

# Atomic-sized Conductors: Chains of Atoms and Hydrogen Molecules

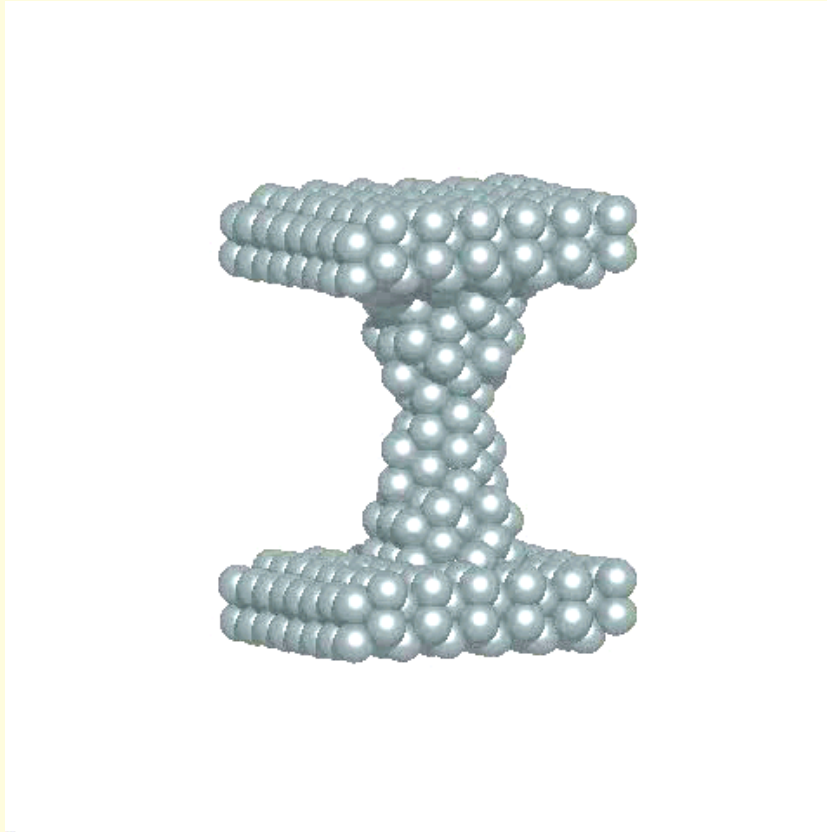
*Jan van Ruitenbeek*

*Kamerlingh Onnes Laboratorium*



# What will be discussed

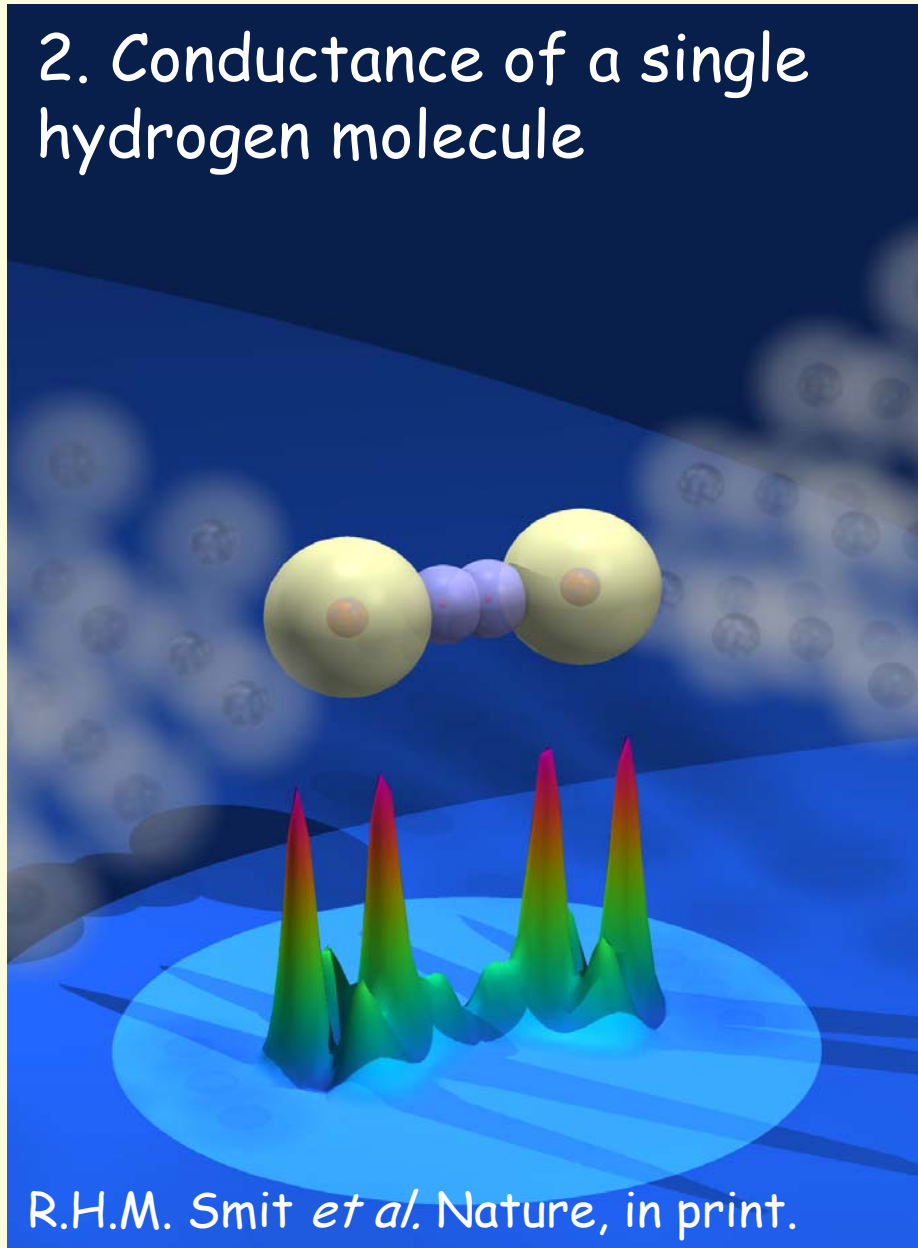
## 1. Chains of metal atoms



MD simulation Au, 12 K. Sørensen  
*et al.*, PRB **57**, 3283 (1998)

# What will be discussed

## 2. Conductance of a single hydrogen molecule



# In collaboration with ...

**Leiden:** Helko van den Brom, Martijn Krans, Bas Ludoph, Chris Muller, Yves Noat, Niko van der Post, Roel Smit, Carlos Untiedt, Alex Yanson.

