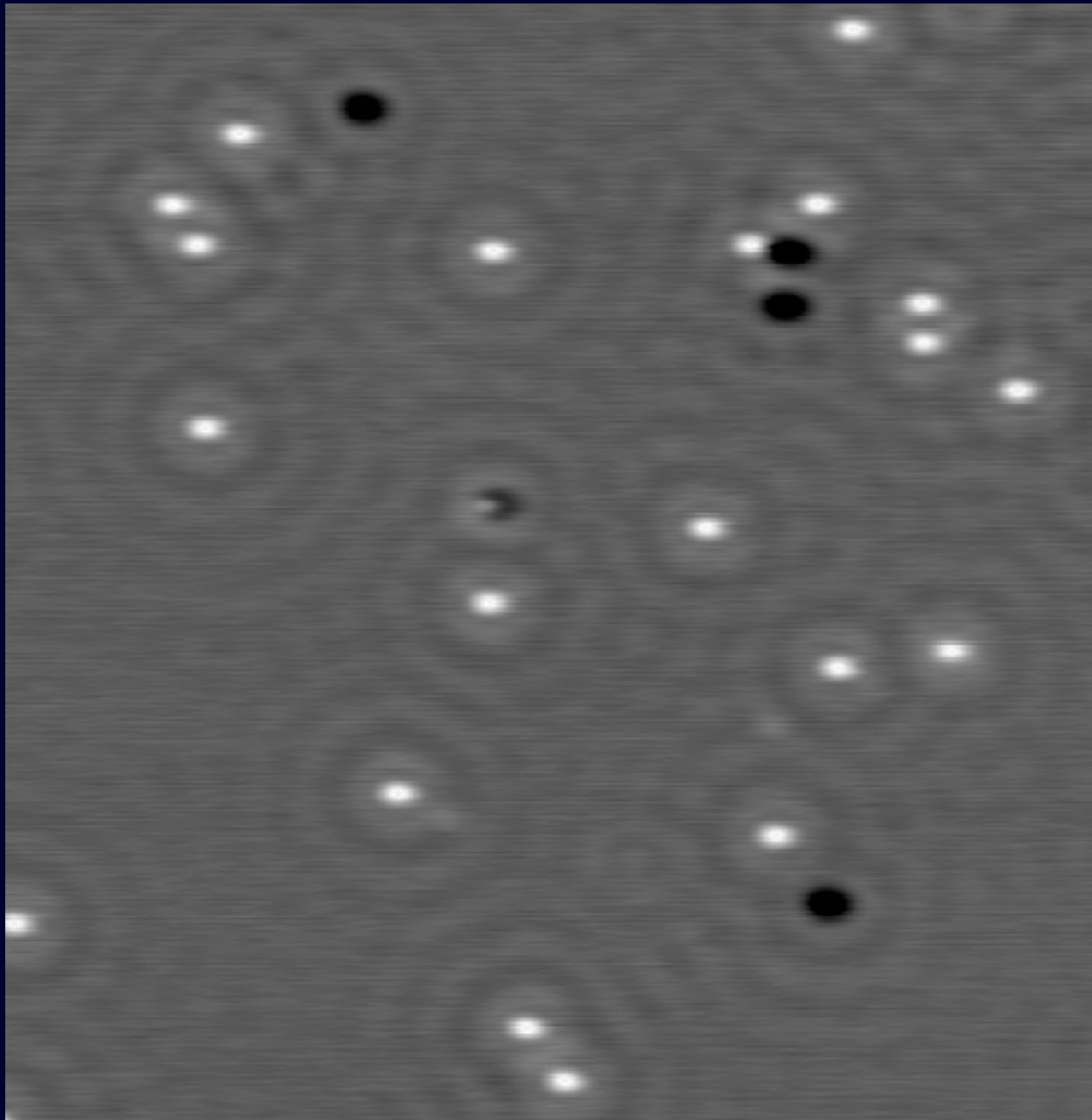
$\lambda_F = 75$ Å

LDOS $\approx \cos(2k_F r)/r^2$

Brune *et al*. EPL **13** (1990).

N. Knorr *et al*. PRB **65** (2002).

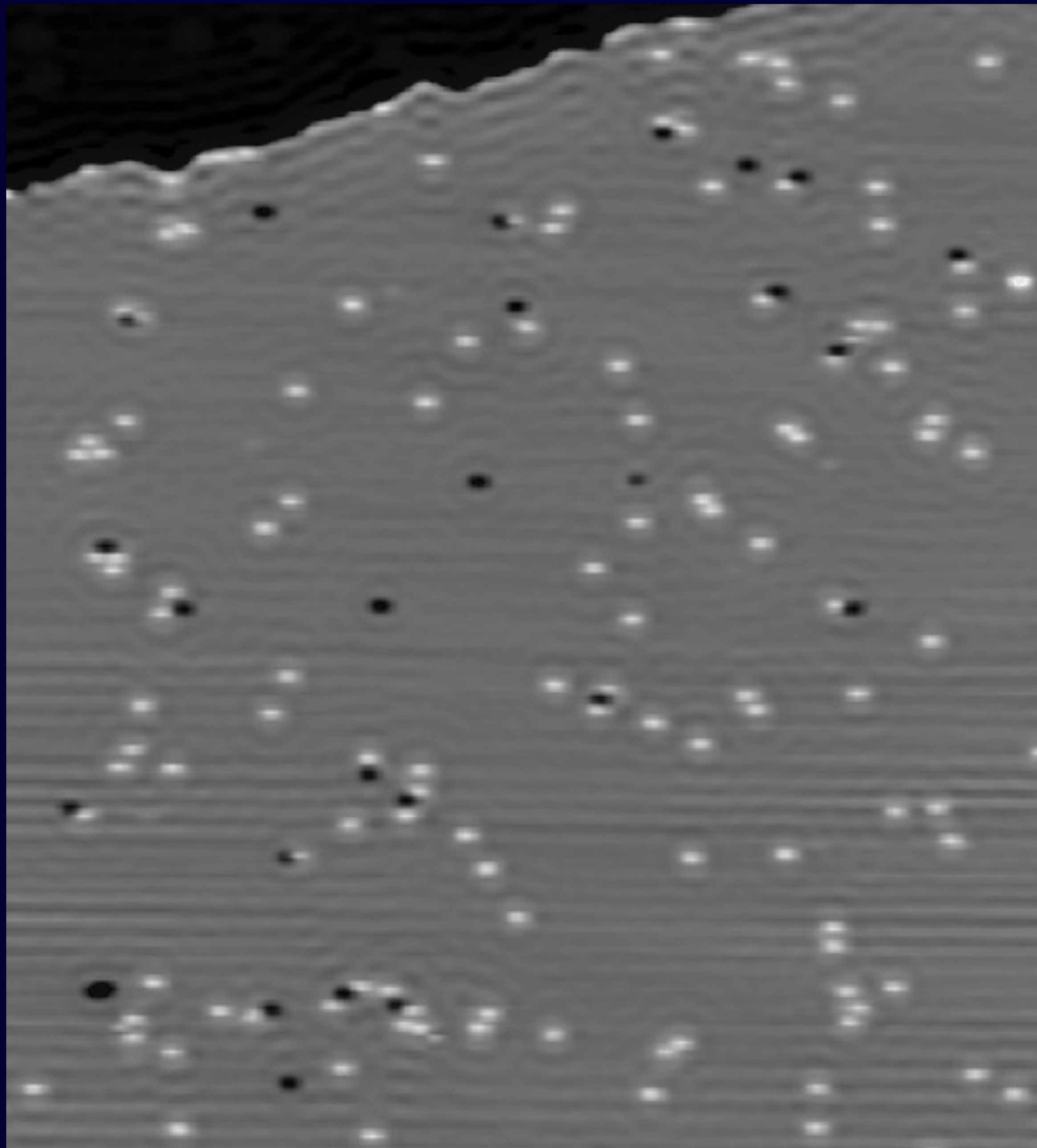
Watching tracer diffusion: Cu/Cu(111)



100 Å

T = 13.5 K, Θ = 1.4 x 10^{-3} ML

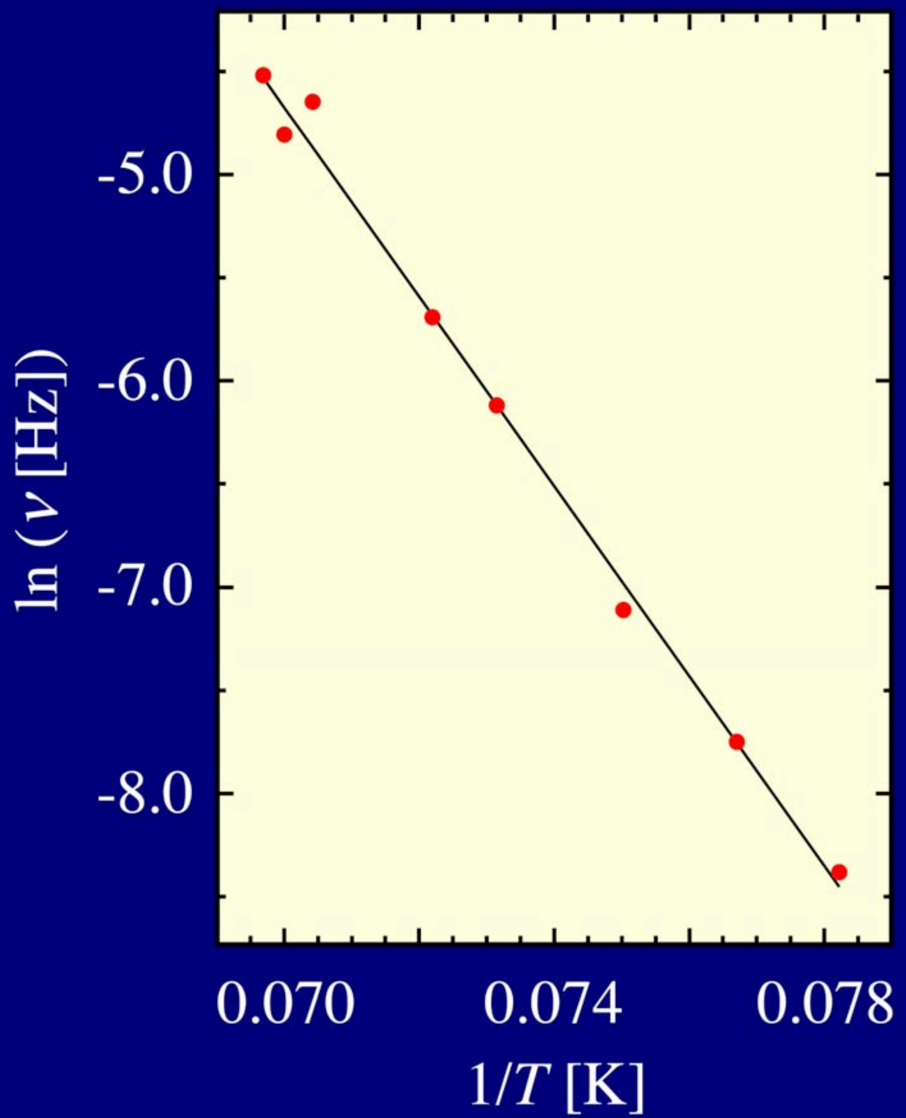
Watching tracer diffusion: Cu/Cu(111)



