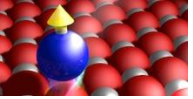


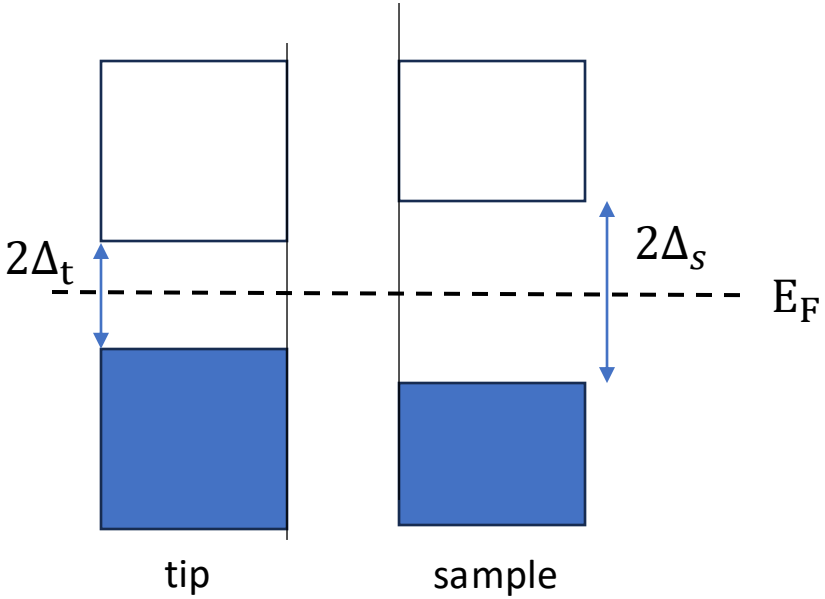
4.1 SIS junction

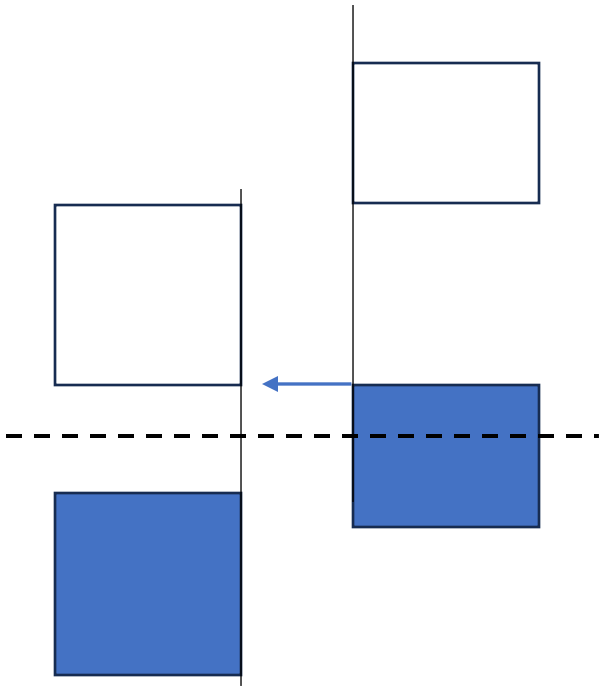
Consider a superconductor-insulator-superconductor (SIS) junction.

Sketch the energy barrier scheme at the relevant bias voltages and deduce qualitatively the dI/dV spectrum.

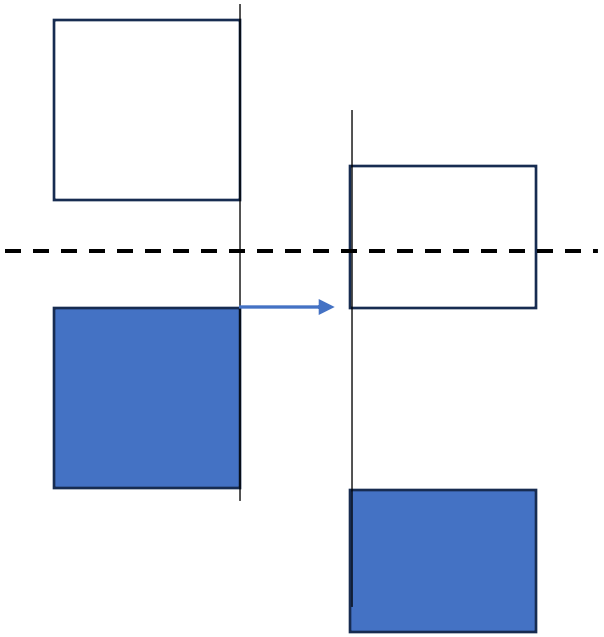
Which quantity can be determined?

4.1 SIS junction - Solution



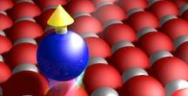


$eV_{Bias} = -\Delta_s - \Delta_t$



$eV_{Bias} = +\Delta_s + \Delta_t$

The observed gap is equal to 2 times the sum of the superconducting gaps.
This sum is the quantity that can be determined



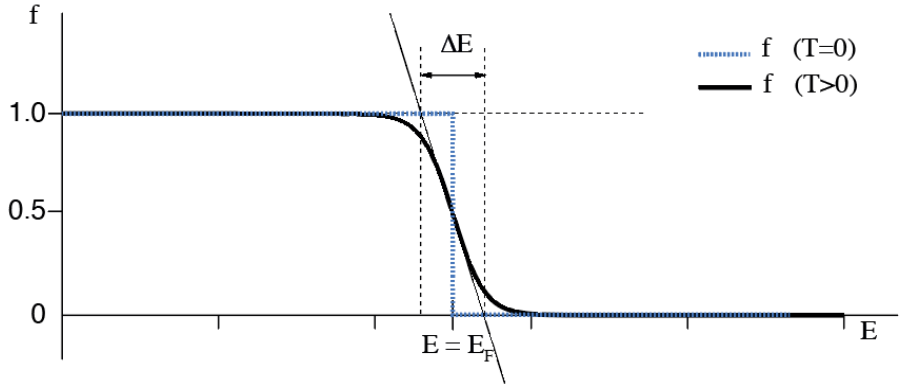
4.2 Quantum states and thermal energy

a) The width of the Fermi-Dirac function is $\sim 4k_BT$.

$$f(E) = \frac{1}{1+\exp[(E-E_F)/k_BT]}$$

Evaluate it (in meV) at
- room temperature: $\sim$ 300 K
- liquid nitrogen temperature: $\sim$ 77 K
- liquid helium temperature: $\sim$ 5 K

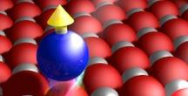
$k_B = 0.086$ meV K^{-1}



b) Consider the Cu chains on Cu(111) discussed in the lecture.

Calculate the difference in energy between the two first states for a chain of length $L = 5$ nm.
Is it possible to resolve these two states at room temperature?

$m^* = 0.68\, m_e$
$m_e = 9.1 \cdot 10^{-31}$ kg
$\hbar = 1.05 \cdot 10^{-34}$ J s



4.2 Quantum states and thermal energy - Solution

a)

- room temperature: ~ 300 K $\Delta E \sim 100$ meV
- liquid nitrogen temperature: ~ 77 K $\Delta E \sim 25$ meV
- liquid helium temperature: ~ 5 K $\Delta E \sim 1.7$ meV

b)

$$E_n = \frac{\hbar^2}{2m^*}\left(\frac{\pi}{L}\right)^2 n^2, \qquad n > 0$$

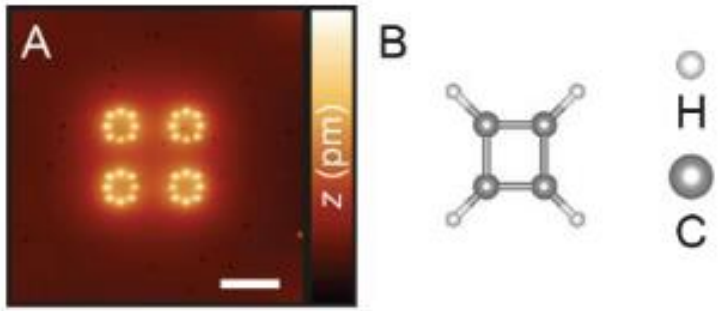
$$E_2 - E_1 = 3\frac{\hbar^2}{2m^*}\left(\frac{\pi}{L}\right)^2$$