Marc van Hemert

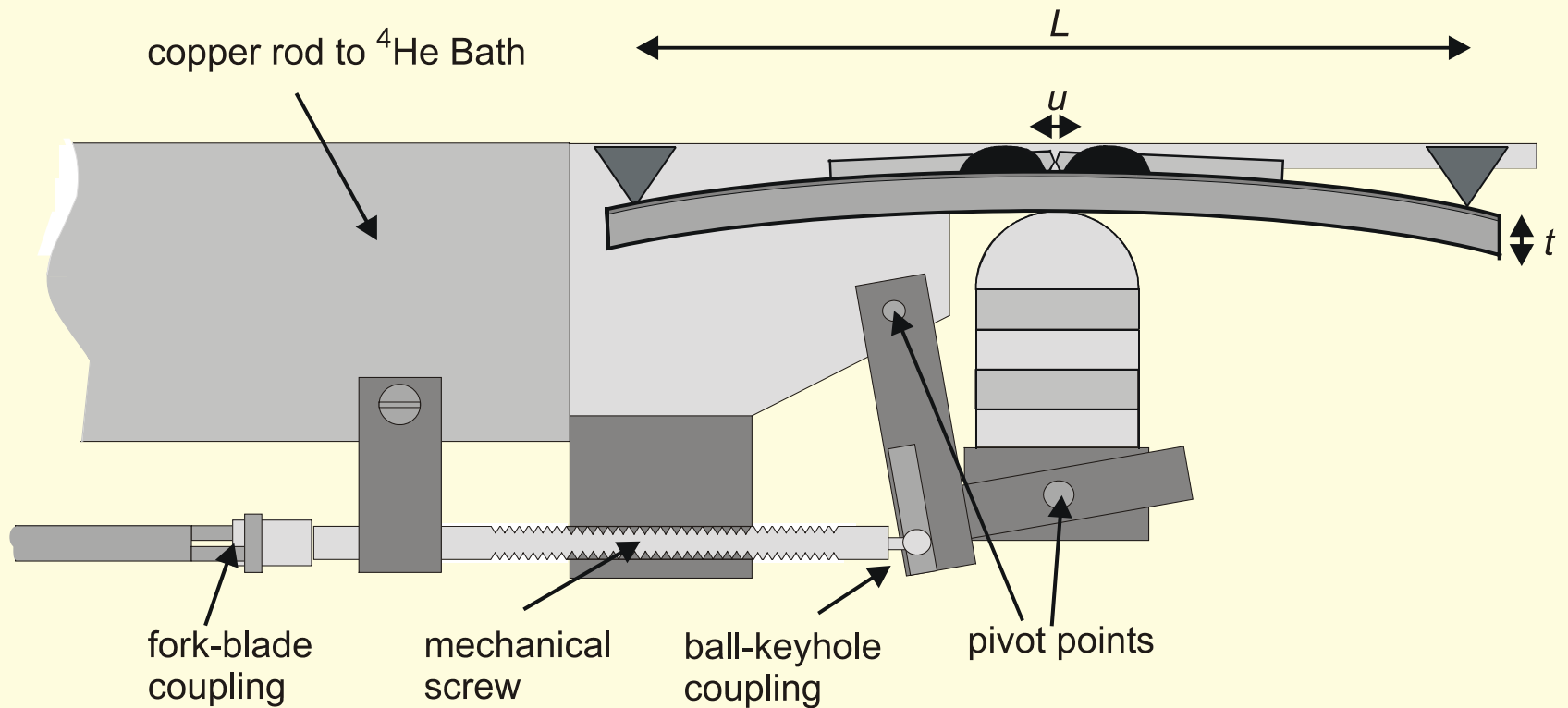
**IBM Yorktown Heights:** Norton Lang

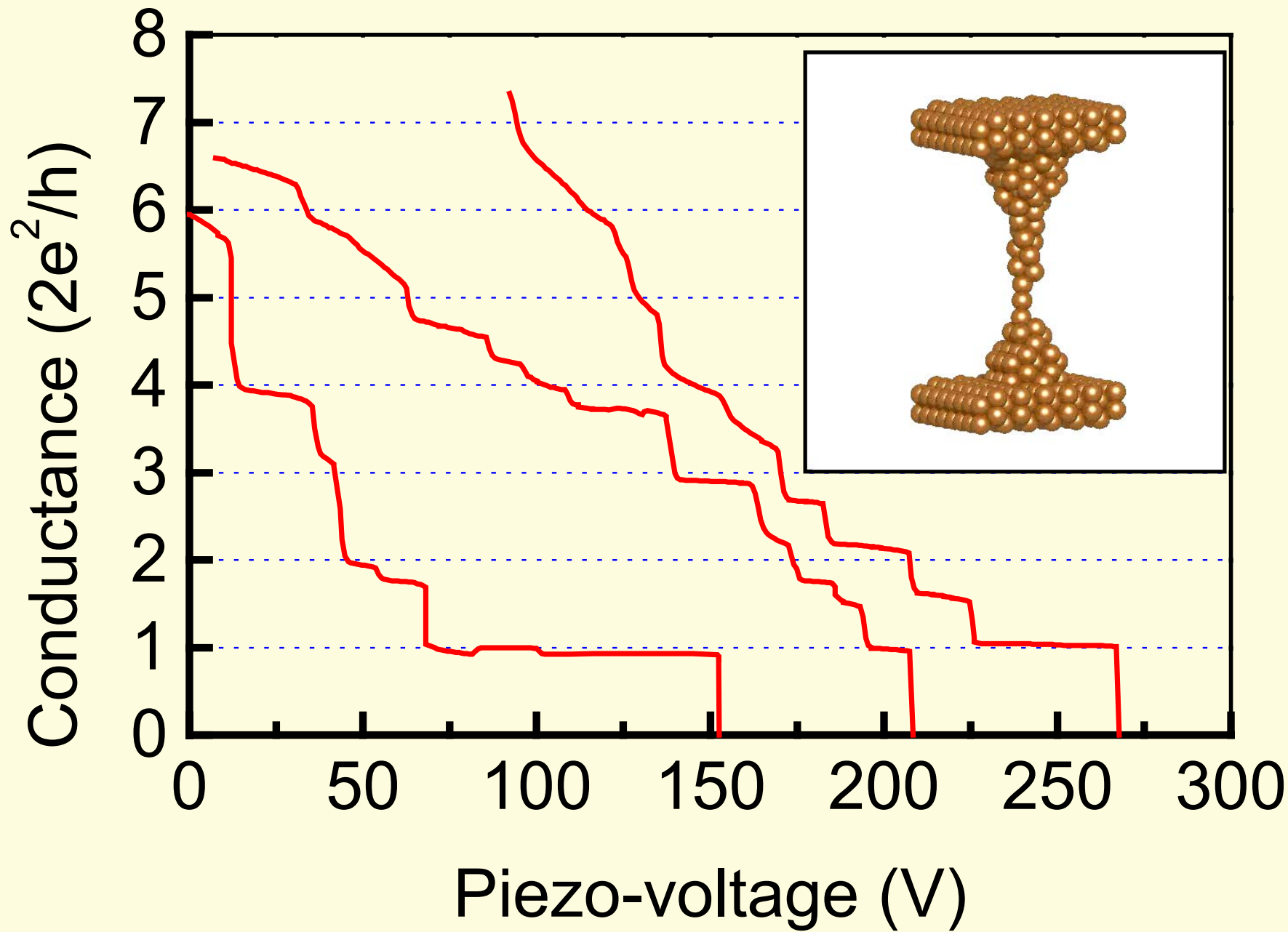
**Madrid:** Nicolas Agraït, Gabino Rubio, Juan-Carlos Cuevas, Alfredo Levy Yeyati, Alvaro Martin-Rodero

**Saclay:** Michel Devoret, Daniel Esteve, Cristian Urbina

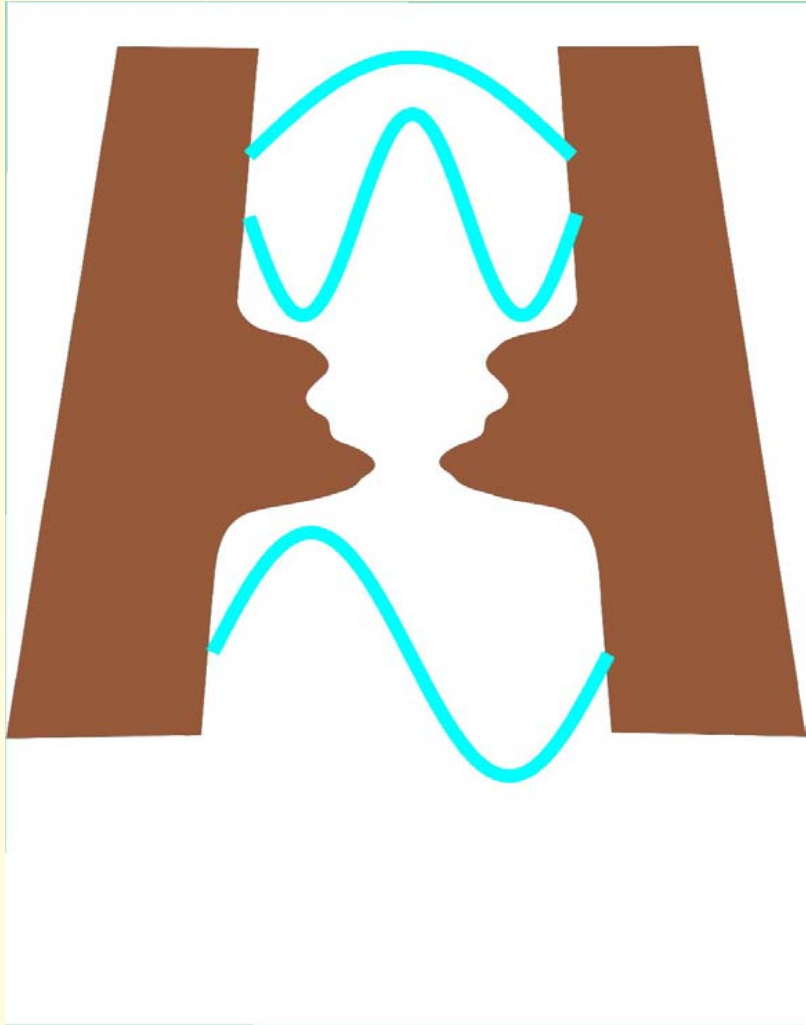
**Konstanz:** Elke Scheer

# Mechanically Controllable Break Junction





# Quantum conductance (2 dimensions)



Incoming and reflected  
modes

Scattering at the contact

Transmitted modes

# Conductance is transmission

Vector of incoming waves from the left, on a basis of quantum modes:

$$\vec{i}_l$$

Vector of outgoing waves to the right, on a basis of quantum modes:

$$\vec{o}_r$$

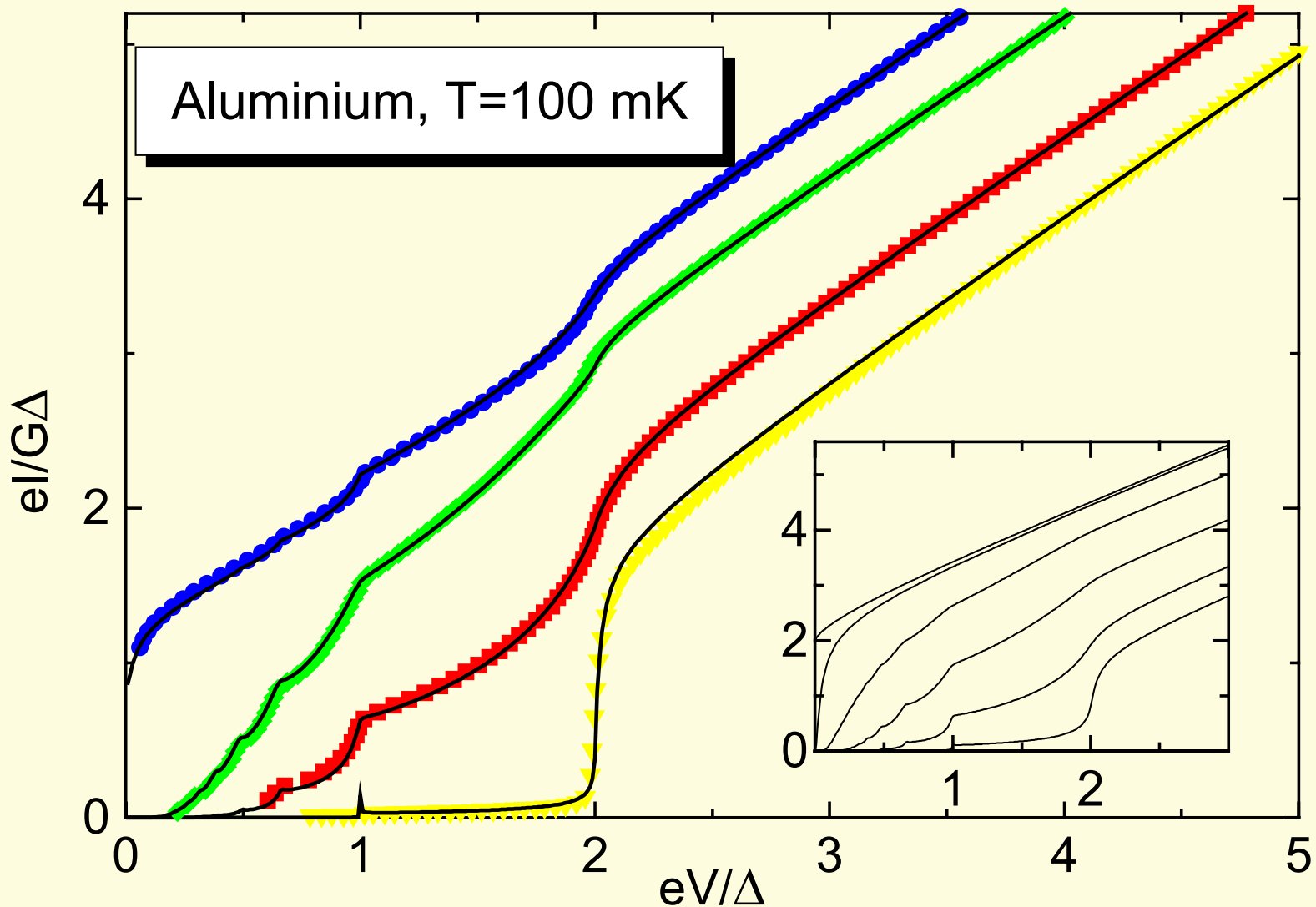
Matrix of transmission amplitudes:  $\vec{o}_r = \hat{t} \vec{i}_l$

Landauer:

$$G = \frac{2e^2}{h} \text{Tr}(\hat{t}^\dagger \hat{t}) = \frac{2e^2}{h} \sum_n T_n$$