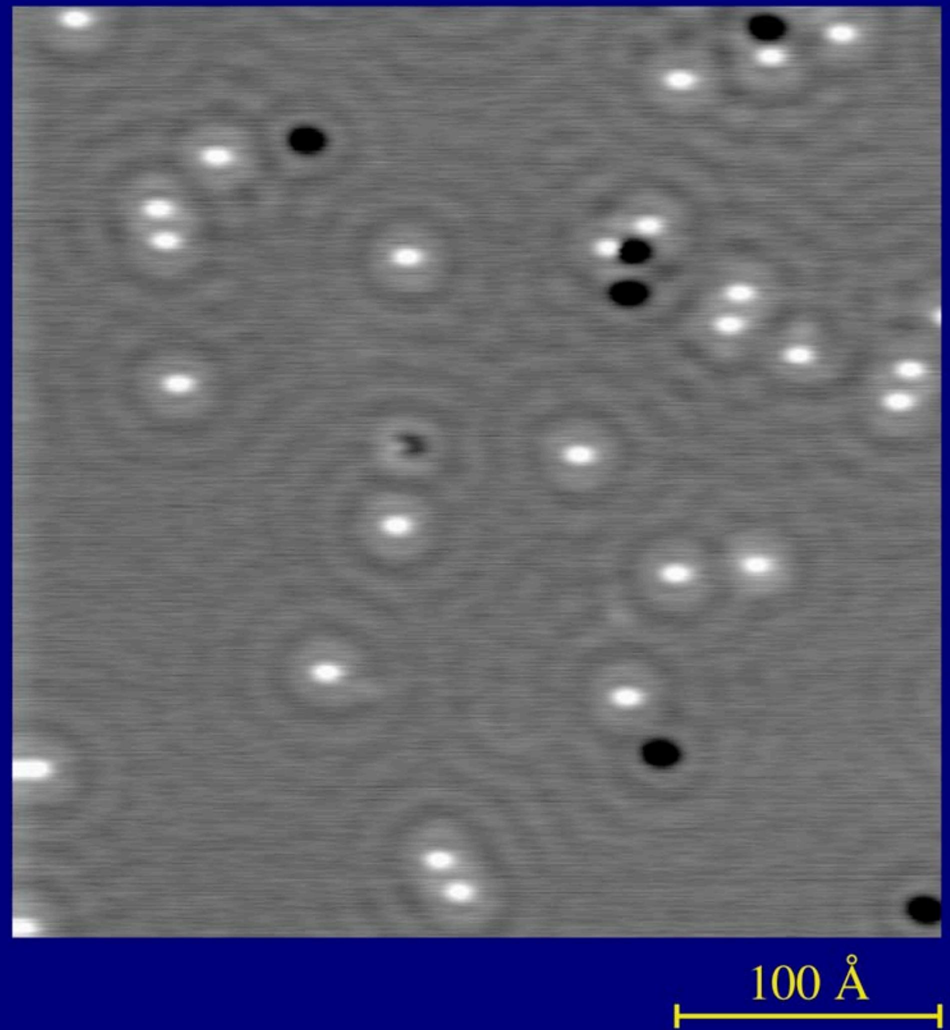
T = 15.6 K, Θ = 1.4 x 10^{-3} ML

100 Å

Tracing Cu monomer diffusion Cu(111)



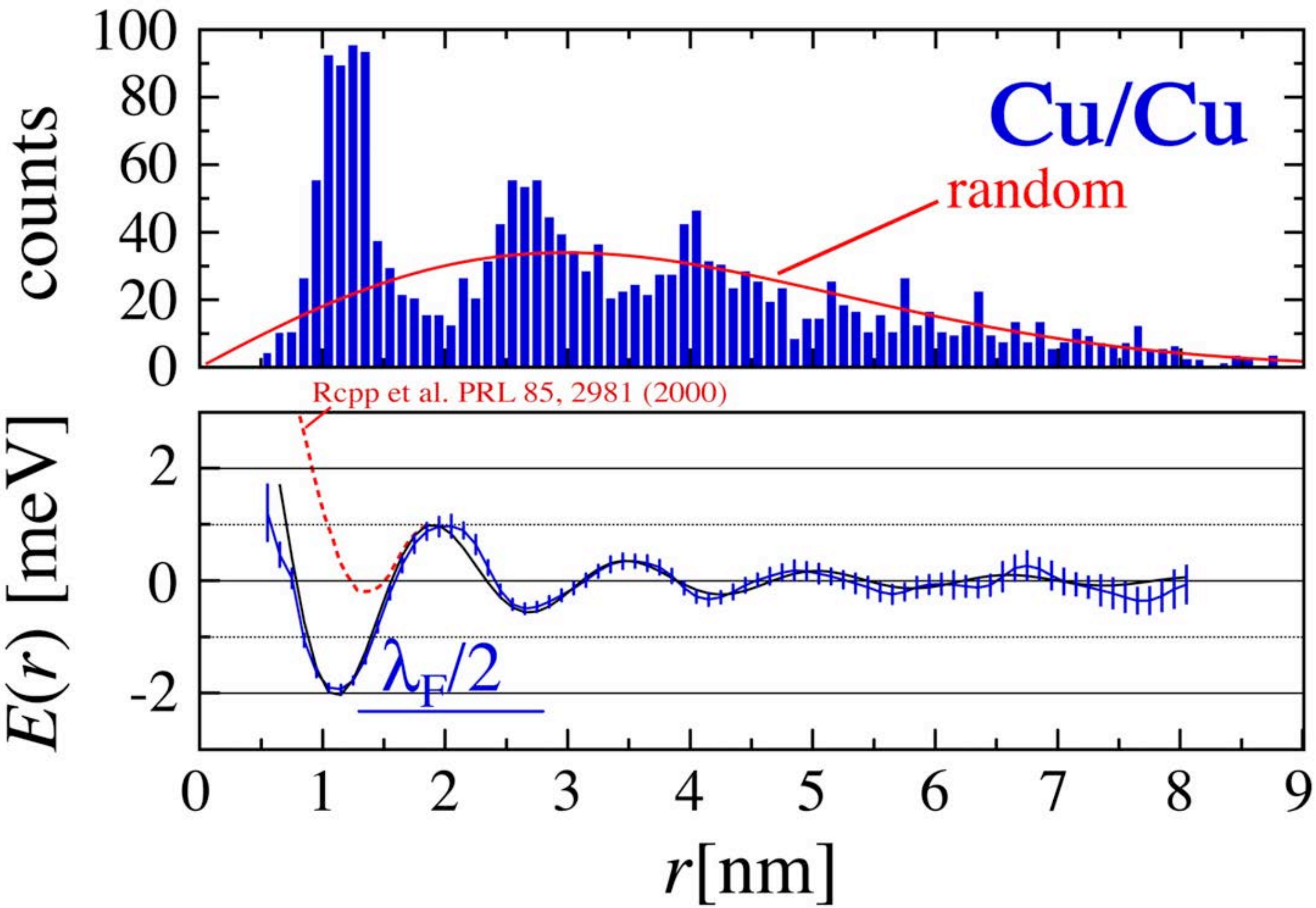
$E_m = 40 \pm 1$ meV $\nu_0 = 1x10^{12.0\pm0.5}$ s^{-1}



$T = 13.5$ K, $\Theta = 1.4x10^{-3}$ ML
$V_t = 0.1$ V, $I_t = 0.1$ nA

N. Knorr *et al*. PRB **65** (2002).

Long range interactions show up in pair–distribution



$\Phi = (0.50 \pm 0.07)\ \pi,\ \ q = (0.20 \pm 0.01)\ \text{Å}^{-1},\ \ k_{F,\,Cu(111)} = 0.21\ \text{Å}^{-1}$

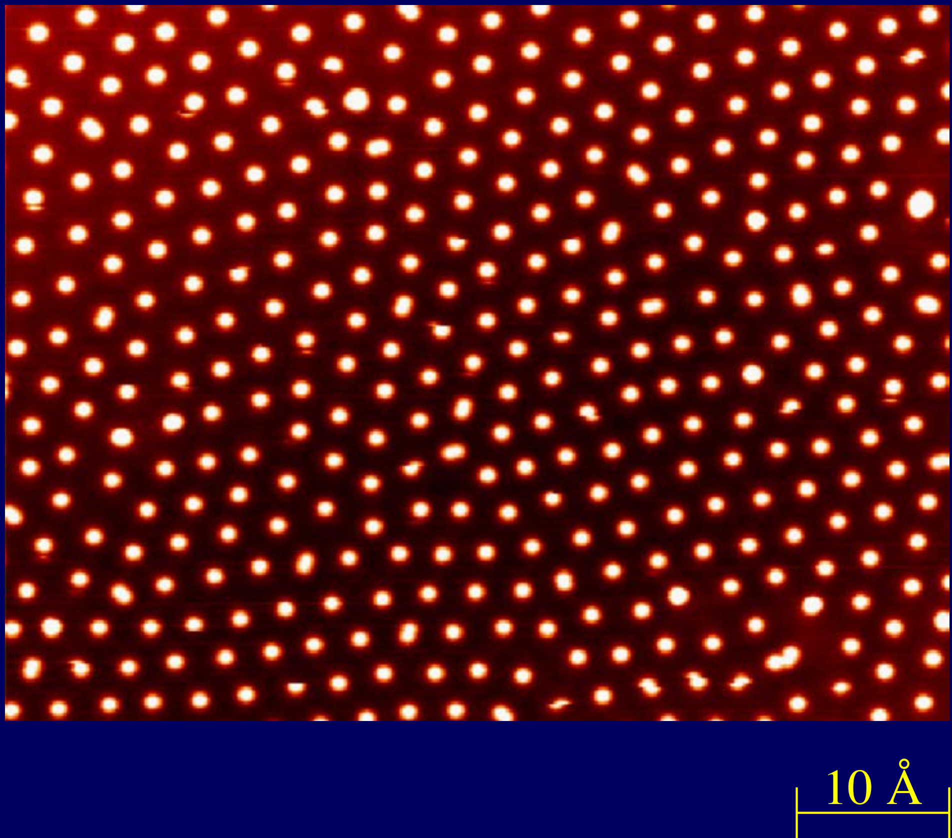
prediction: Lau & Kohn (1978), model: Hyldgaard & Persson, JPCM (2000)