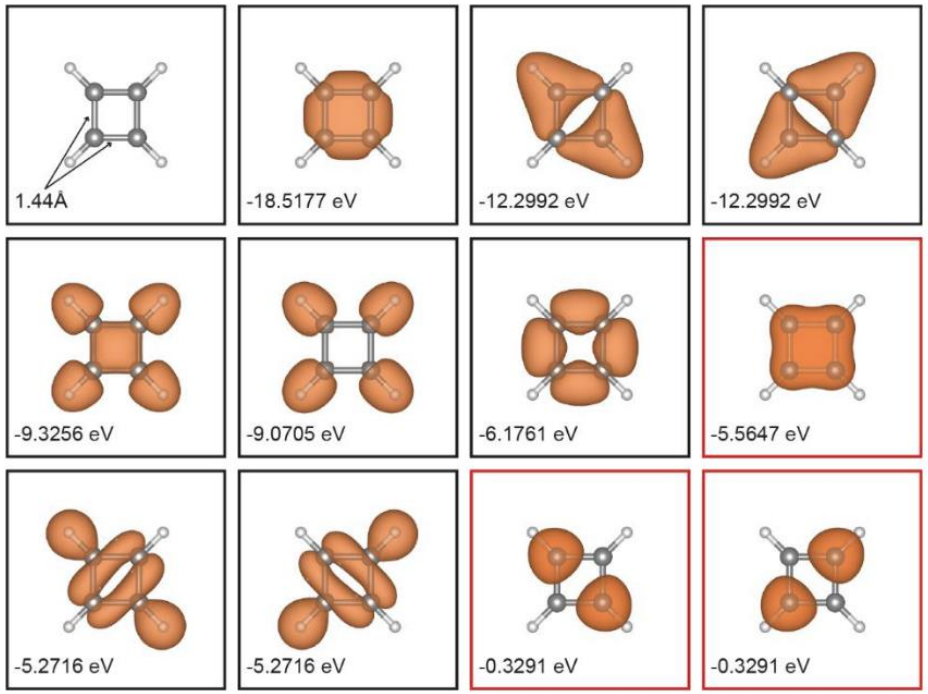
$$E_2 - E_1 \approx 60 \text{ meV}$$

At room temperature $4k_BT \approx 100$ meV
Therefore, it's not possible to resolve the two first states.
Measurements at low temperature are needed.

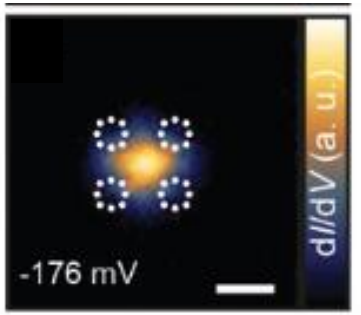
4.3 Artificial cyclobutadiene

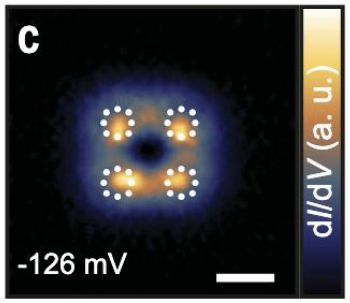
The cyclobutadiene molecule has been simulated with the help of four artificial atoms on InSb, placed at a distance $d \approx 11$ nm (lateral scale 10 nm).

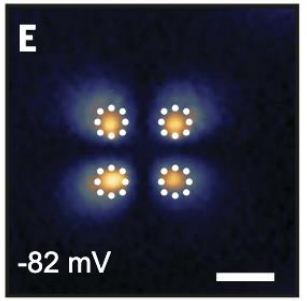


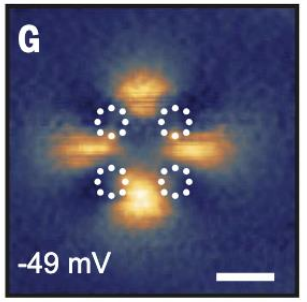


Using the calculated molecular orbitals shown on the left, identify which ones are observed in the dI/dV maps on the right.
(Energy scales are not comparable.)



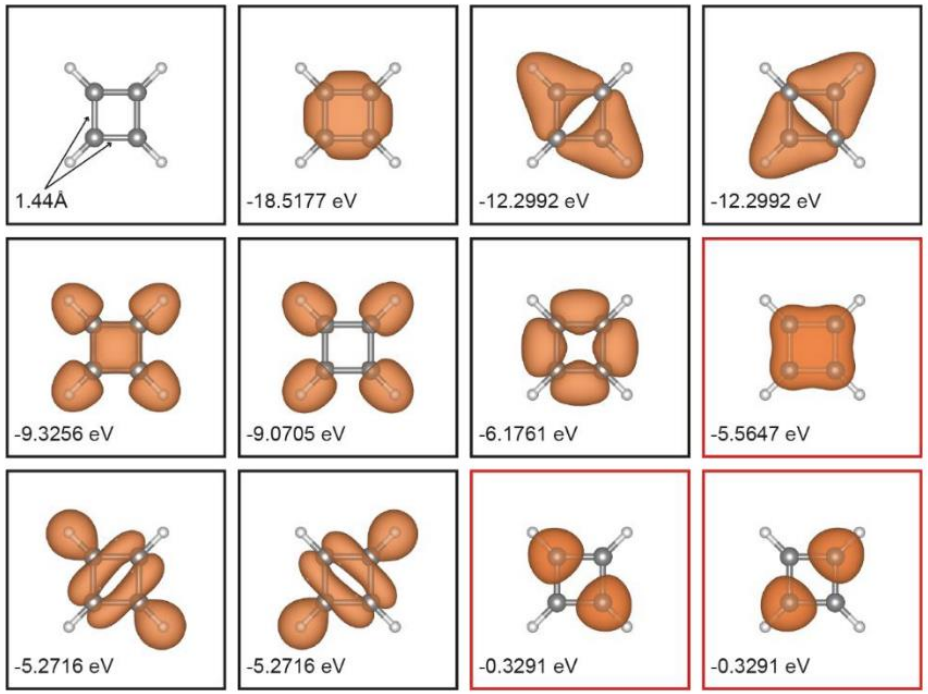




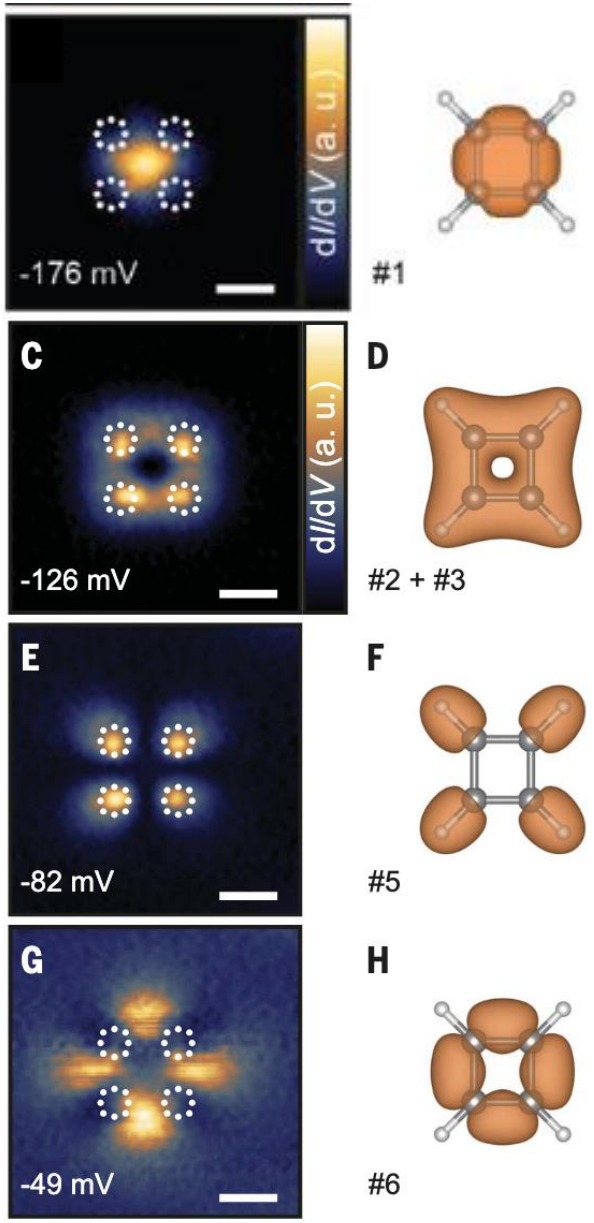


4.3 Artificial cyclobutadiene - Solution

Lowest energy state at -176 mV: LDOS centered in the square and delocalized over all four artificial atoms, in agreement with the first cyclobutadiene MO.
State at -126 mV: ring of LDOS with no intensity in the center of the square, in agreement with a superposition of the degenerate second and third MO.
State at -83 mV: LDOS located at the center of each artificial atom, but with intensity extending outward at 45 degrees with respect to the horizontal and vertical axes of the structure. This state could be identified as the fifth cyclobutadiene MO of the DFT calculation.
State at -49 mV: LDOS concentrated in between the artificial atoms, in good agreement with the sixth MO:



Some states and the higher energy states are not detected, likely because of hybridization with the 2D electron gas and/or with the bulk states



4.4 The surface state of Ag(111)

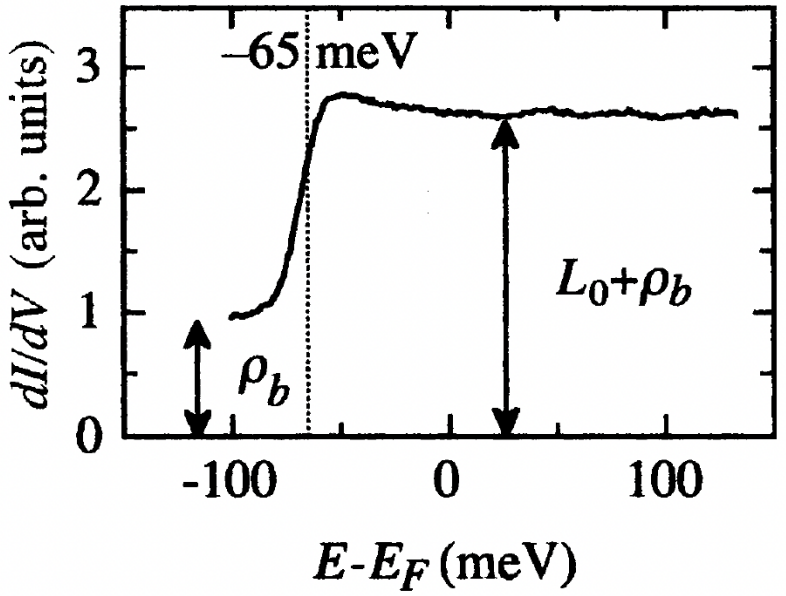
The figure shows a dI/dV spectrum acquired on a Ag(111) surface.

The step observed at $E_0 = -65$ meV corresponds to the onset of the surface state. The surface state is a 2D free-electron gas, consequently its DOS is constant, indicated here as $L_0 = m^*/\pi\hbar^2$.

Consider for simplicity that also the bulk DOS ρ_b as well as the tip DOS ρ_t are constant, and that $T = 0$.

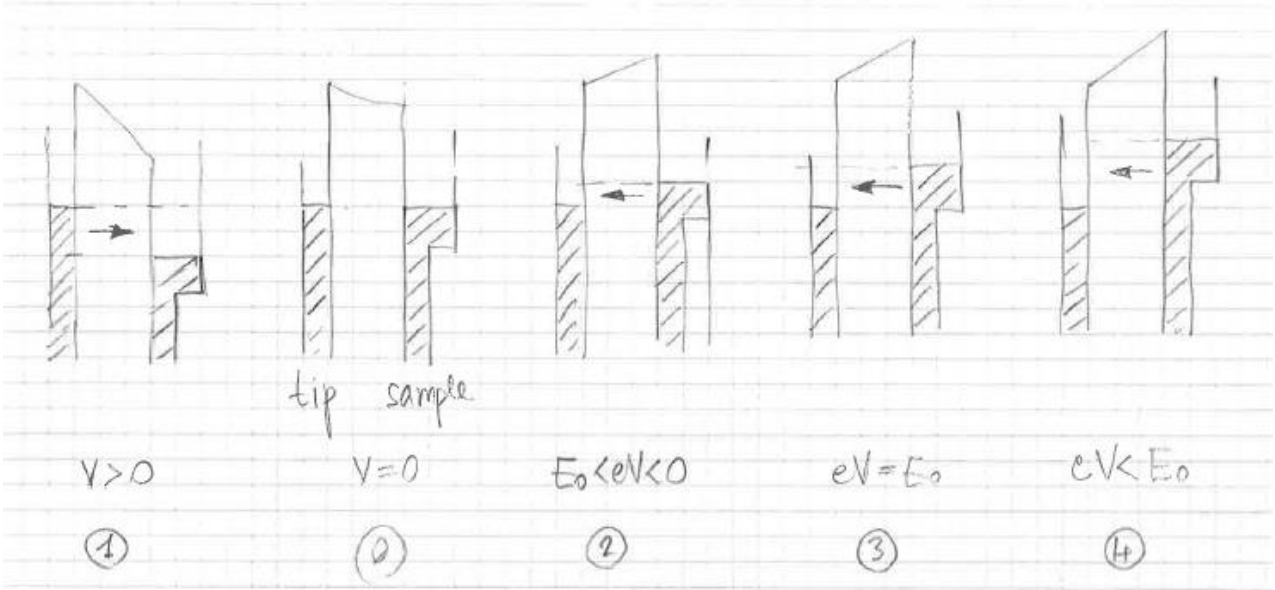
a) Sketch the energy barrier scheme at the relevant bias voltages corresponding to the different regions of the dI/dV spectrum.

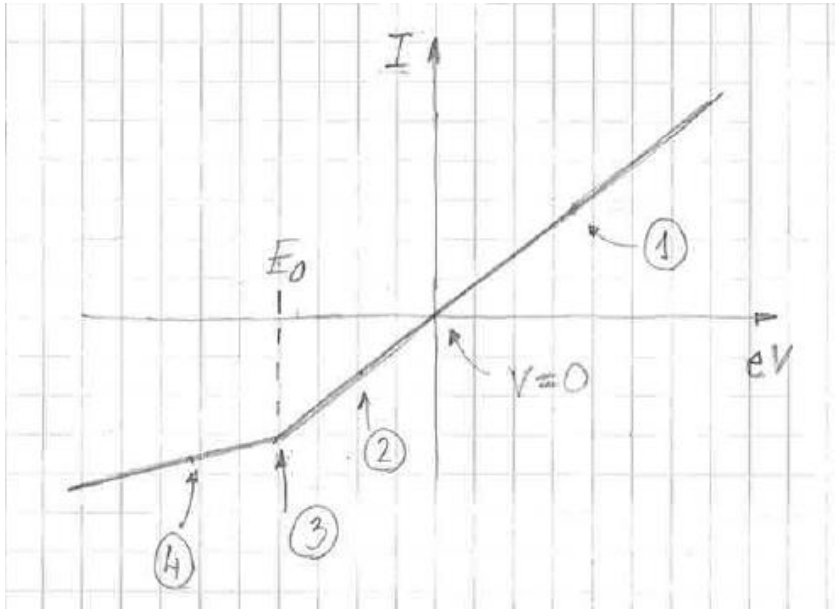
b) Sketch the corresponding current vs bias voltage (I vs V) curve.