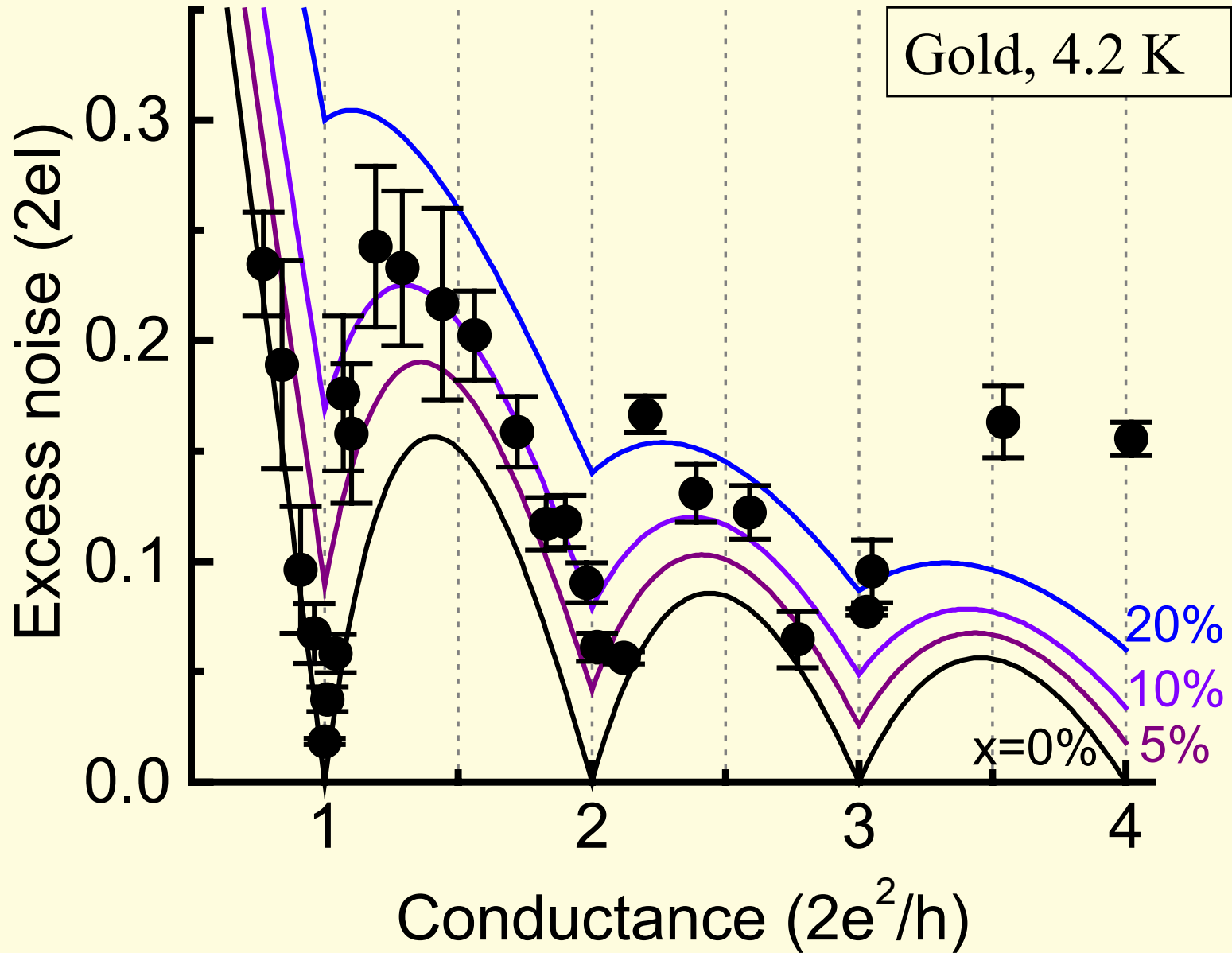


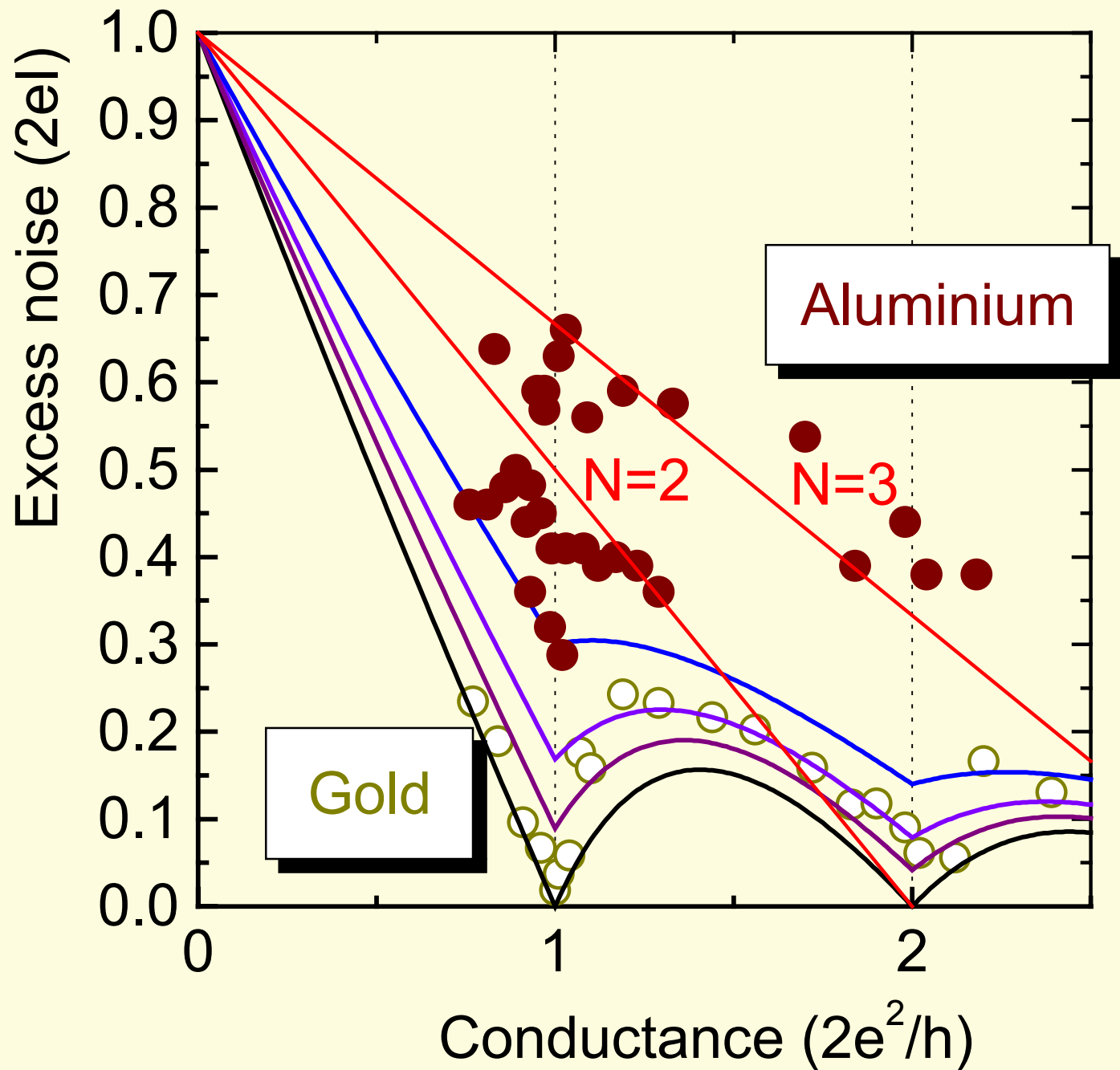
# Superconducting subgap structure



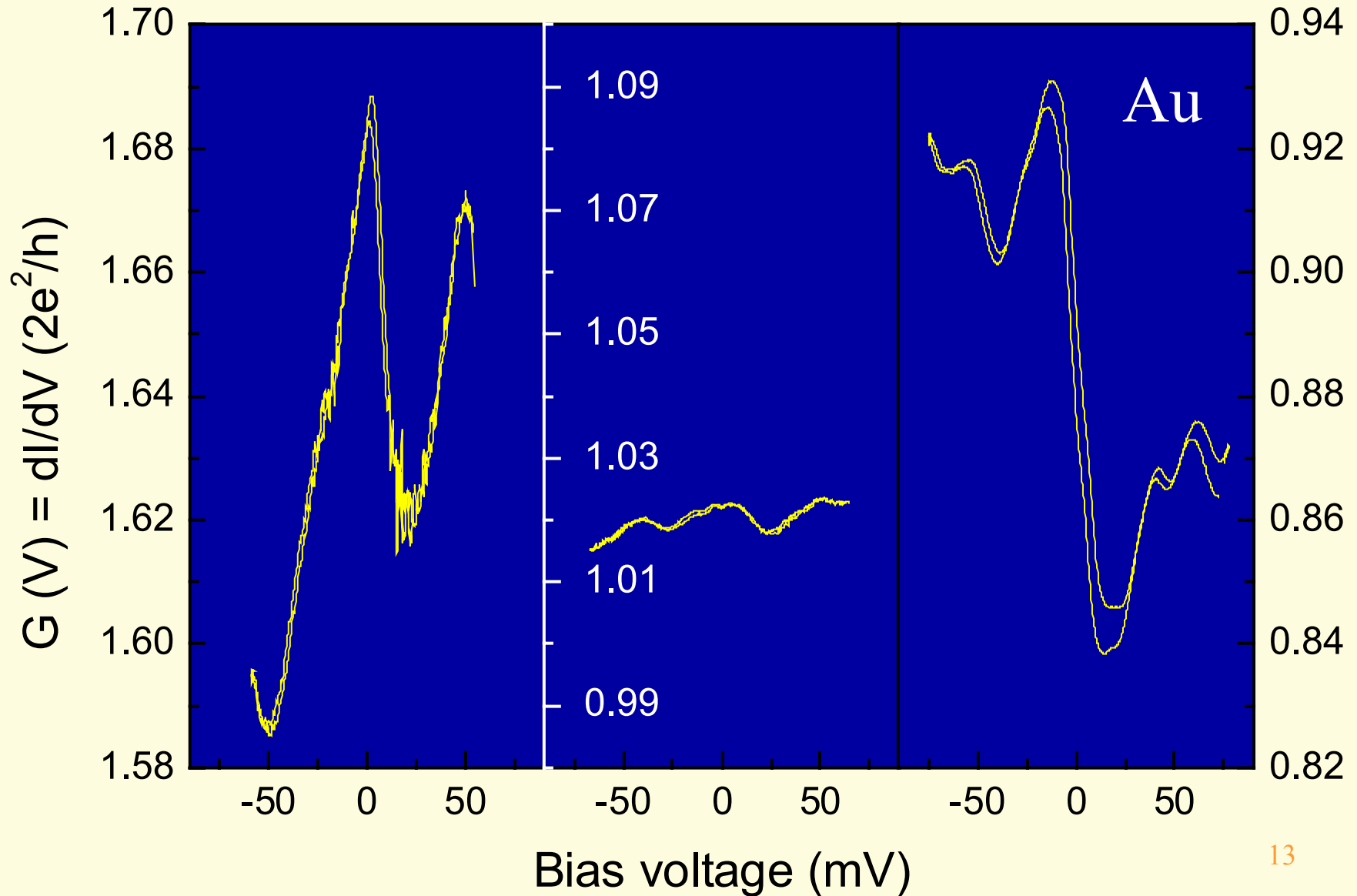
# Fitting procedure: demonstration

# Shot noise

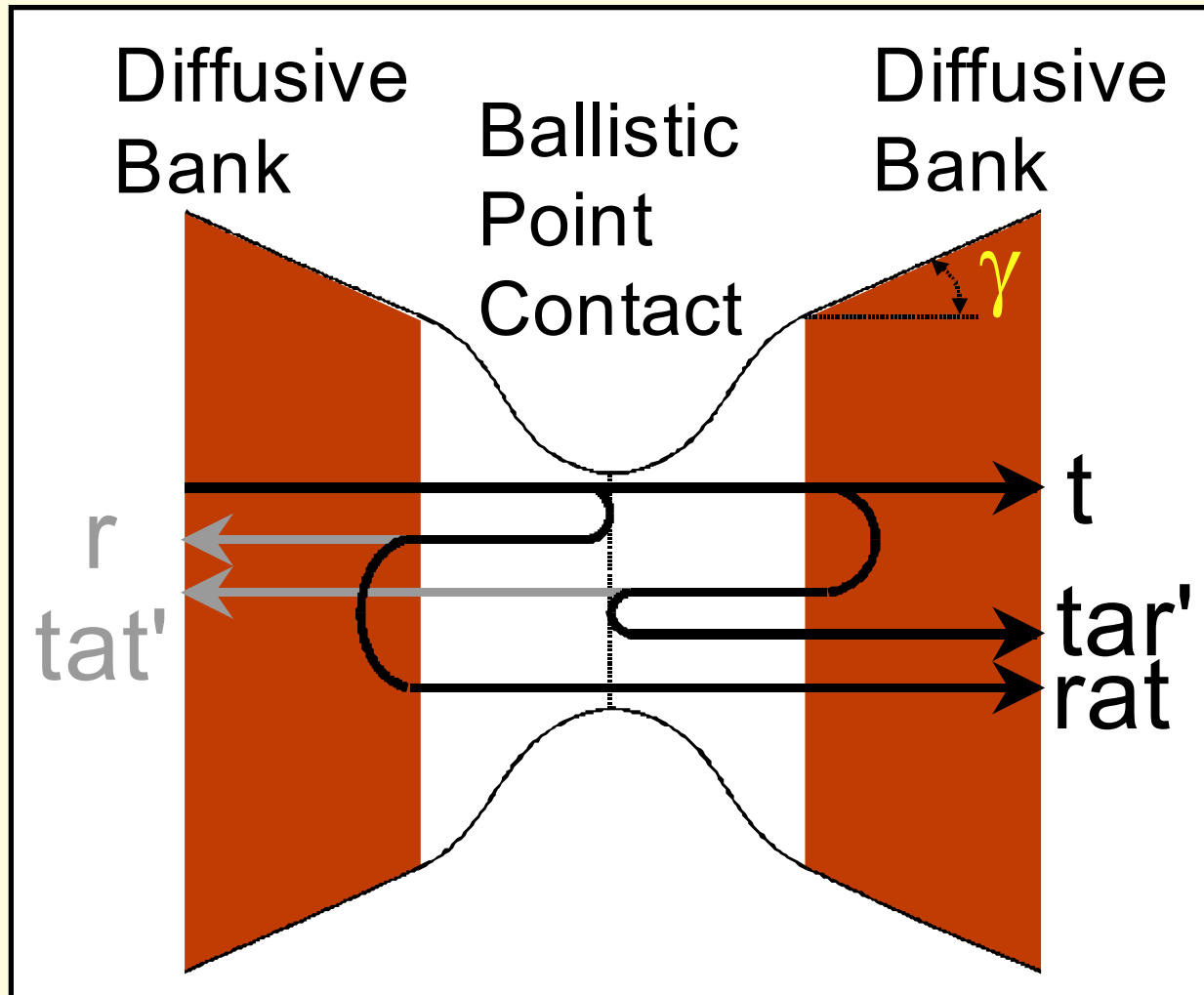




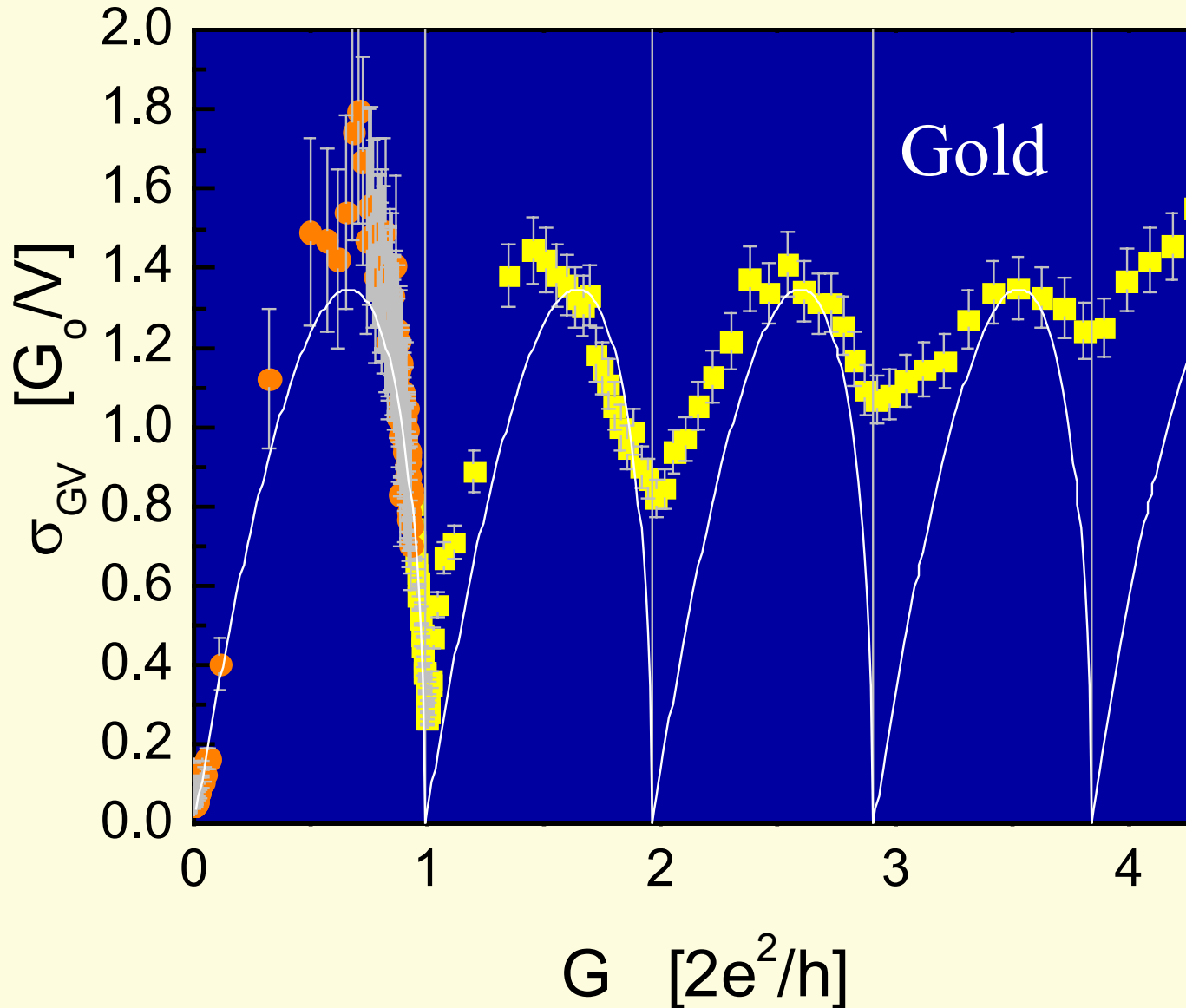
# Conductance fluctuations: 3 examples



# Principle of conductance