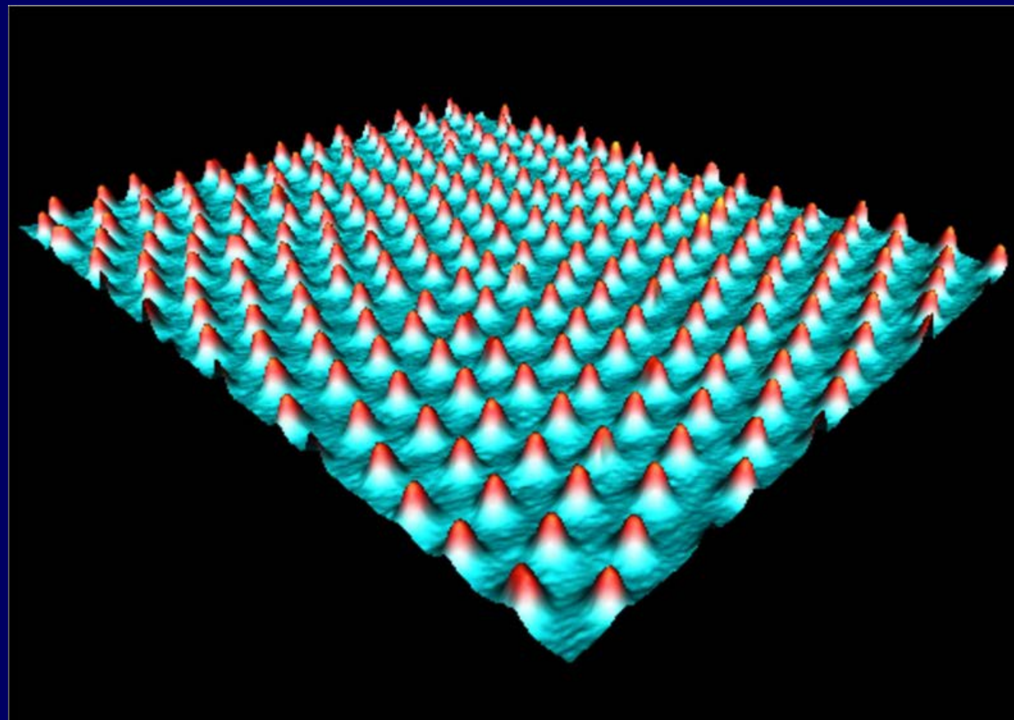
Short-range repulsion of 14 meV !

J. Venables & H. Brune PRB **66** (2002).

N. Knorr *et al*. PRB **65** (2002).

Ce/Ag(111)