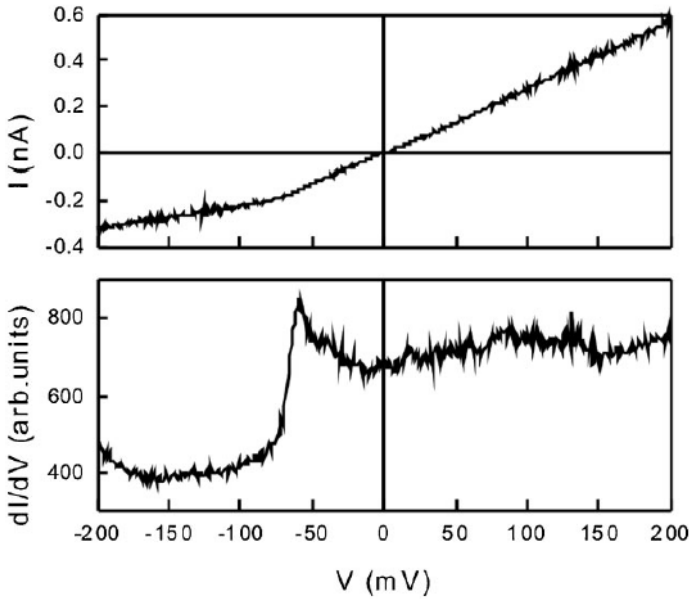


Adapted from
Appl. Phys. A **75**, 141–145 (2002)

4.4 The surface state of Ag(111) - Solution







The tunneling current is linear with the same slope for all biases where the surface state contributes to the current (1 and 2): constant dI/dV (constant LDOS) → linear I. Once the surface state onset energy E_0 is reached (3), the tunneling current continues to increase (in absolute value) but with a smaller slope (4), since the density of states contributing to the current for $eV < E_0$ is lower.

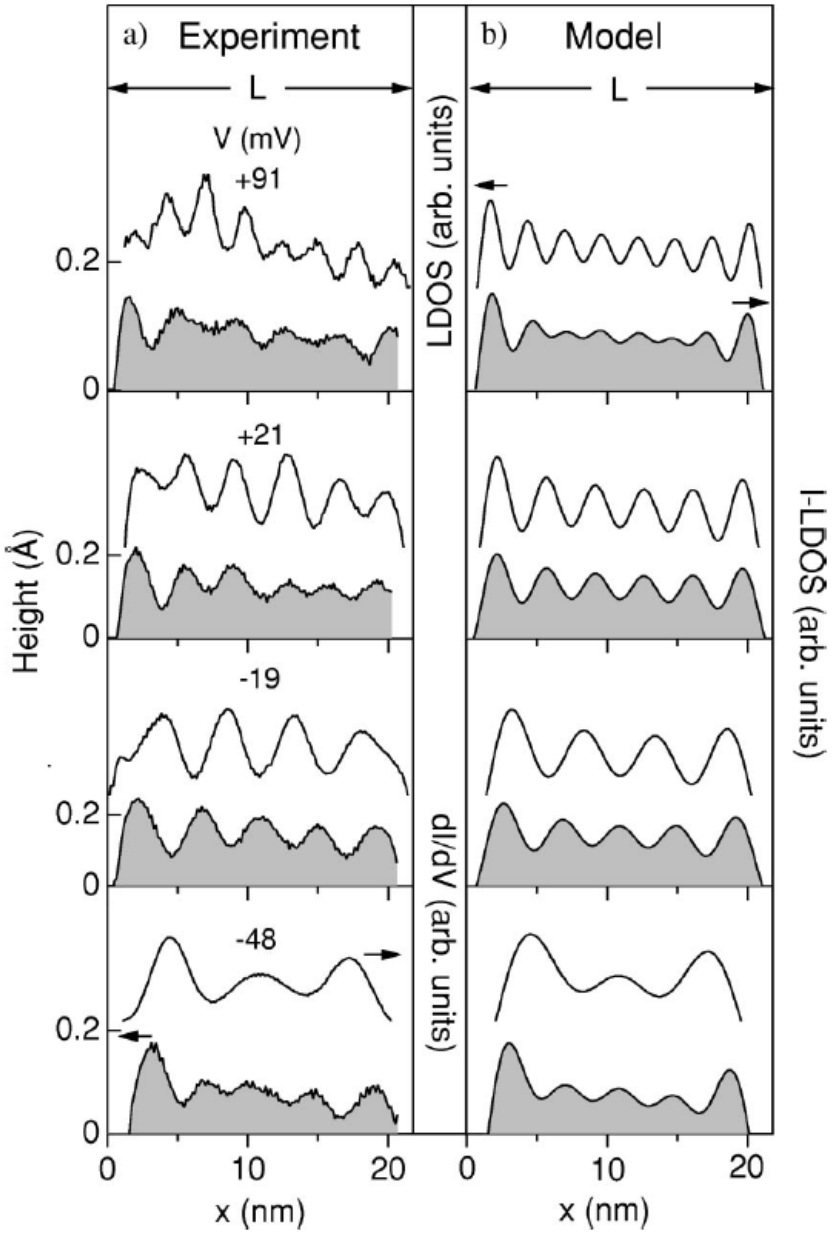
The figure on the left presents a measurement of the Ag(111) surface state taken from another reference, where both $I(V)$ and dI/dV vs V are shown.

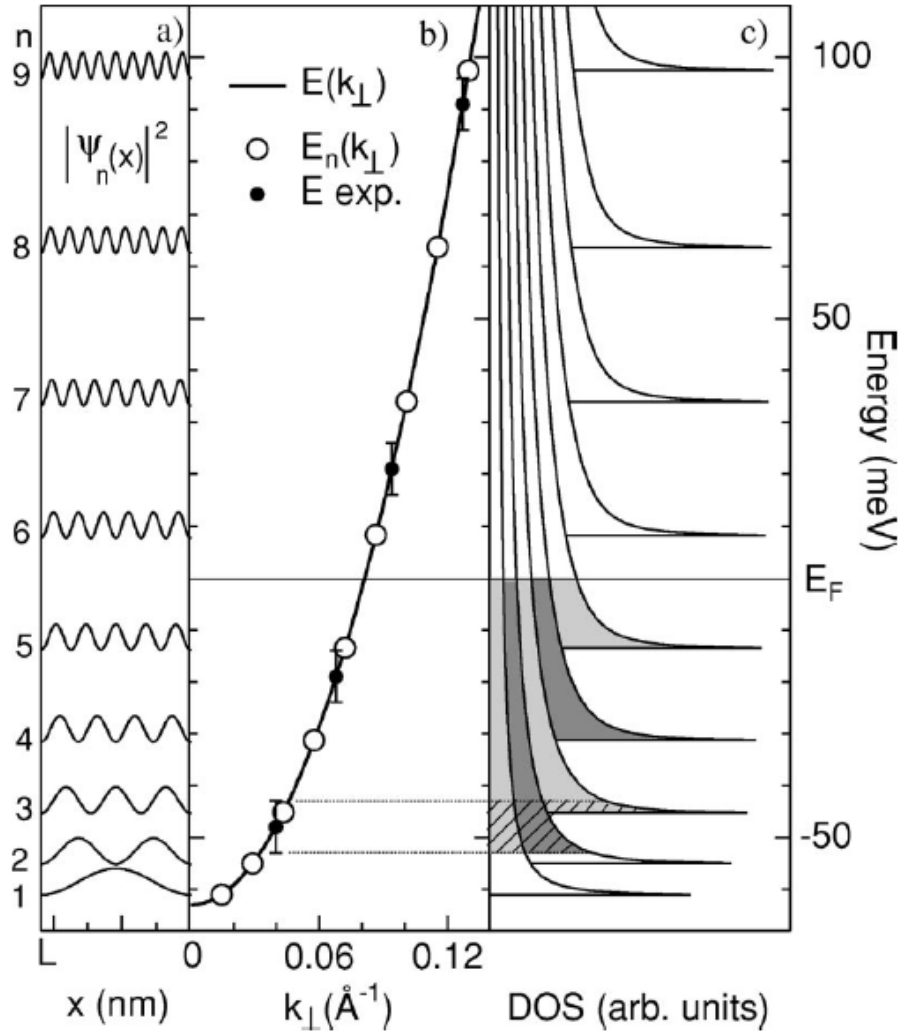
K. Morgenstern et al., Phys. Status Solidi B **250**, 1671 (2013)

4.5 Ag(111) surface state confinement in 1D

Interpret the experimental data (dI/dV maps and topography) considering the energy diagram and DOS shown in the figure further on the right .