fluctuations in ballistic contacts



# RMS fluctuations measured for Au



# The modes determined by valence orbitals

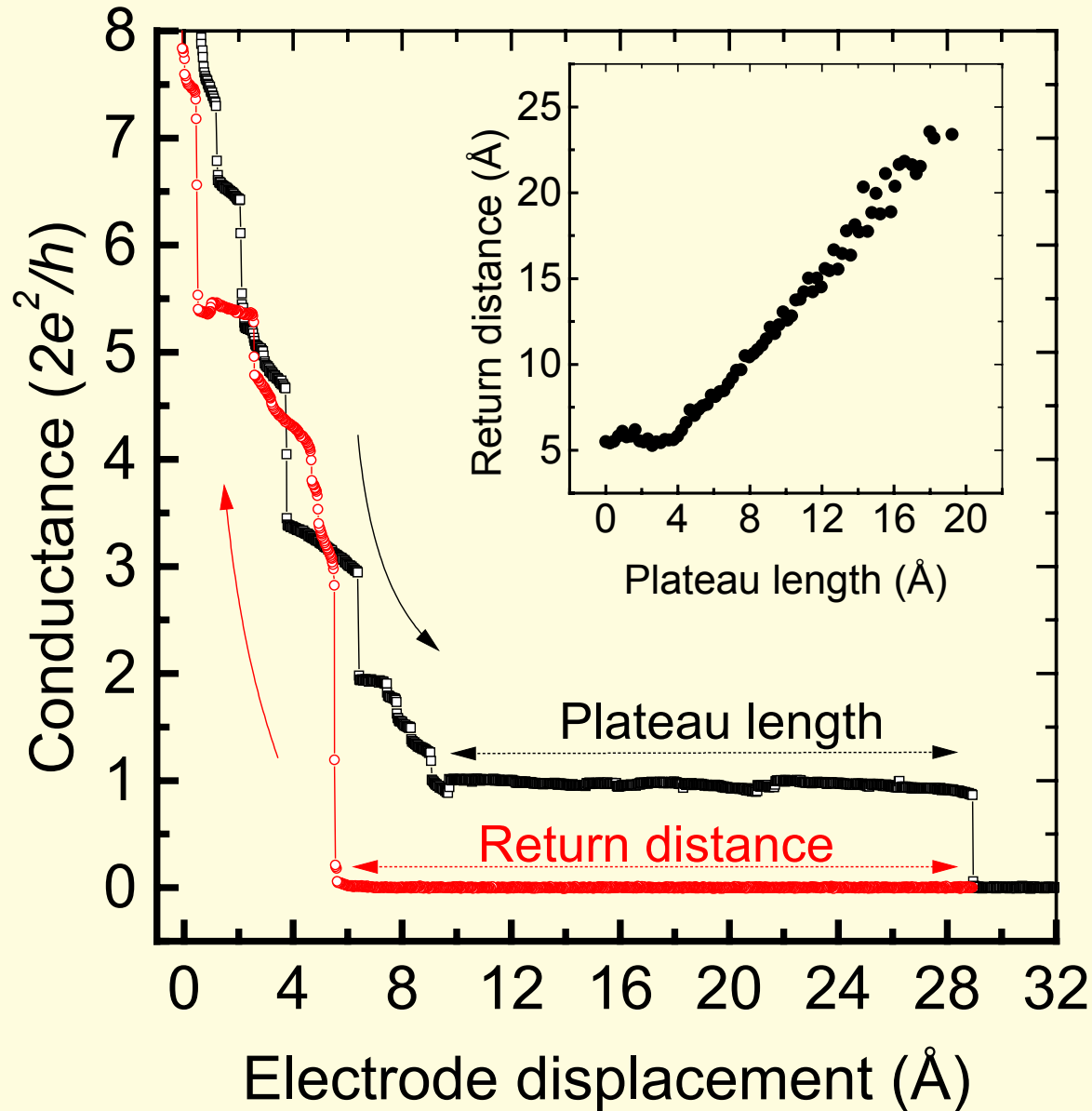
<i>Element</i>	<i>Type of atom</i>	<i>Number of modes</i>	<i>Conductance for one atom</i>
<b>Au</b>	<i>s</i>	1	1 $G_0$
<b>Al</b>	<i>s-p</i>	3	~0.8-1.2 G
<b>Pb</b>	<i>s-p</i>	3	~2.5-3 G
<b>Nb</b>	<i>s-d</i>	5	~2.5-3 G