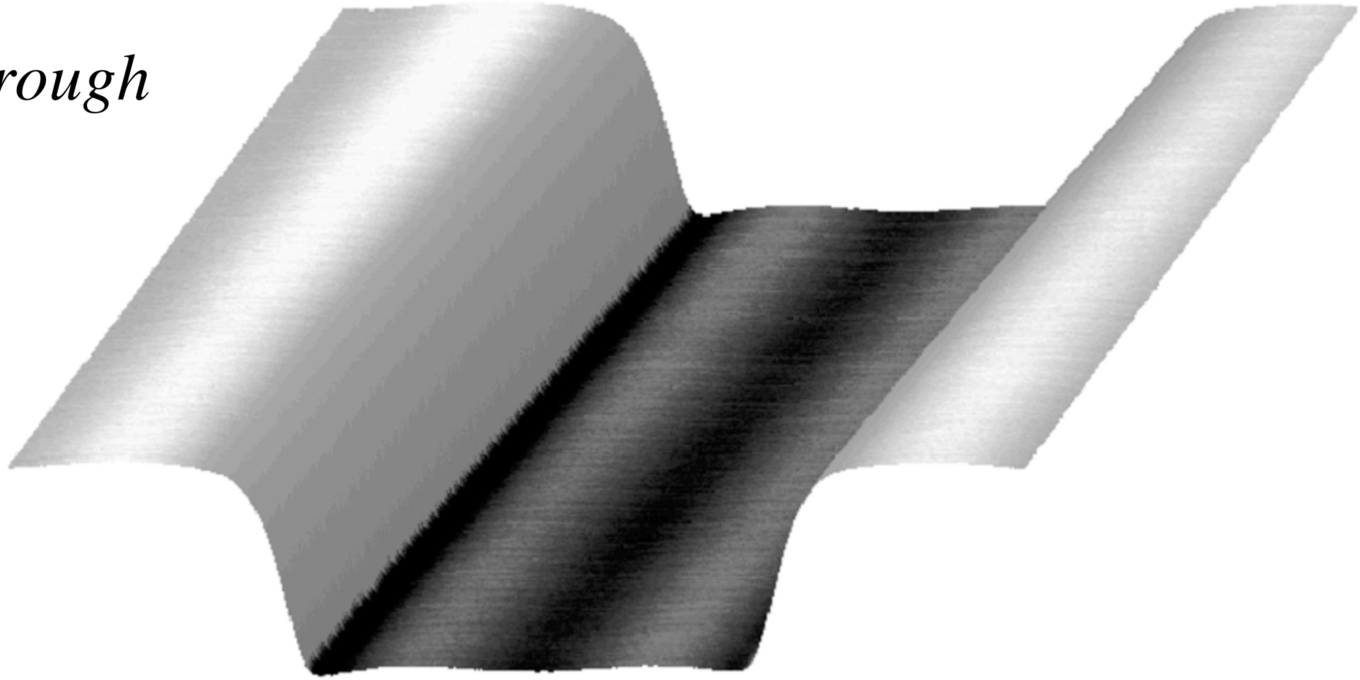


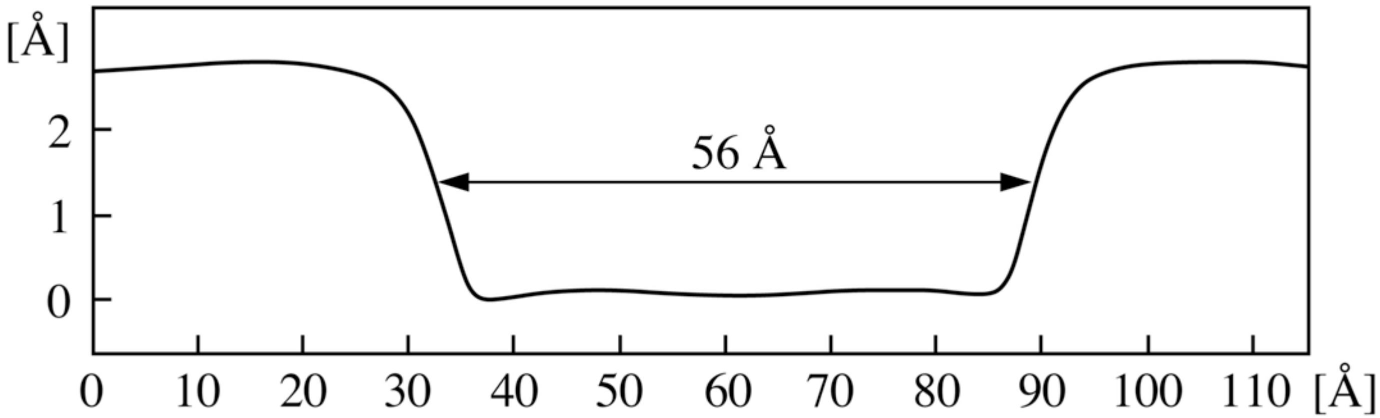


F. Silly *et al*. Phys. Rev. Lett. **92** (2004).

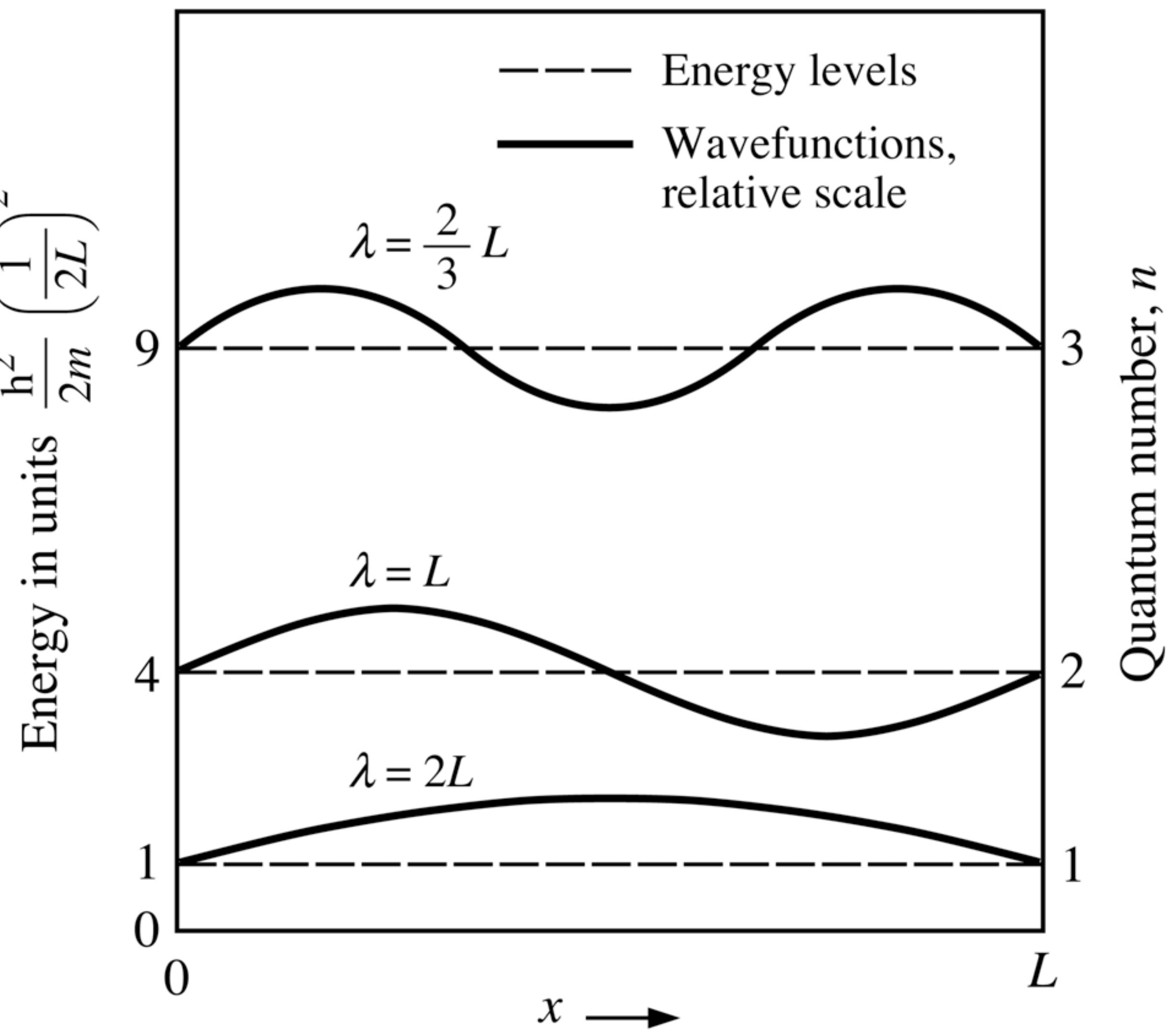
Quantum Confinement

Quantum trough on Ag(111)



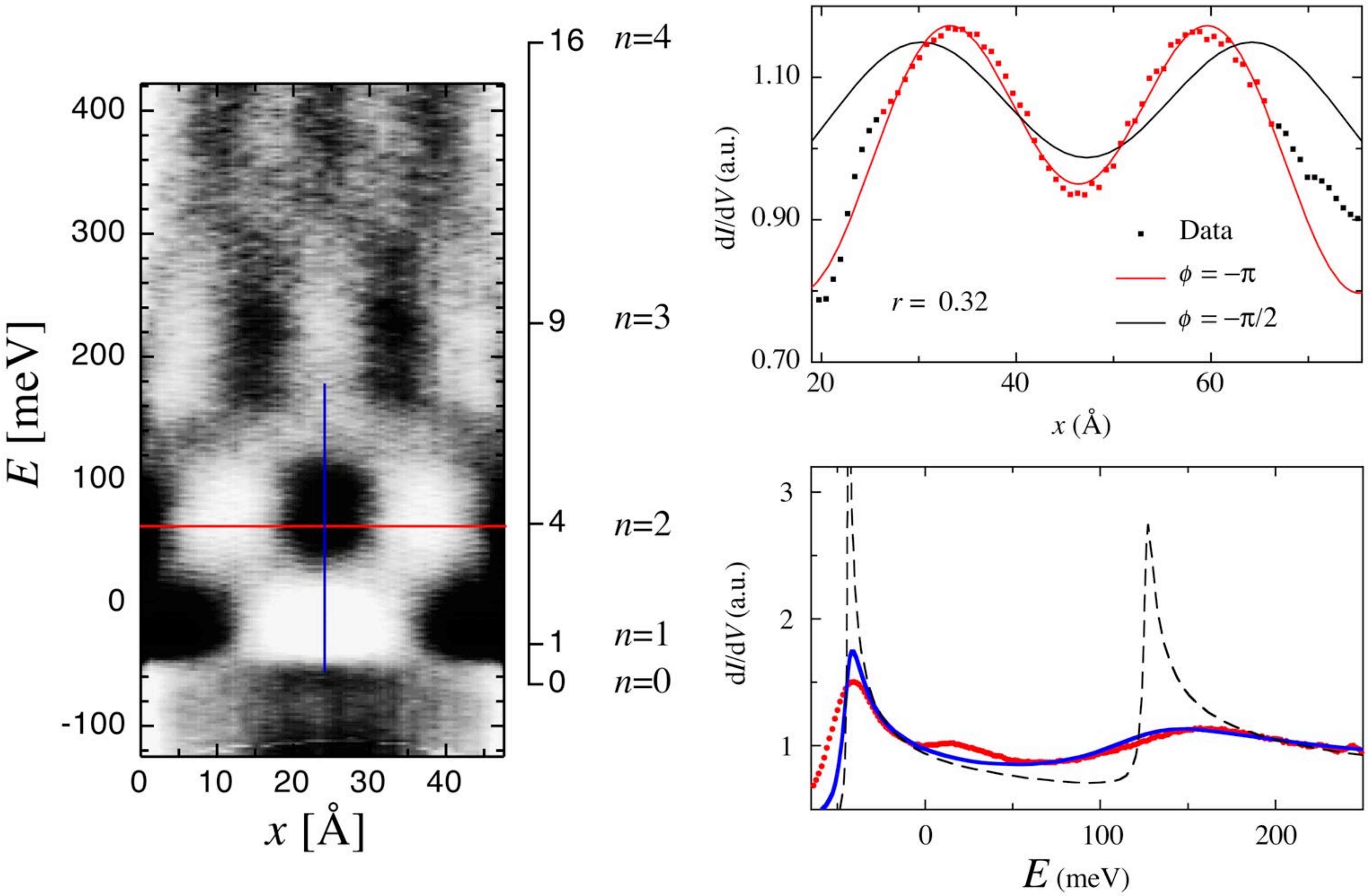


Particle in box of width L

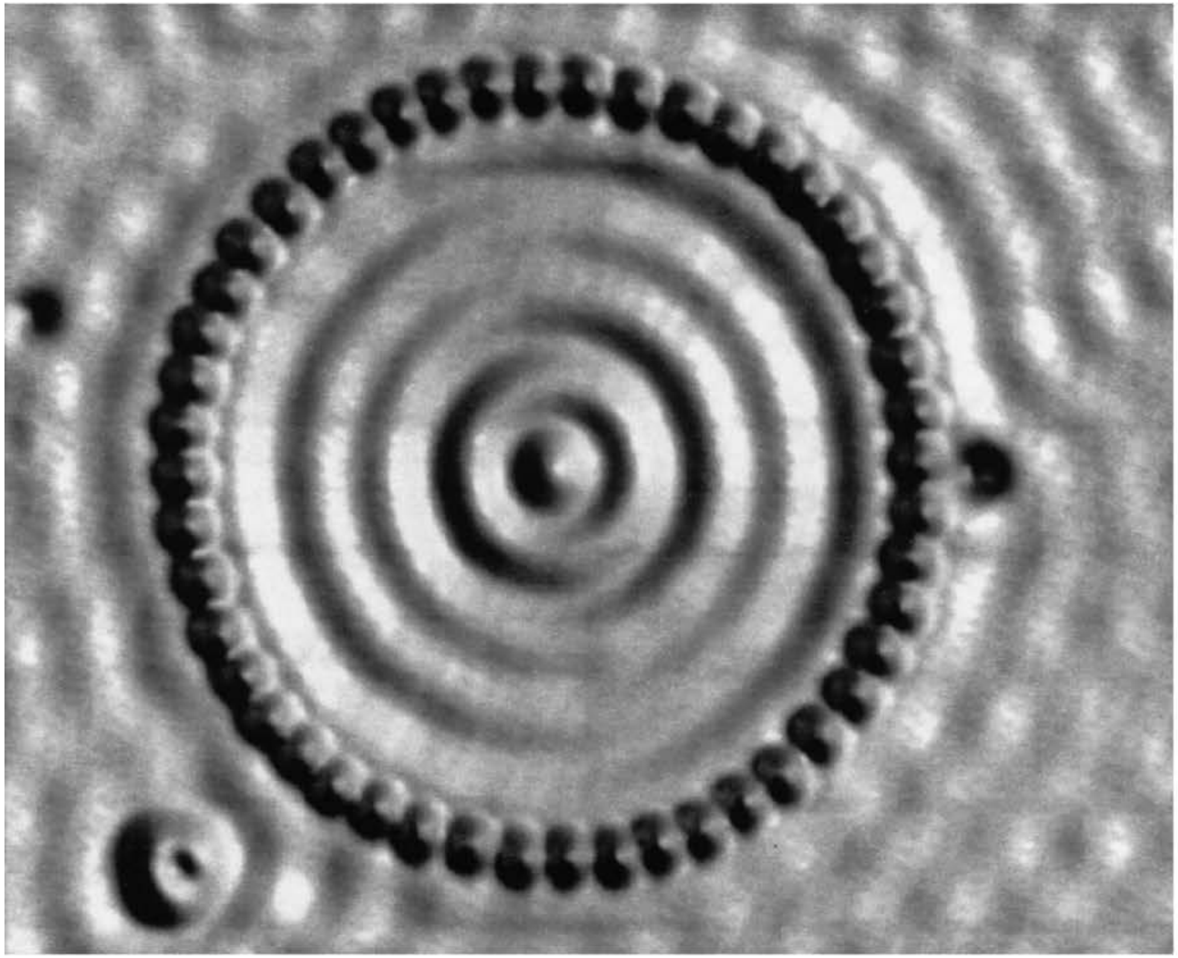


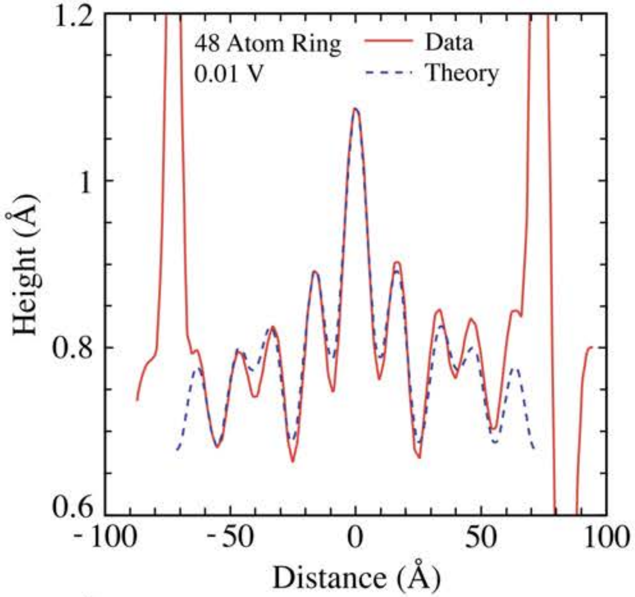
$$E_n = \frac{\hbar^2}{2m}k_n^2 = \frac{\hbar^2}{2m}\left(\frac{2\pi}{\lambda_n}\right)^2 = \frac{h^2}{2m}\left(\frac{n}{2L}\right)^2$$