Lock-in acquisition:
$V_{mod} = \pm 5$ mV

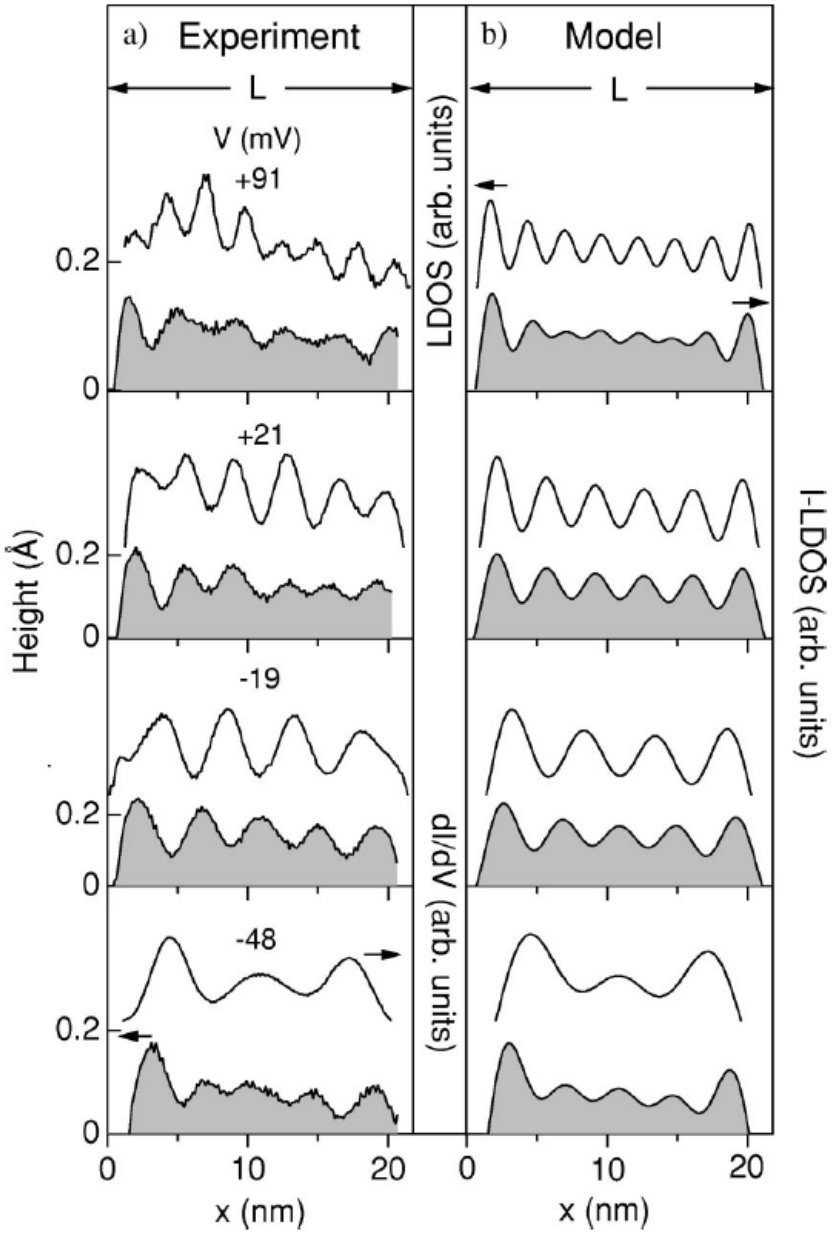


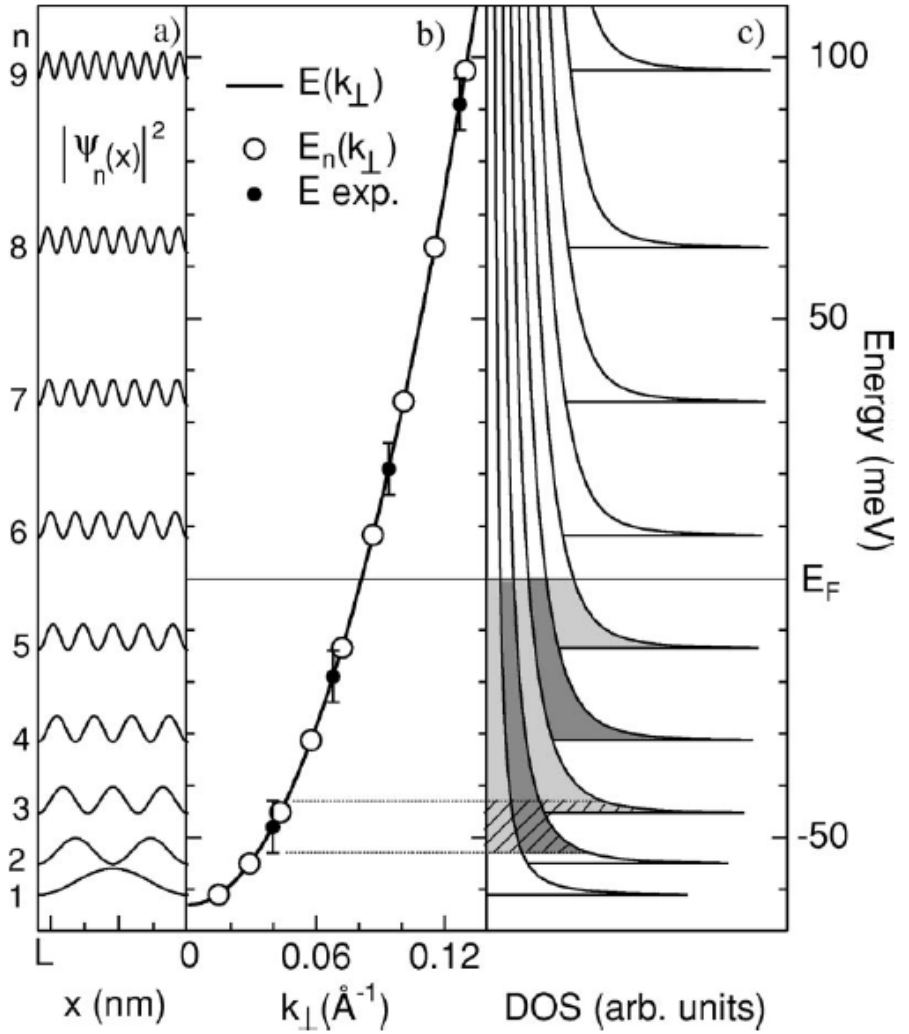


DOI: 10.1103/PhysRevB.67.193402

4.5 Ag(111) surface state confinement in 1D - Solution

The difference between dI/dV and topography is explained by considering the contribution of different states.
For example, the topography measurement at -19 mV includes contributions from
all five occupied subbands, while the n=5 one is excluded from the dI/dV measurement.
Therefore, a different number of maxima appear in the profiles. A similar reasoning applies to the measurement at -48 mV.
The measurement at +21 mV show little difference between dI/dV and topography, indicating that most of the contribution comes from a single state, n=6, in both cases.