Cuevas *et al.*, PRL **80** (1998) 1066

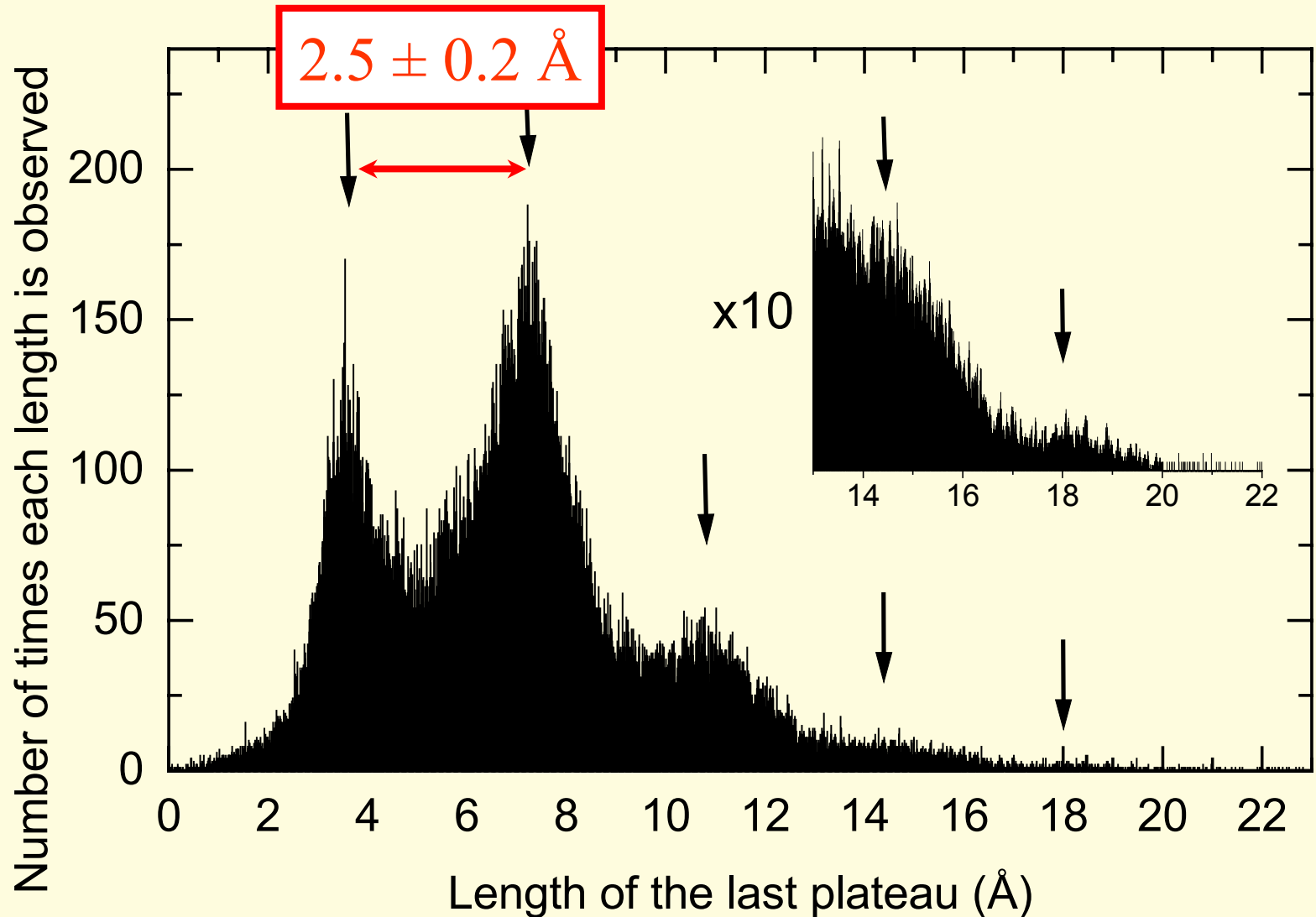


# Chains of single atoms

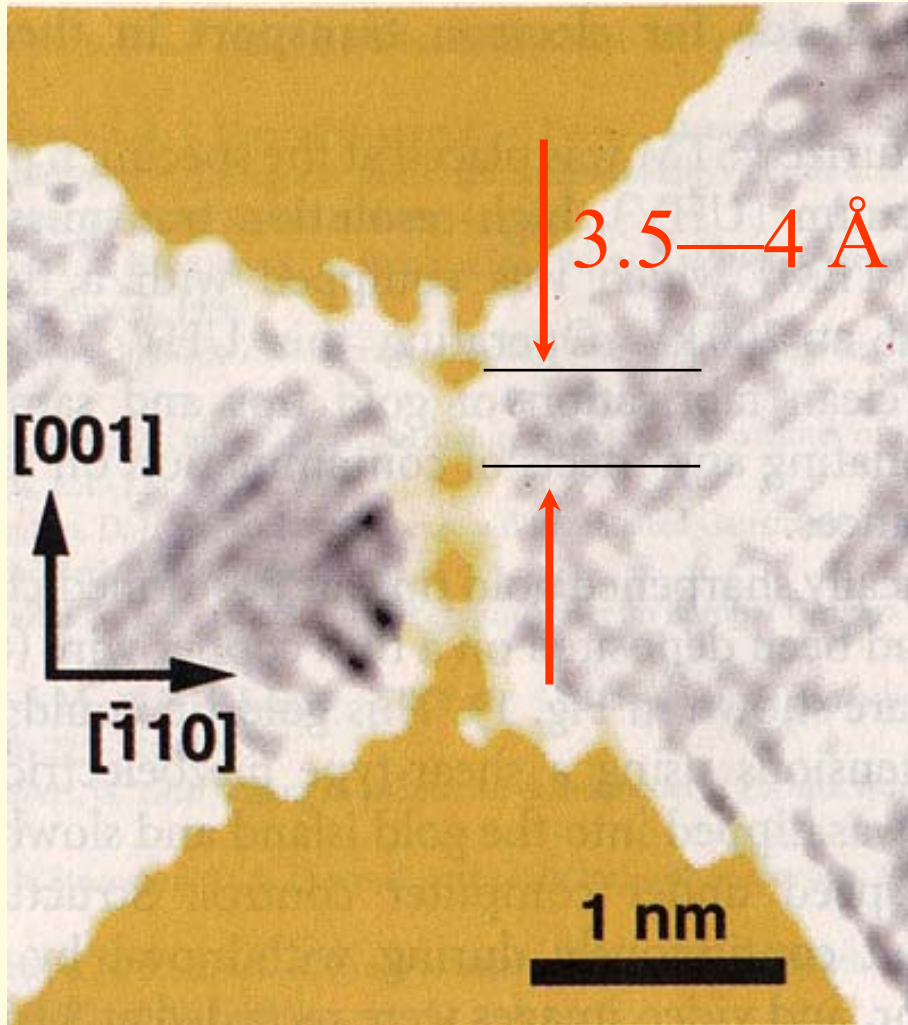
# Conductance curves for gold contacts at 4.2 K



# Histogram of lengths of last plateau, Au 4.2 K

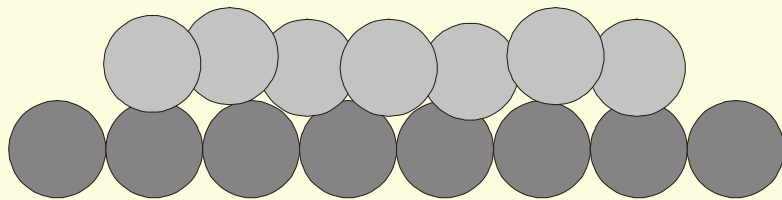
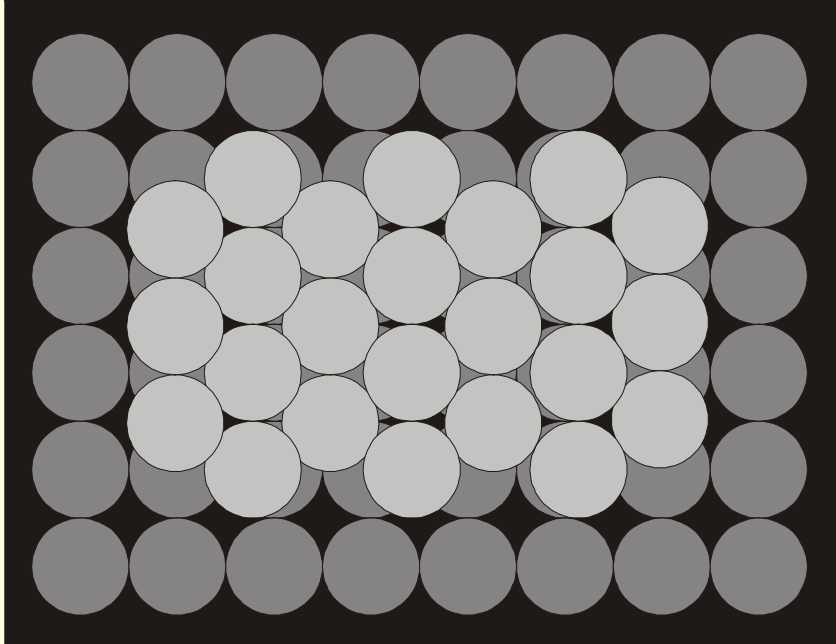