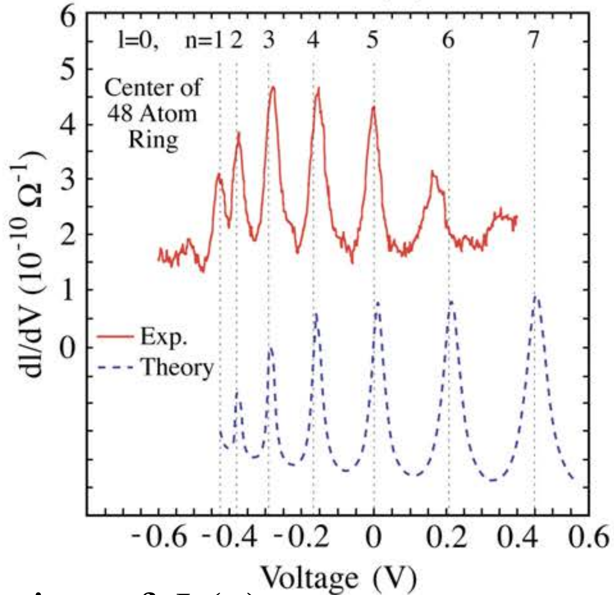
LDOS in Quantum trough



Electrons in Quantum Corral: Fe/Cu(111)







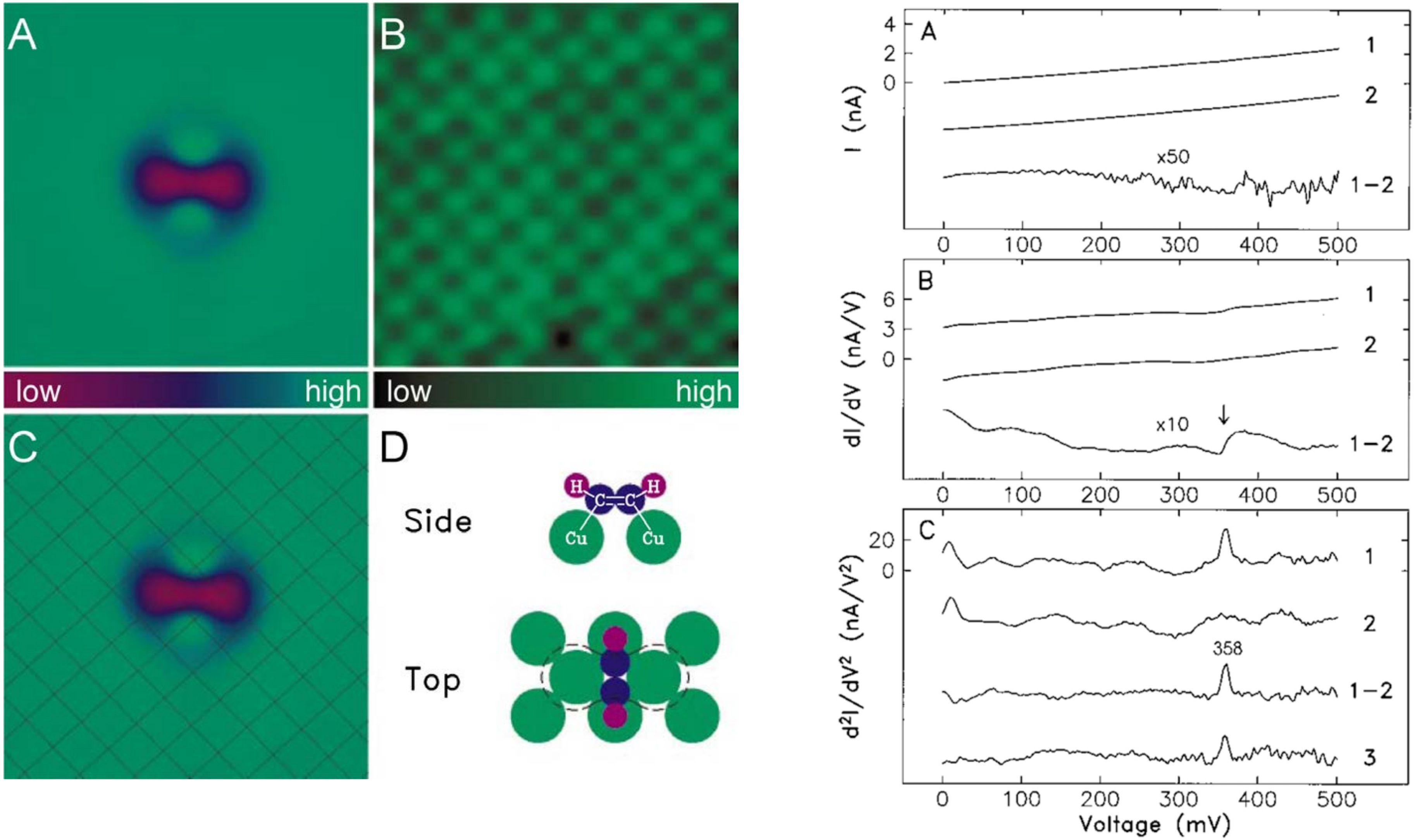
$$\Delta LDOS(x) = \frac{1}{kx}\left(\cos^2(kx - \frac{\pi}{4} + \delta_0) - \cos^2(kx - \frac{\pi}{4})\right), k = \sqrt{\frac{2m^* E}{\hbar^2}}$$

$$\Psi_{n,l}\left(x,\Phi\right) = const.\ J_l(k_{n,l}x)e^{il\Phi},\ \text{with } k_{n,l} = \frac{z_{n,l}}{r}, z_{n,l} \text{ n'th zero-crossing of } J_l(z)$$

M.F. Crommie, C.P. Lutz, D.M. Eigler, Science **262**, 218 (1993).

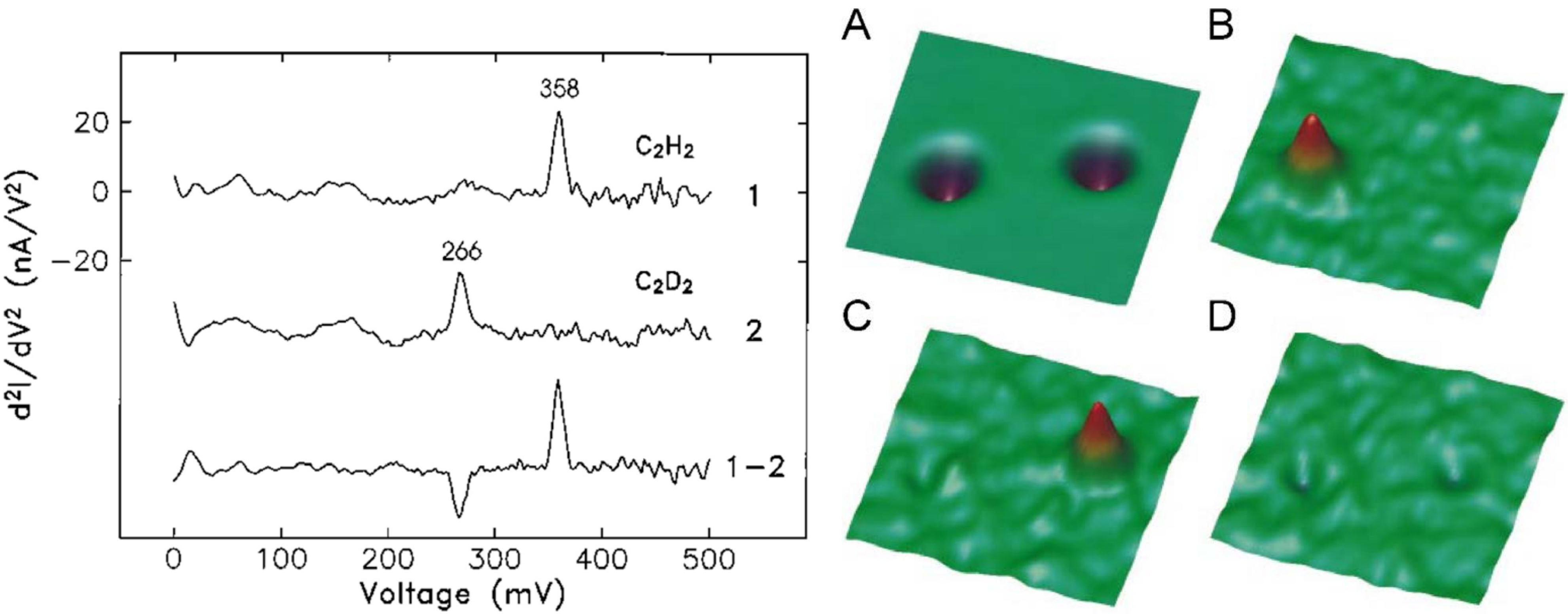
Inelastic Electron Tunneling Spectroscopy (IETS)