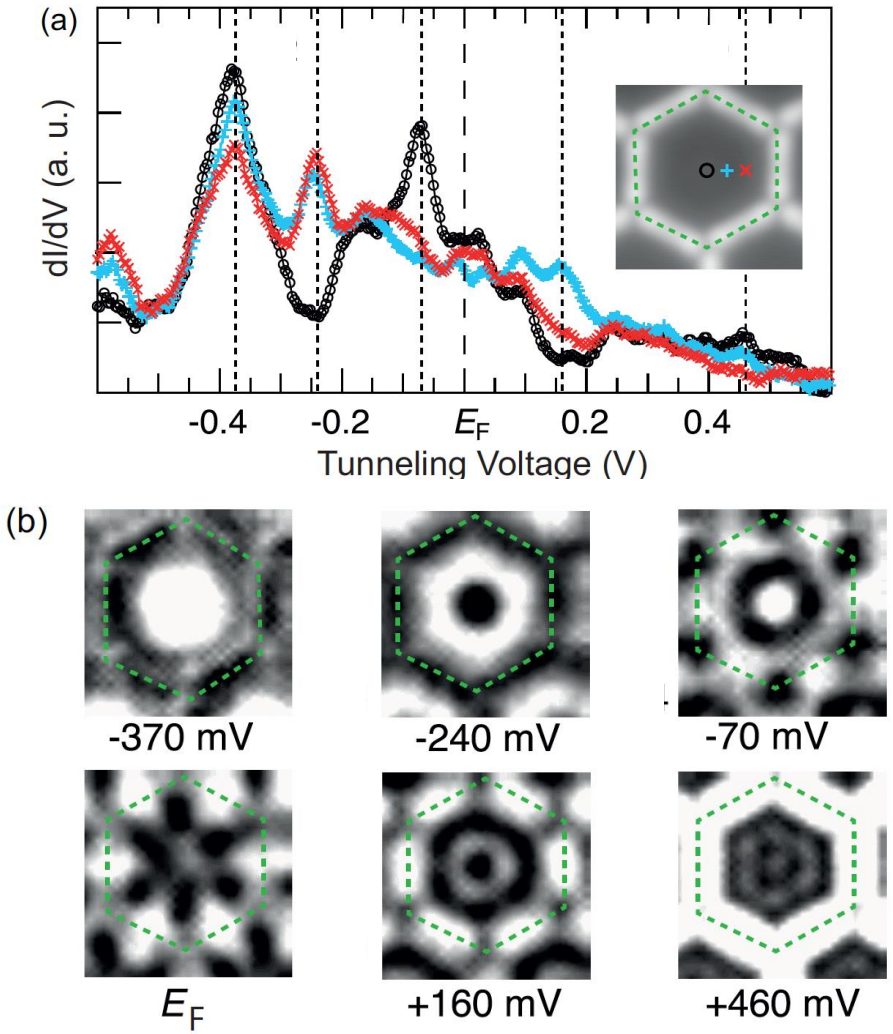


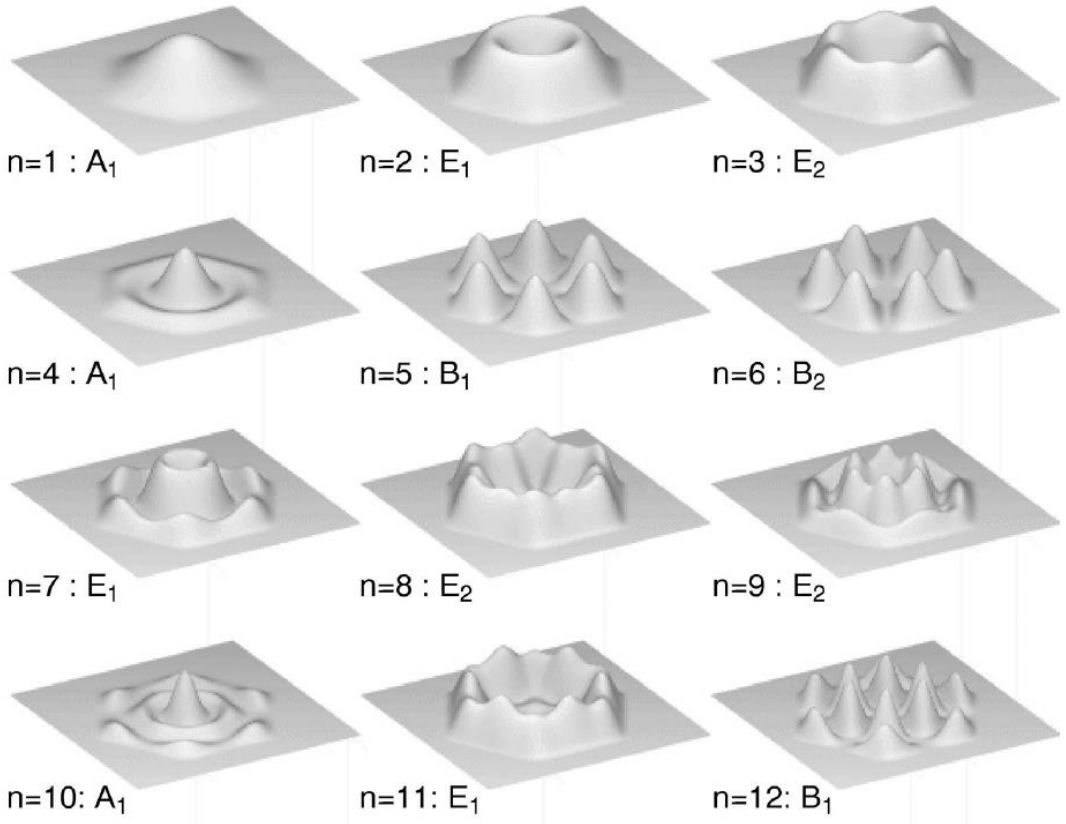


DOI: 10.1103/PhysRevB.67.193402

4.6 Ag(111) surface state confinement in 2D

The surface state can be confined by molecular structures grown at the surface. Compare the experimental data (maps) with the calculated state densities of the lowest eigenstates of a particle in a hexagonal box and identify the observed states.