# Combined TEM and STM

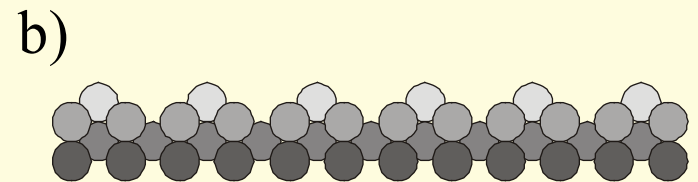
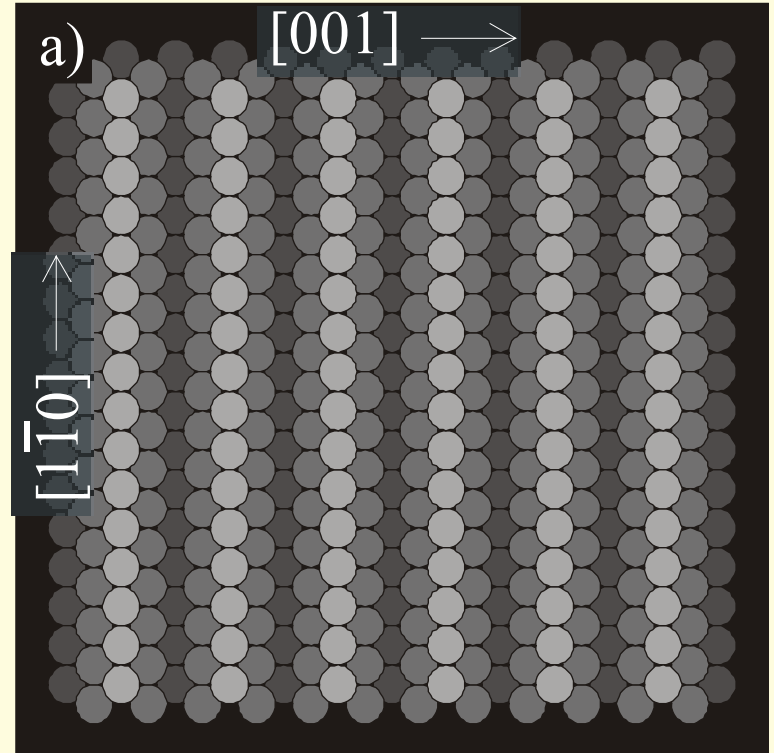


Ohnishi, Kondo and  
Takayanagi Nature  
**395**, 780 (1998)