Detecting vibrational quantum levels for $C_2H_2/Cu(100)$



B. C. Stipe *et al*. Science (1998).

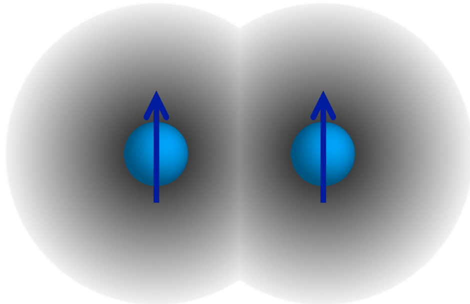
Isotope Effect – C_2H_2 vs. C_2D_2/Cu(100)



B. C. Stipe *et al*. Science (1998).

W. Heisenberg, Z. Phys. **41**, 239 (1927).

Para and Ortho Species in Homonuclear Diatomics



$$\Psi_{\mathrm{tot}} = \Psi_{\mathrm{el}}\,\Psi_{\mathrm{vib}}\,\Psi_{\mathrm{nuc}}\,\Psi_{\mathrm{rot}}$$

The first preparation of pure para H_2 enabled the confirmation by emission spectra and heat conductivity measurements in the gas phase

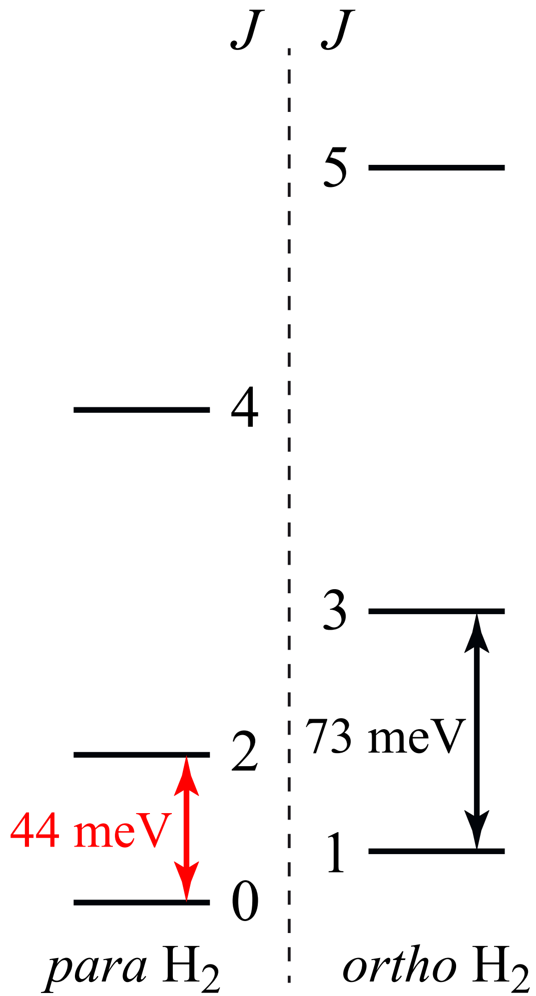
K. F. Bonhoeffer and P. Harteck, Z. Phys. Chem. B **4**, 113 (1929).

Example: Hydrogen and Deuterium

$I_N = 1/2$ Fermions

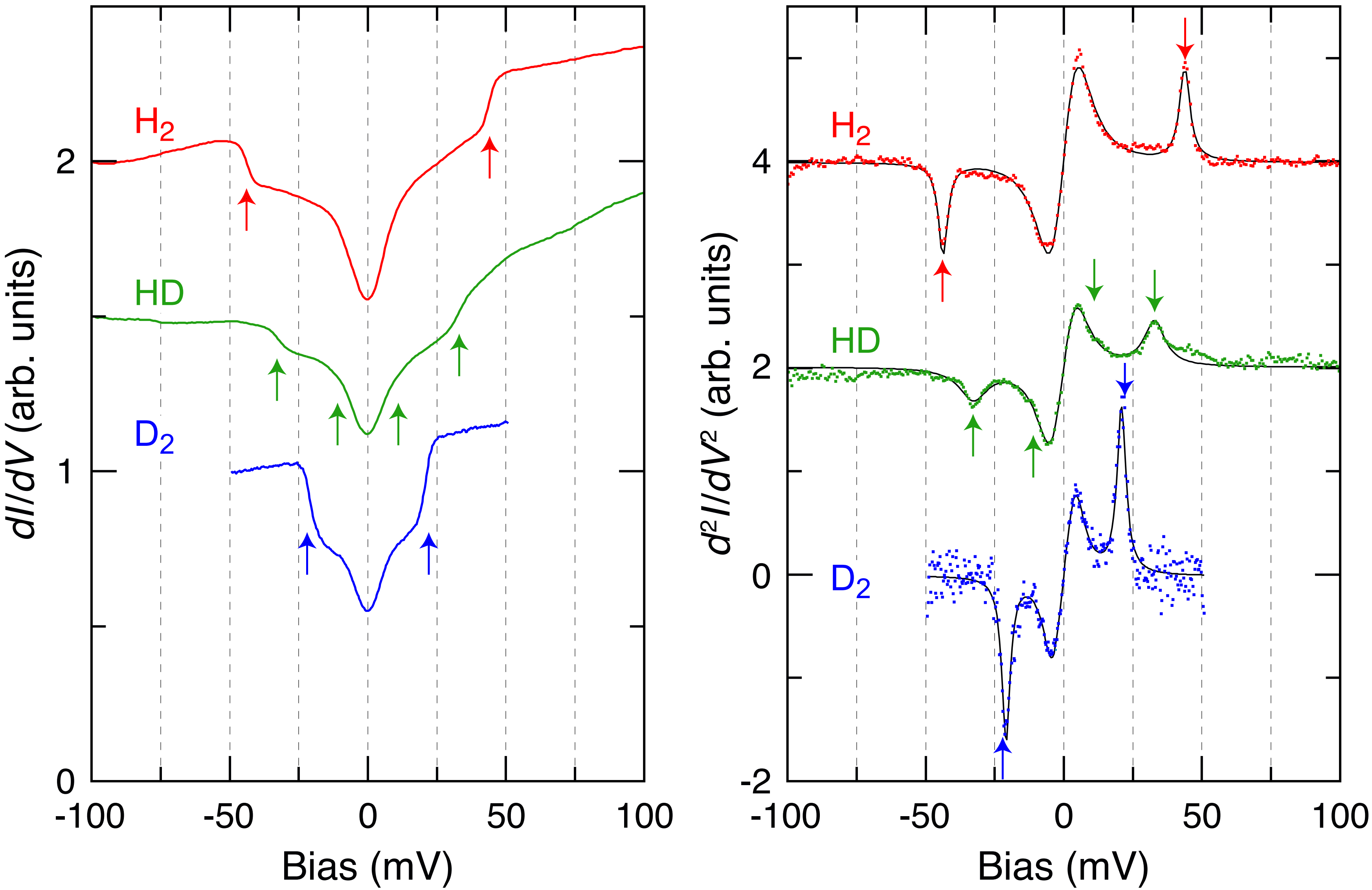
Molecule	Ψ_{tot}	Ψ_{nuc}	Ψ_{rot}
para–H_2	AS	AS	S (even J)
ortho–H_2	AS	S	AS (odd J)
ortho–D_2	S	S	S (even J)
para–D_2	S	AS	AS (odd J)

$I_N = 1$ Bosons



Detection of rotational quantum levels

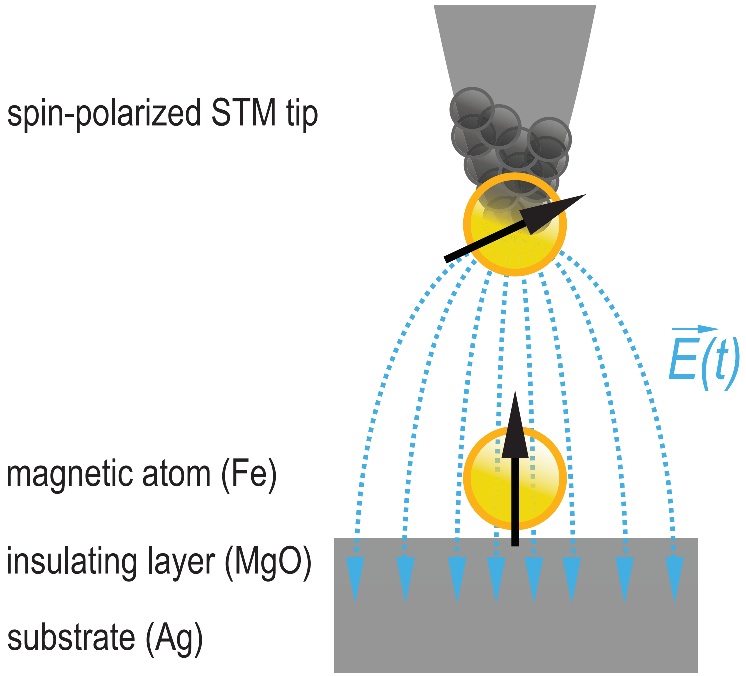
STM-IETS on H_2, D_2, and HD/h-BN/Ni(111)