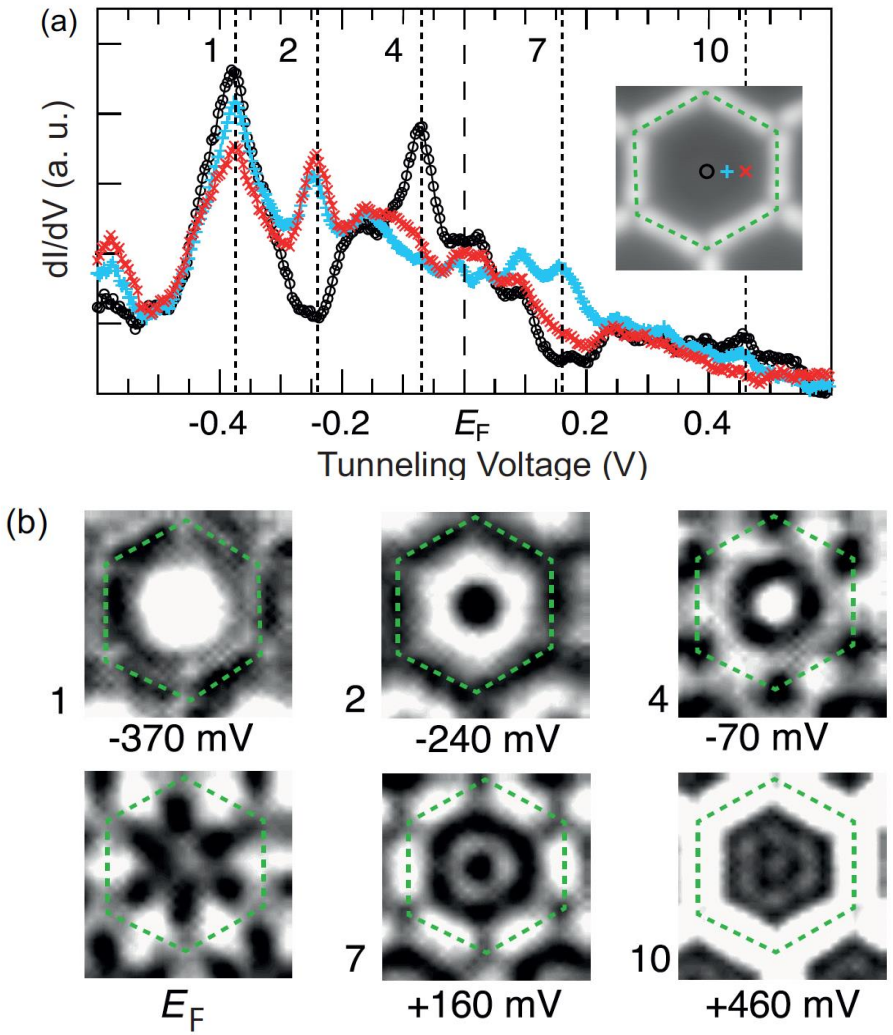


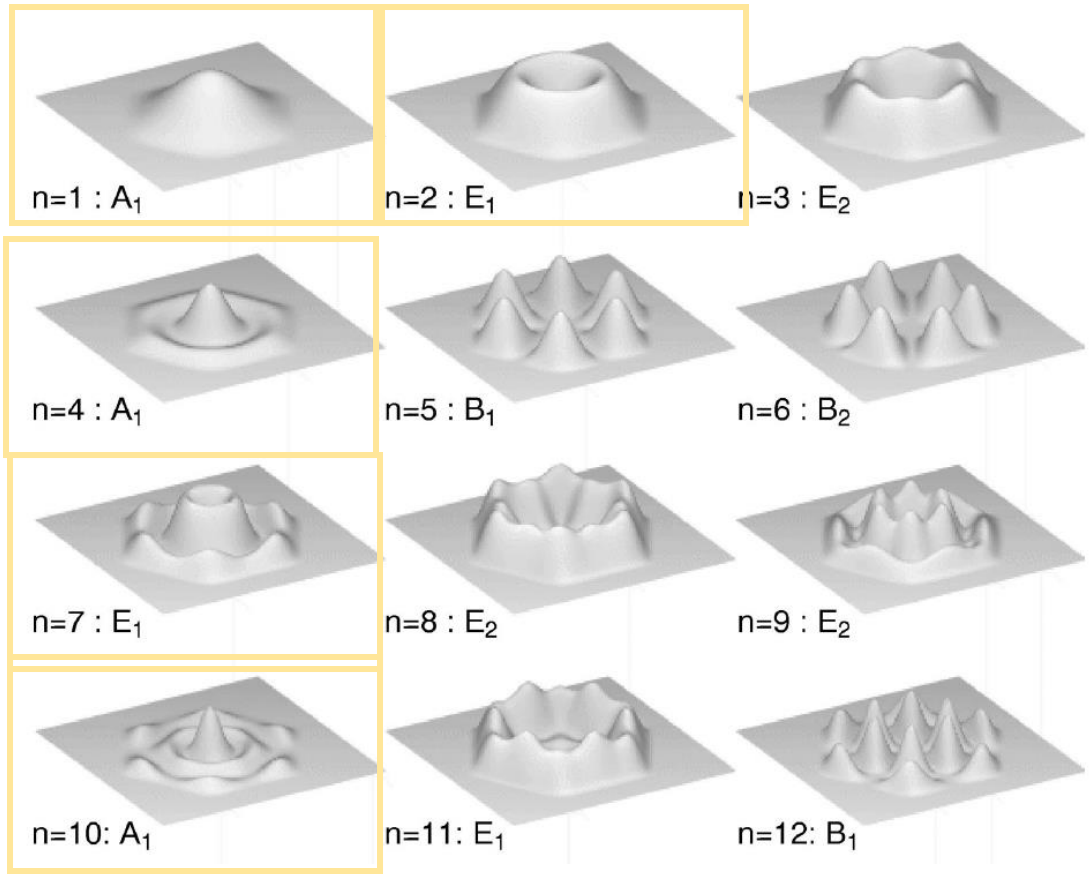


DOI: 10.1103/PhysRevLett.110.086102

DOI: 10.1016/S0039-6028(98)00890-5

4.6 Ag(111) surface state confinement in 2D - Solution





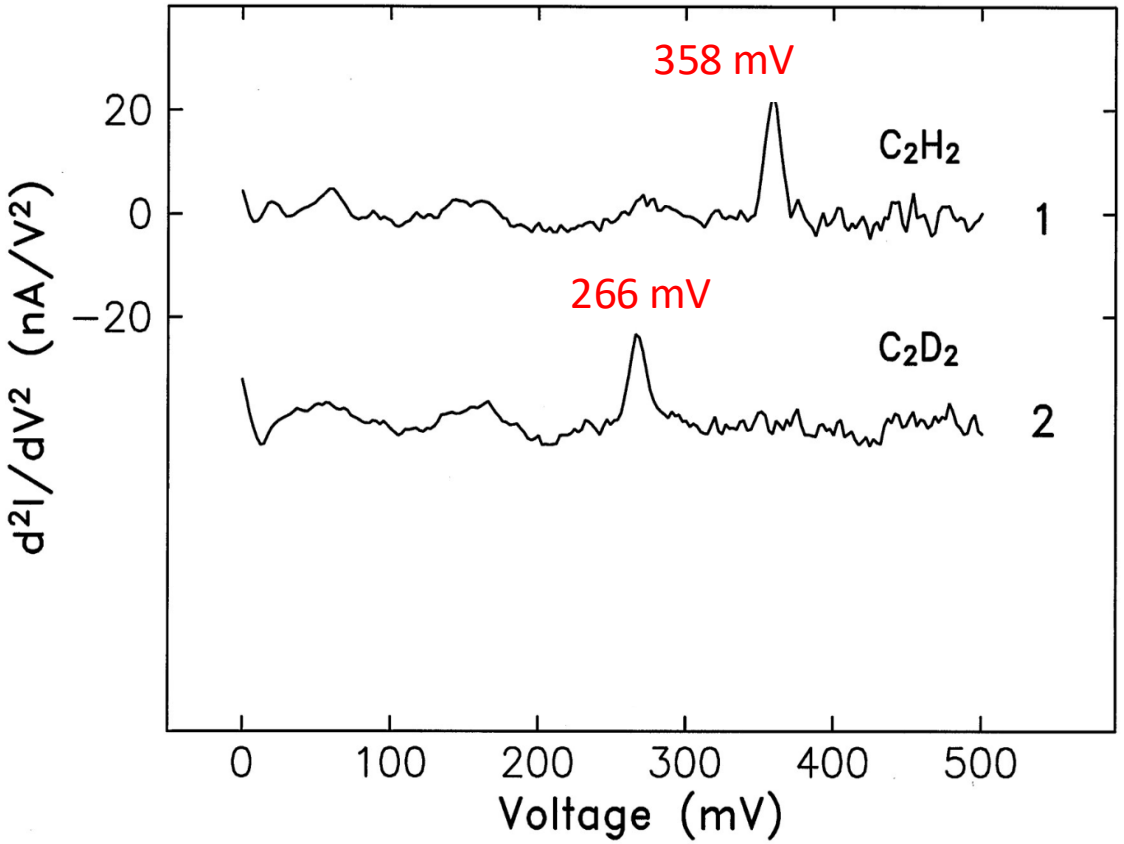
DOI: 10.1103/PhysRevLett.110.086102

DOI: 10.1016/S0039-6028(98)00890-5

4.7 IETS: Vibrational modes

Verify the scaling of the observed stretching mode when replacing hydrogen with deuterium

Hints:
- assume the same spring constant K for the C-H and the C-D bonds
- use the masses of H, D, and C in atomic units



Adapted from :
B. C. Stipe *et al.,* Science **280**, 1732 (1998)
B. C. Stipe, *et al.,* Phys. Rev. Lett **82**, 1724 (1999)

4.7 IETS: Vibrational modes - Solution

$$\hbar\omega \propto \frac{1}{\sqrt{m_{reduced}}}$$

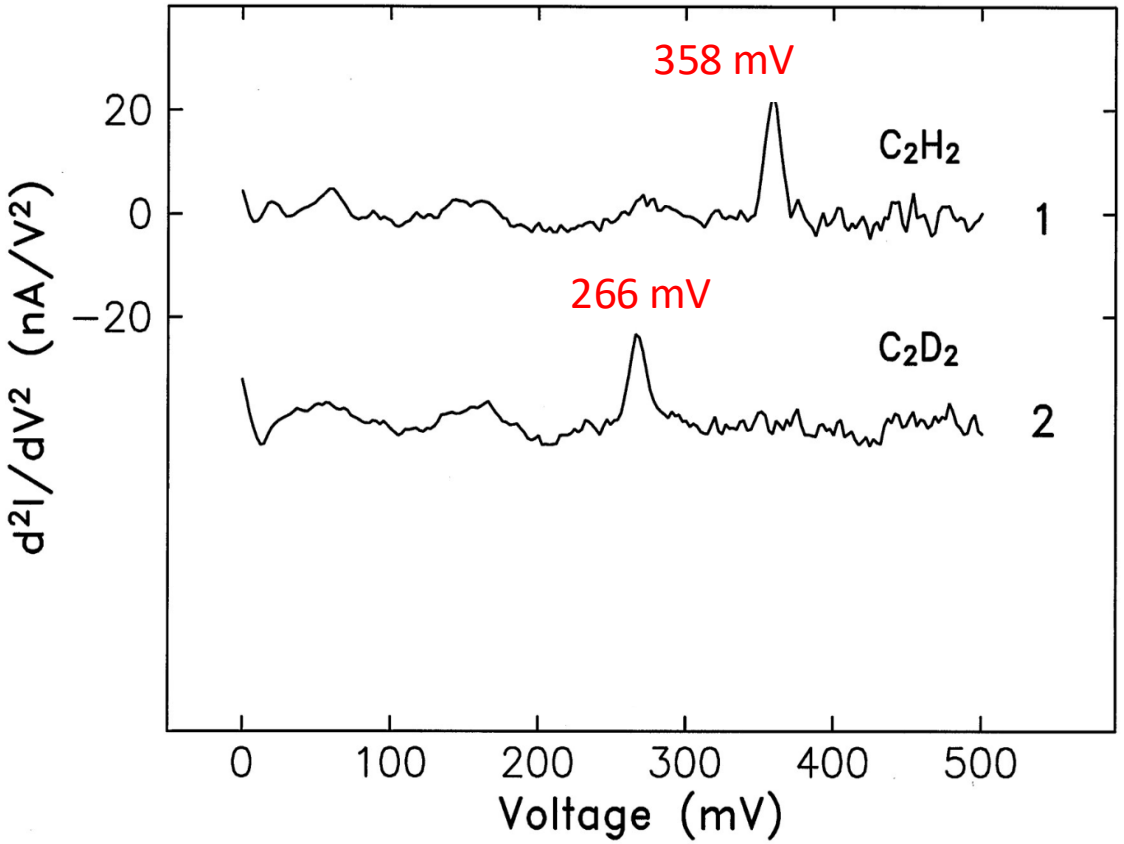
$$\frac{1}{m_{\mathrm{CH}}} = \frac{1}{12} + \frac{1}{1} = 1.08 \rightarrow \sqrt{m_{\mathrm{CH}}} \approx 0.96$$