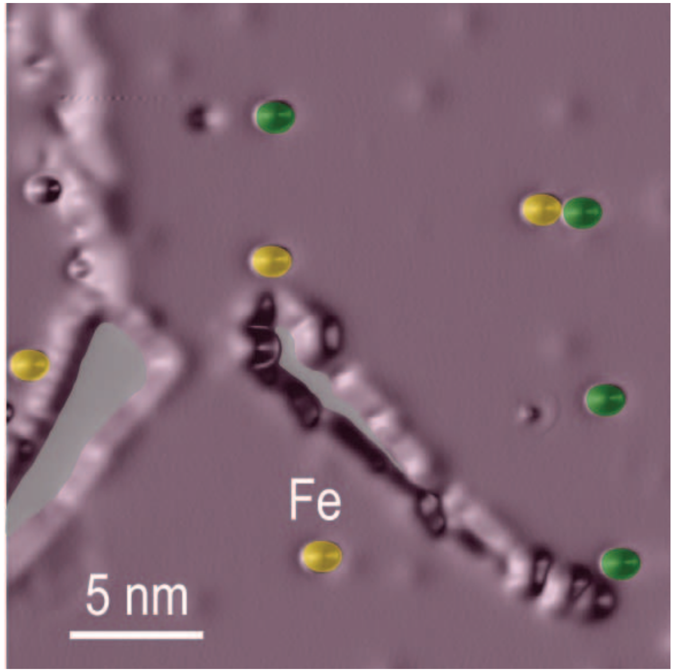


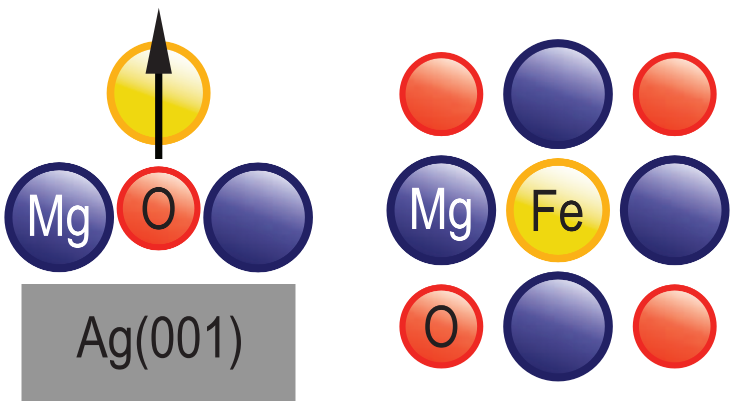
$R_g = 10^9\ \Omega$, $T = 4.2$ K

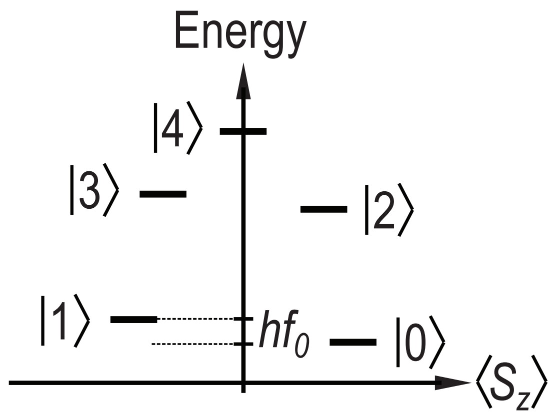
F. D. Natterer *et al.* PRL **111**, 175303 (2013).

Electron Spin Resonance (ESR) with the STM



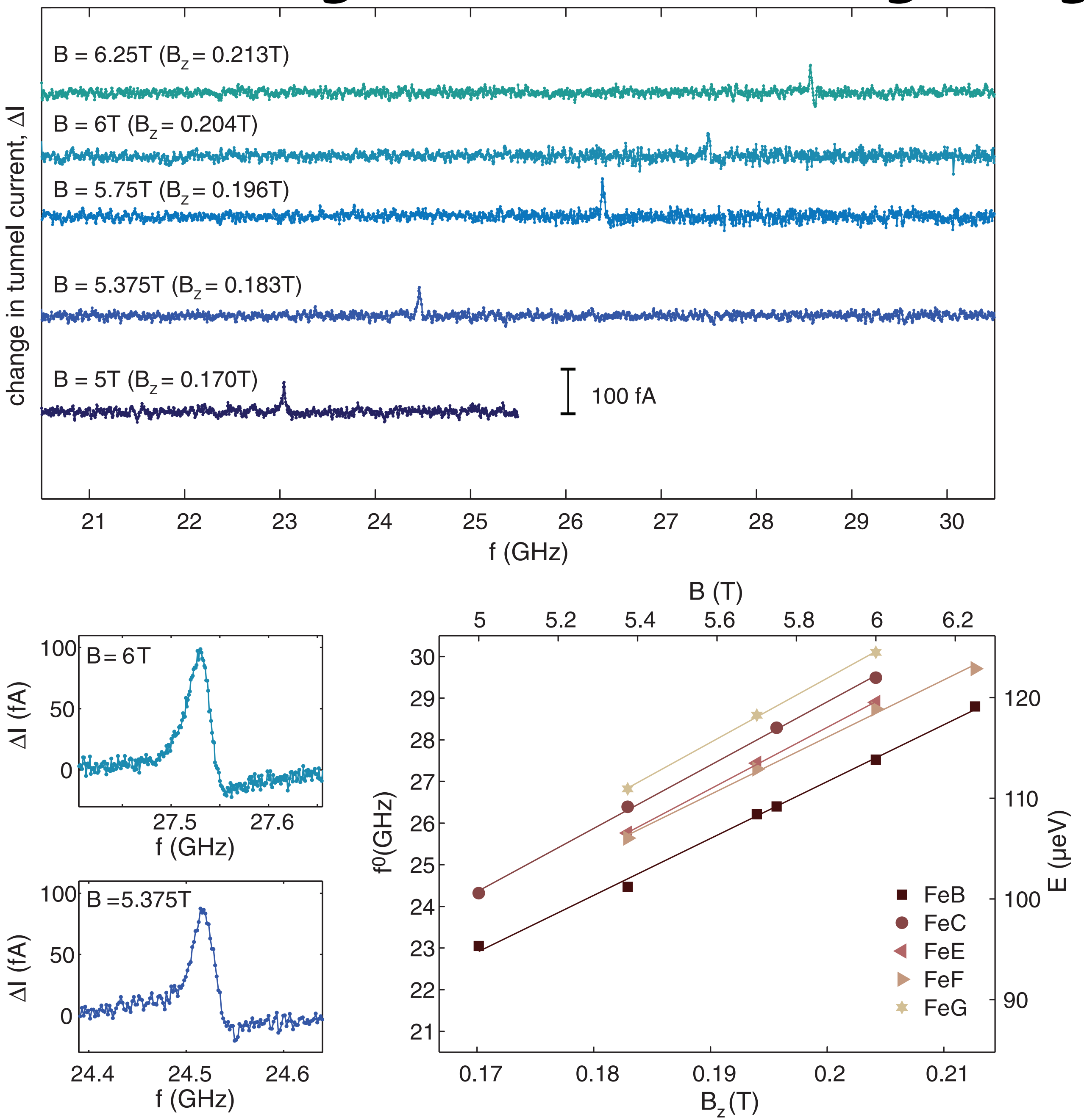






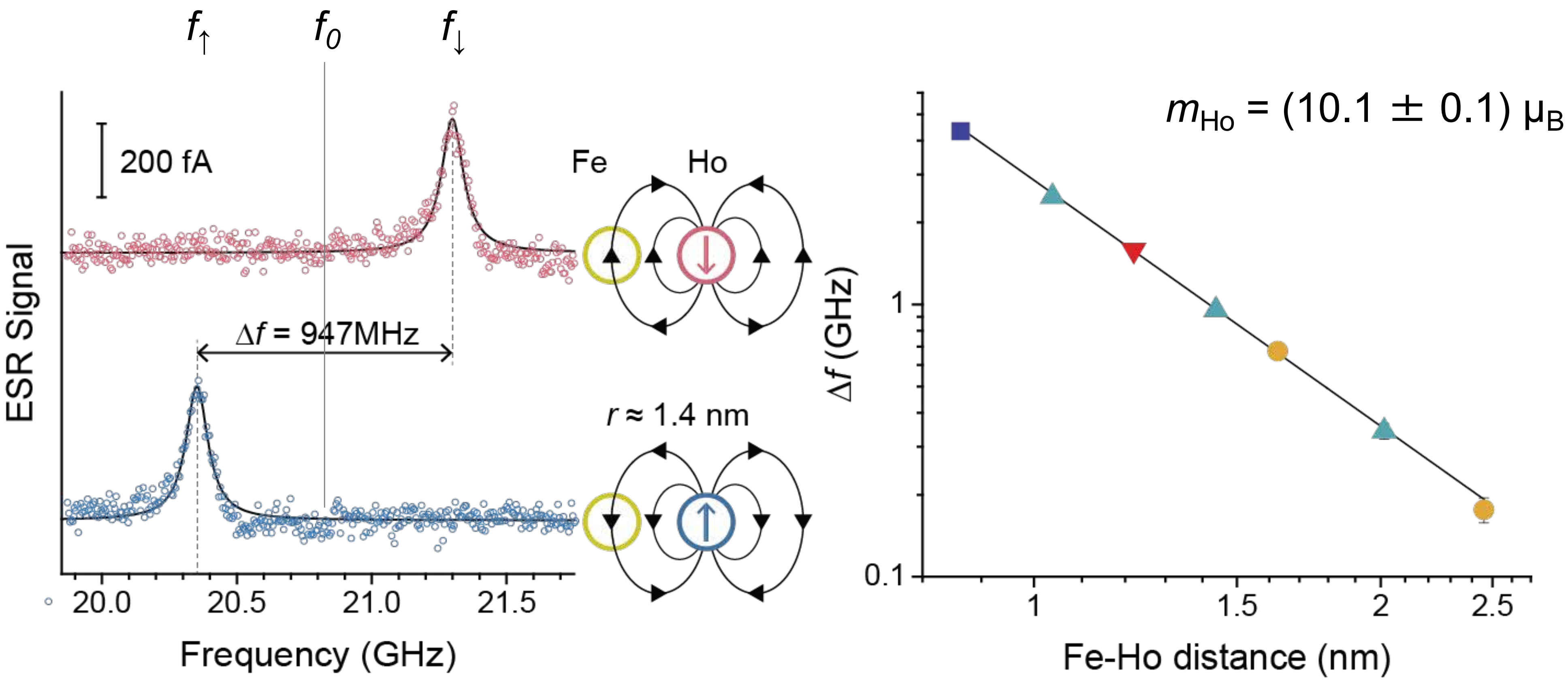
S. Baumann *et al.* Science **350**, 417 (2015).

ESR-STM on single Fe atoms on MgO/Ag(100)



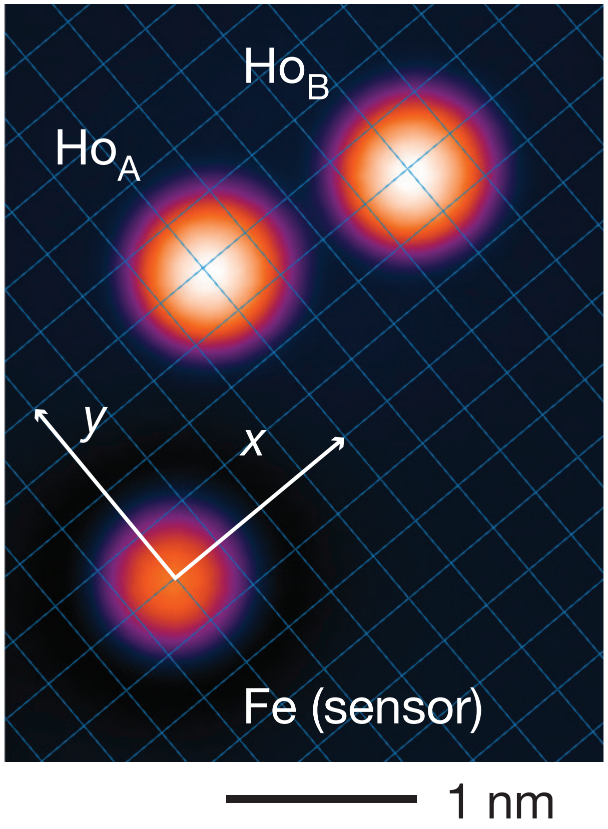
S. Baumann *et al.* Science **350**, 417 (2015).

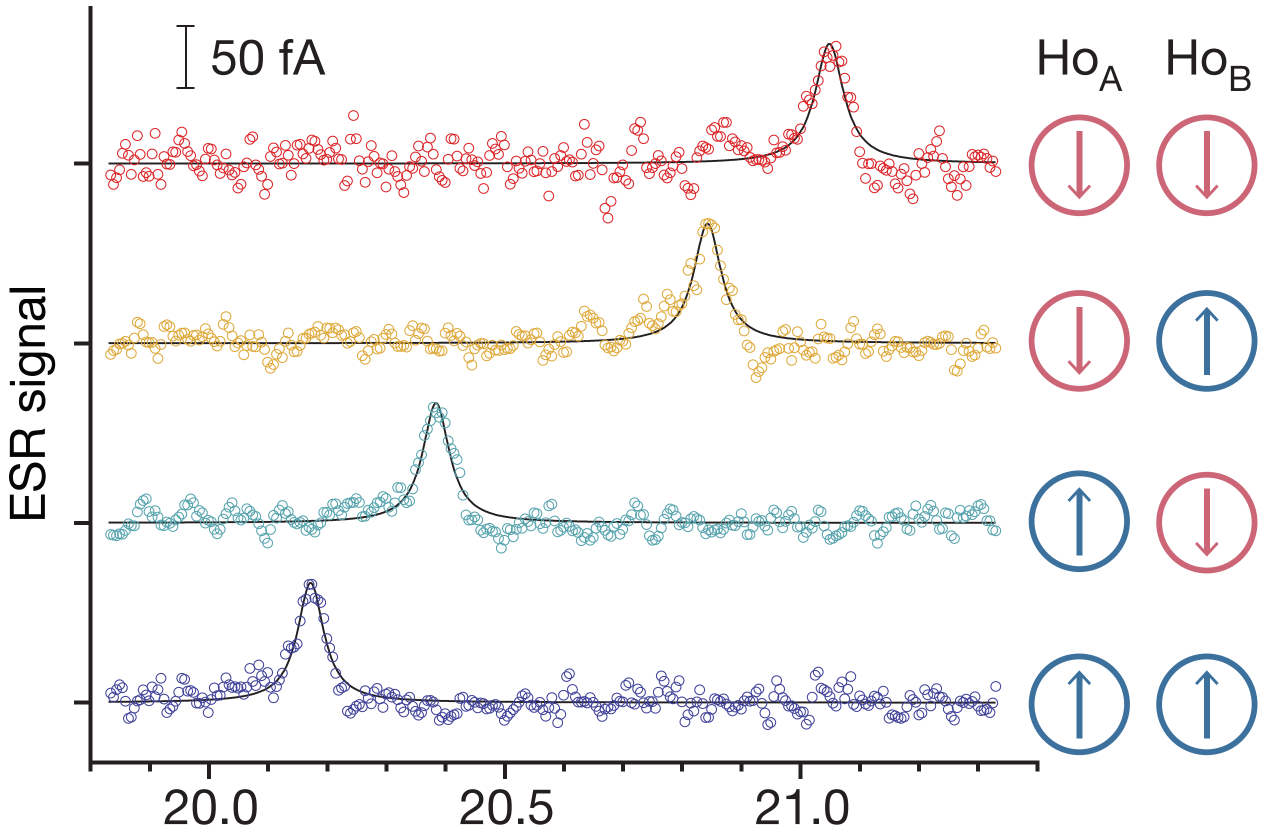
Coupling Ho to an Fe sensor – read with ESR-STM



Ho/MgO/Ag(100) first single atom magnet: F. Donati *et al*. Science **352**, 318 (2016);
Fe to read stray-field of Ho on MgO/Ag(100): F. D. Natterer *et al*. Nature **543**, 226 (2017).

2 bit memory – ESR read-out on Fe sensor atom

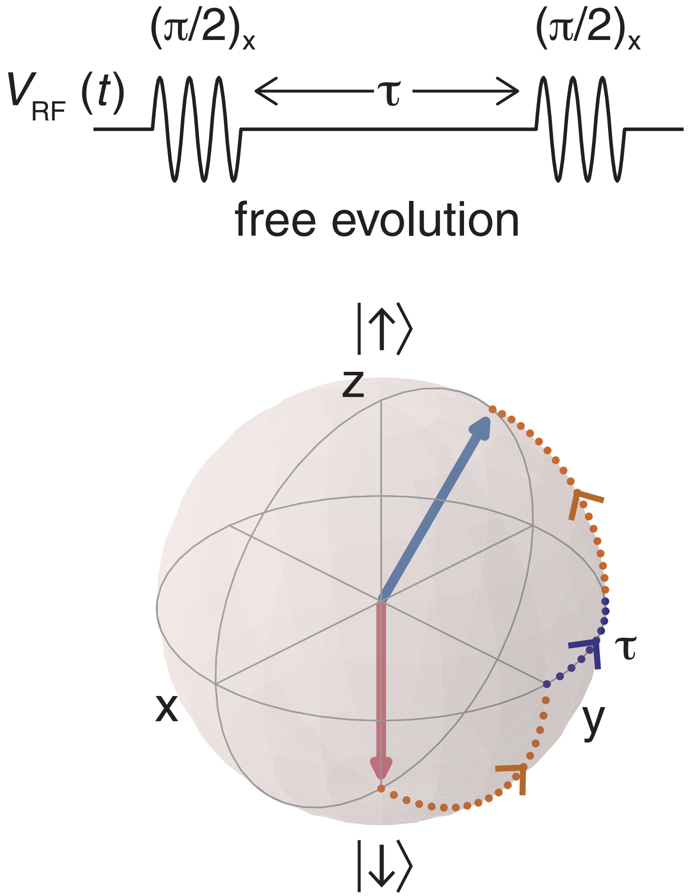


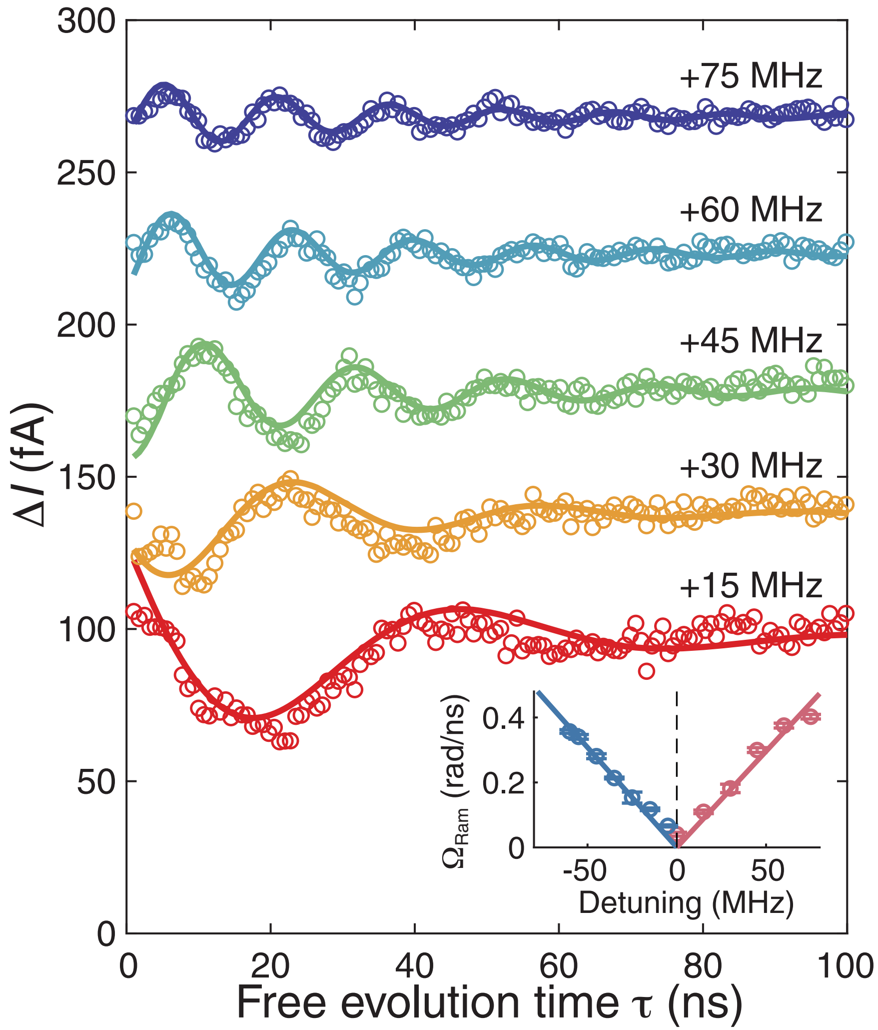


no switching at 1.2 K for 5 h

F. D. Natterer *et al*. Nature **543**, 226 (2017).

TiH/MgO/Ag(100): coherent spin manipulation





$T_{2,\ Rabi}$ = 40 ns $\quad$ T_2 = 189 ± 23 ns

K Yang *et al.* Science **366**, 509 (2019).