$$\frac{1}{m_{\mathrm{CD}}} = \frac{1}{12} + \frac{1}{2} = 0.58 \rightarrow \sqrt{m_{\mathrm{CD}}} \approx 1.31$$

$$\hbar\omega_{\mathrm{CH}} = 358 \text{ meV}$$

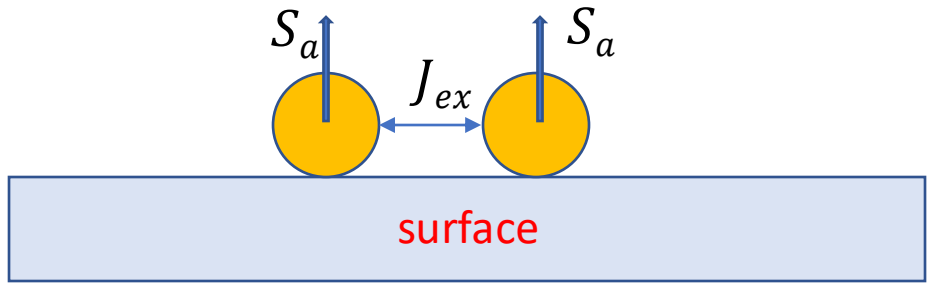
$$\hbar\omega_{\mathrm{CD}} = \hbar\omega_{\mathrm{CH}} \frac{\sqrt{m_{\mathrm{CH}}}}{\sqrt{m_{\mathrm{CD}}}} = 262 \text{ meV}$$

in good agreement with the observation



4.8 Spin excitations in exchange-coupled atoms

Consider two atoms on a surface. For simplicity we assume that each atom has a spin $S_a = 1/2$ which can point up or down. Using the standard notation $|S, M_s\rangle$, each atom can then assume the states $|1/2, 1/2\rangle$ or $|1/2, -1/2\rangle$.

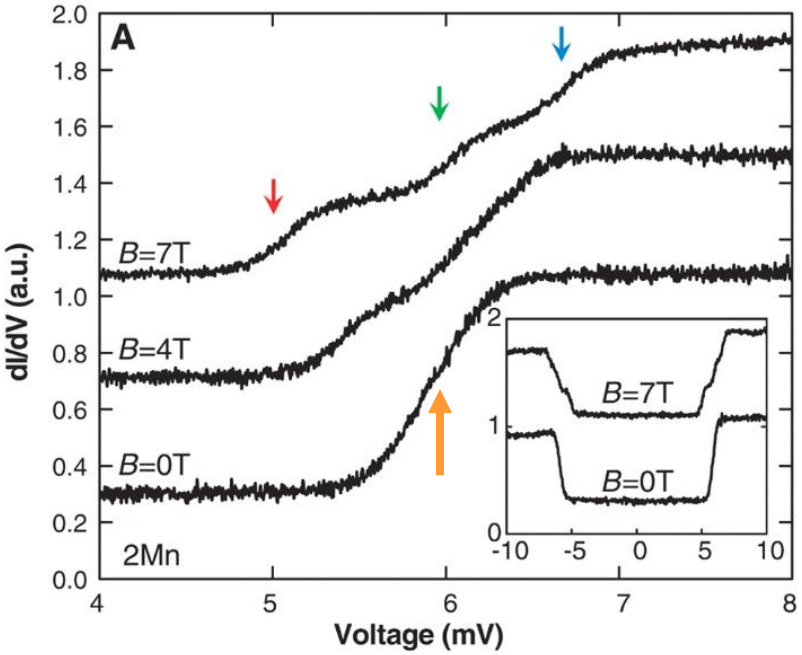


With an STM tip we manipulate the two atoms to form a dimer.
An exchange coupling couples the two spins: the dimer is then described by an Hamiltonian of the form $\mathcal{H} = -2Jex\, \boldsymbol{S_a} \cdot \boldsymbol{S_a}$, where J_{ex} is the exchange constant.

1) What is the total spin S_d of the dimer? Assuming J_{ex} negative (antiferromagnetic coupling) and $B = 0$, describe the ground and excited states of the dimer and their energy separation.

2) We go with the STM tip on top of the dimer, and we perform an IETS experiment. The result is shown in the figure on the right.
Why at $B = 0$ only one excitation (orange arrow) is observed while in field three excitations (red, green, and blue arrows) are observed?
Use the experimental data to estimate the exchange constant J_{ex}.

IETS spectra at different magnetic field B on a Mn dimer



Adapted from : C. F. Hirjibehedin et al., Science 312, 1021 (2006) https://doi.org/10.1126/science.1125398,

4.8 Spin excitations in exchange-coupled atoms - Solution

1) The atom spins in the dimer can be:
parallel to give a dimer spin $S_d = 1$ corresponding to the triplet $|1,-1\rangle$, $|1,0\rangle$, $|1,+1\rangle$ (ferromagnetic coupling) or
antiparallel to give a dimer spin $S_d = 0$ corresponding to the singlet $|0,0\rangle$ (antiferromagnetic coupling).

At $B = 0$ the ground state is given by the singlet $|0,0\rangle$ and the excited state by the three states of the triplet ($|1,M_s\rangle$)which are degenerate in energy. The energy separation between the singlet and the triplet is equal to $2Jex$.

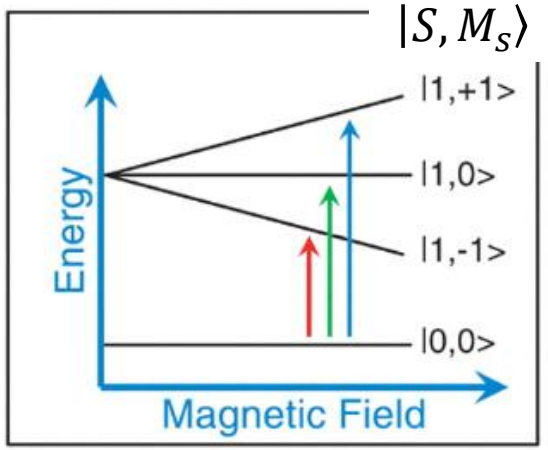
The spin s of the tunneling electron, while scattering with the spin of the dimer, undergoes a change of $\Delta m_s = 0, \pm 1$. To conserve the total momentum, all the transitions in the sketch are possible for the dimer spin: red ($\Delta M_s = -1$), green ($\Delta M_s = 0$) and blue ($\Delta M_s = +1$).

2) At $B = 0$ the three states of the triplet are degenerate in energy and then only the transition corresponding to the orange arrow is observed.

In an external magnetic field, the Zeeman energy splits the three states of the triplet.

The exchange constant can be estimated by the position of the step in the IETS spectrum acquired at $B = 0$, which is roughly 6 meV.
This corresponds to $J_{ex} = 3$ meV

expected



measured