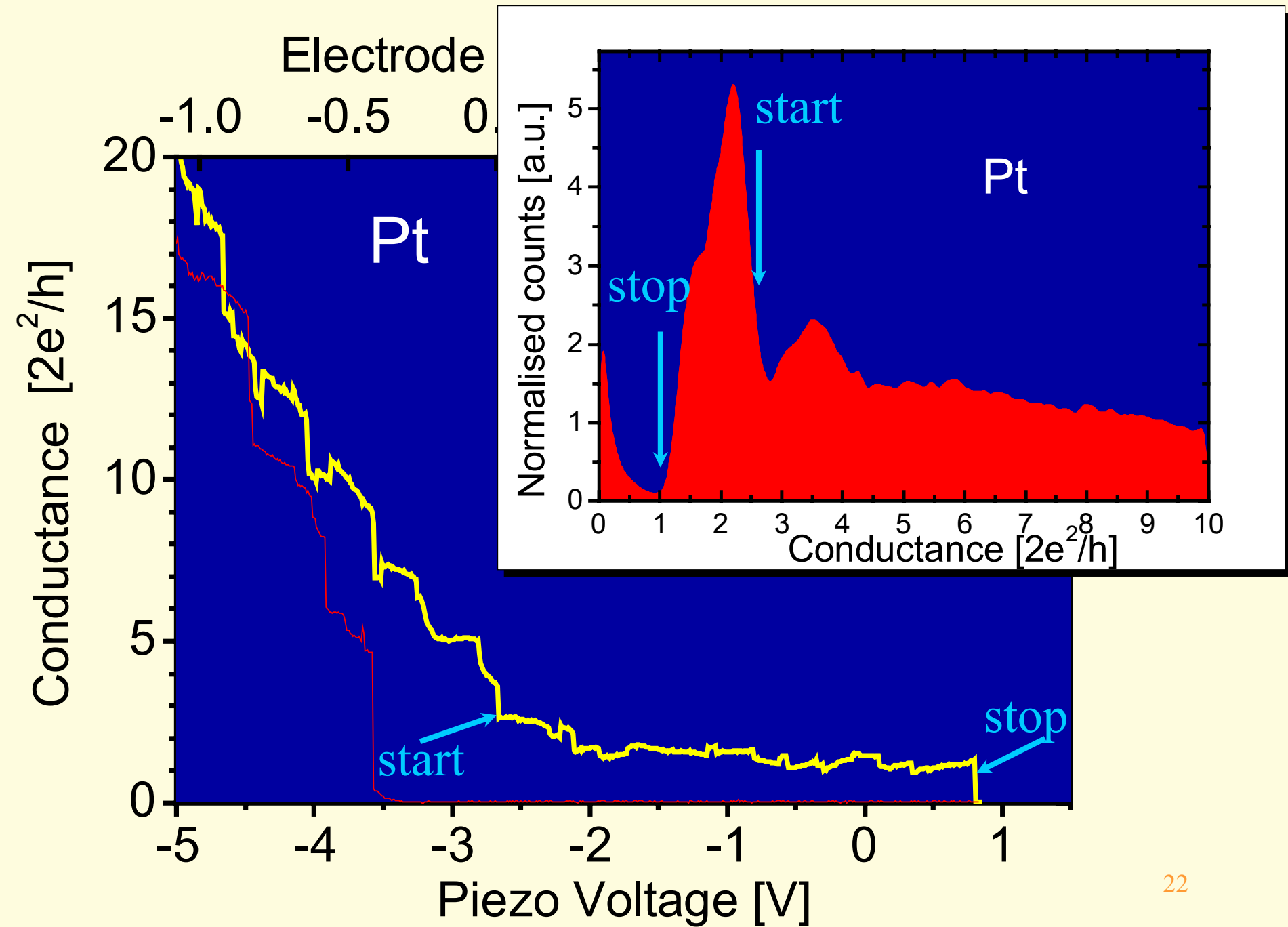
# Surface reconstructions



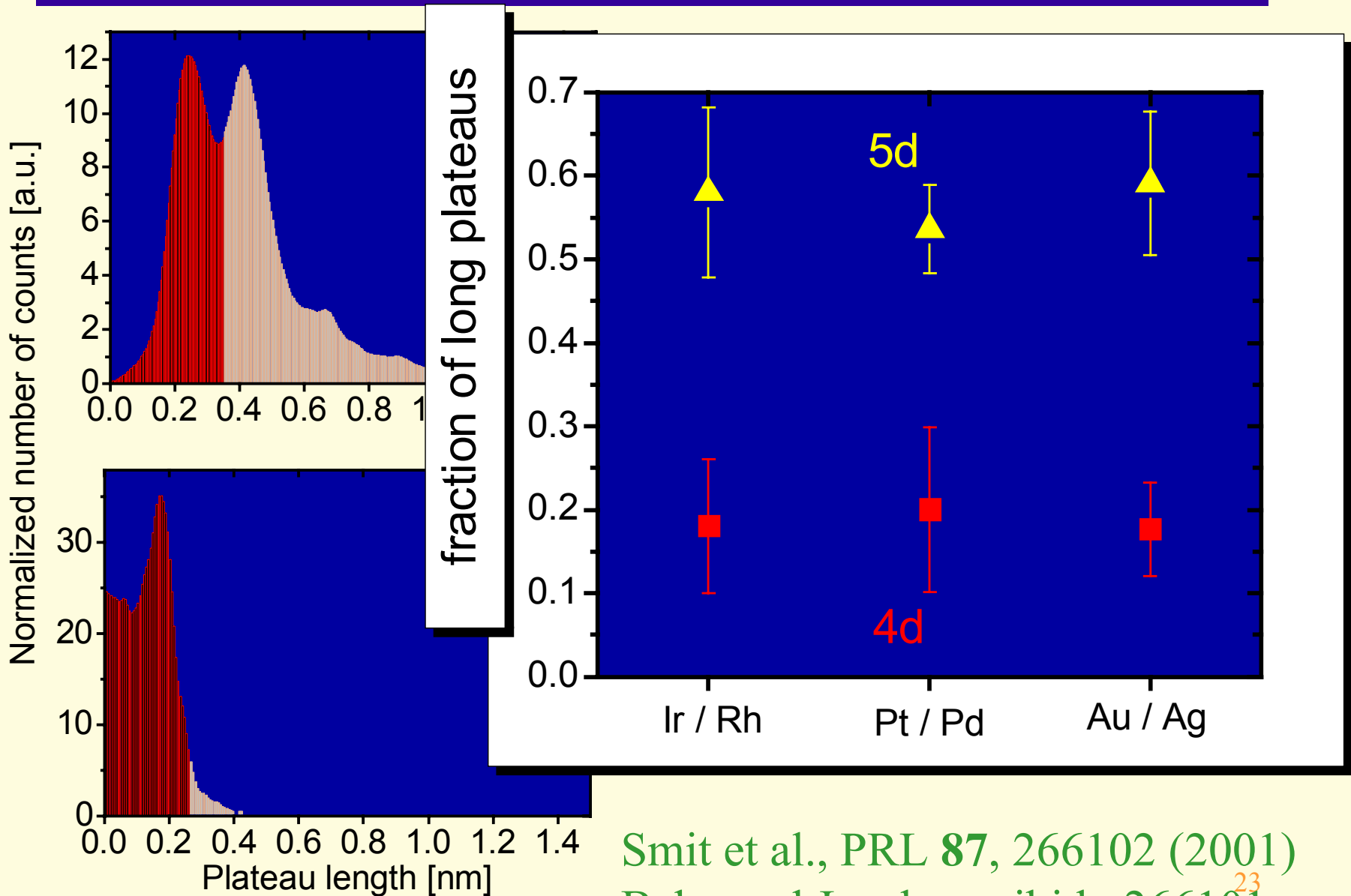
(100) surface



(110) surface

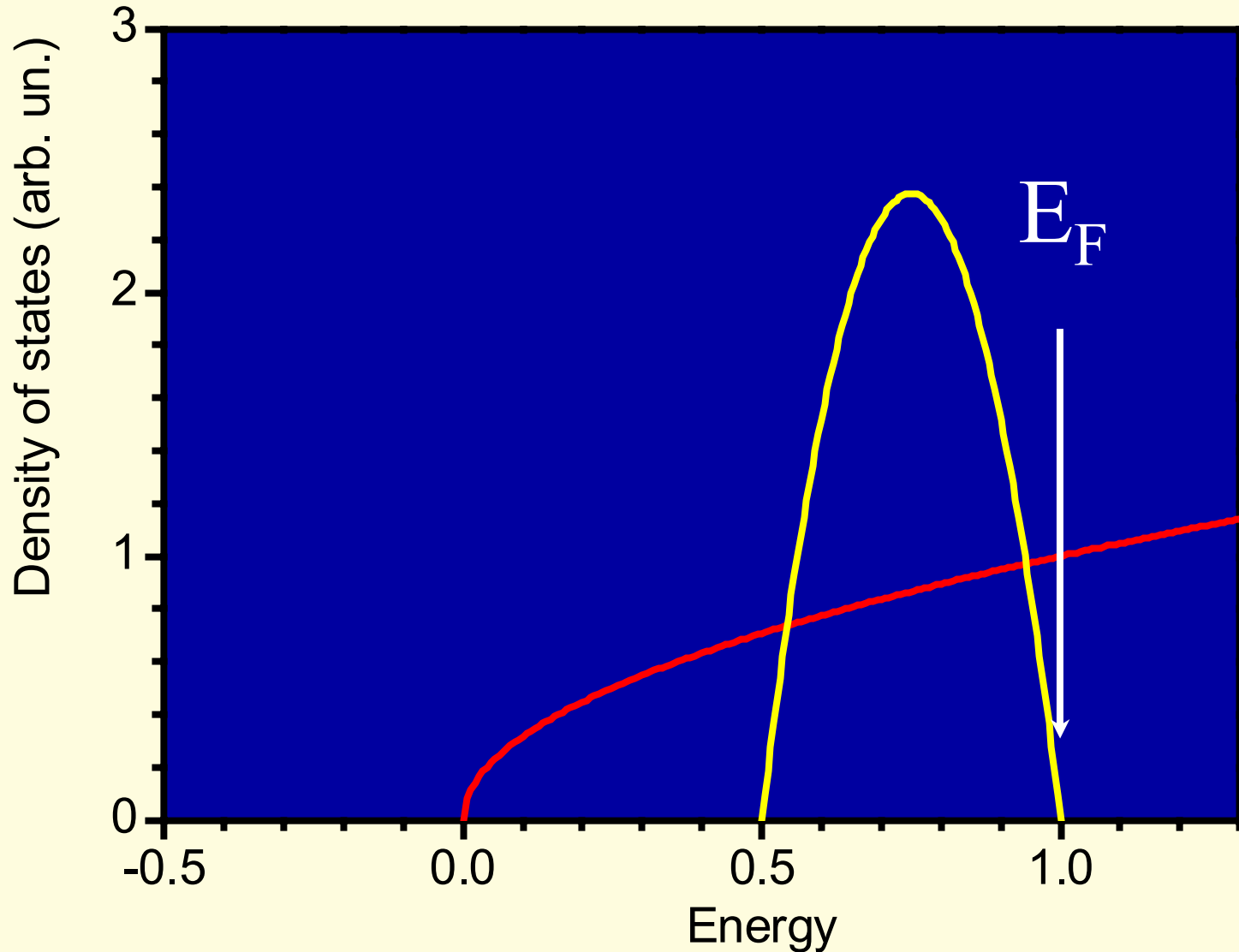


# Test of chain formation for other metals



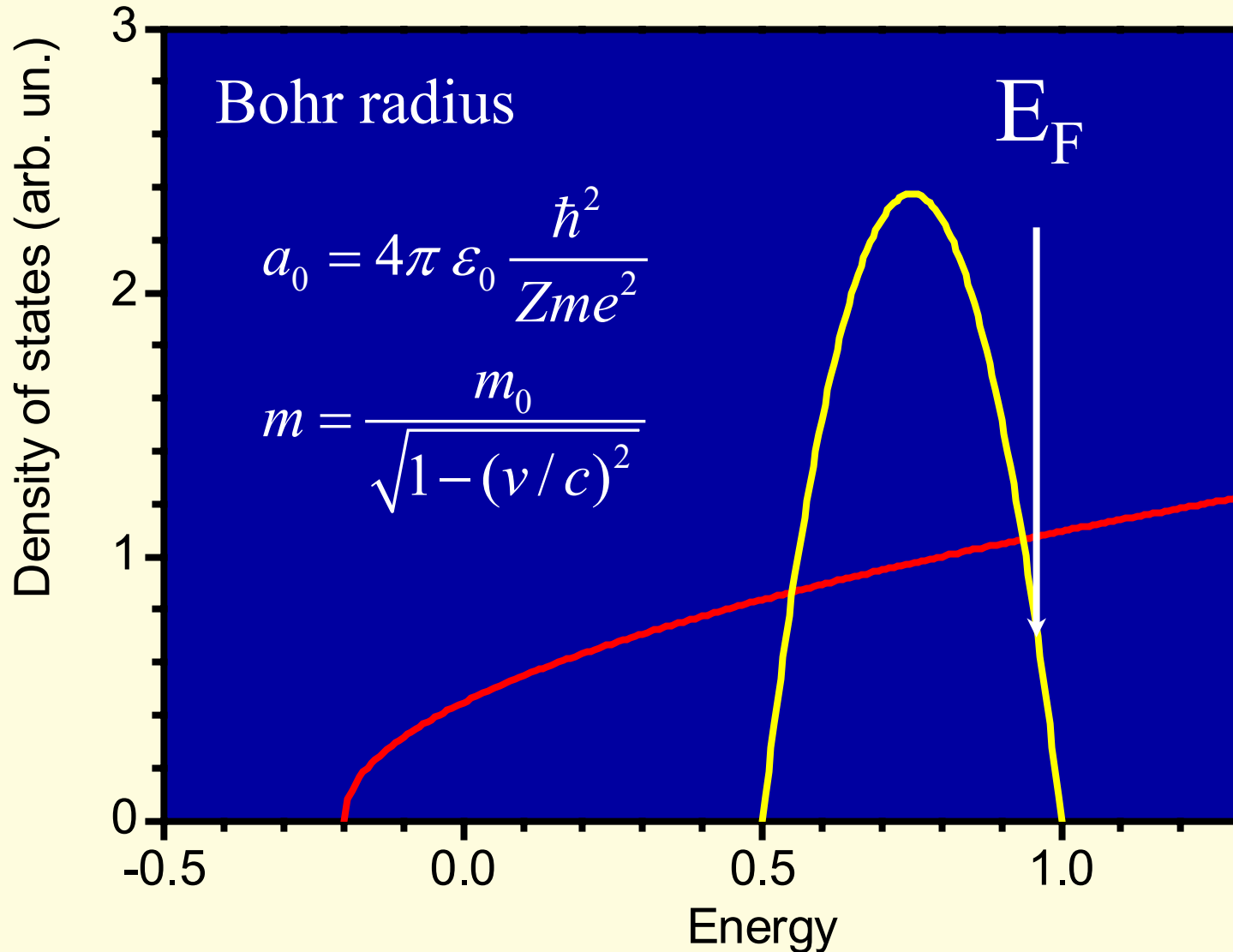
Smit et al., PRL **87**, 266102 (2001)  
Bahn and Jacobsen, *ibid.*, 266101

# Relativistic effects in the bonding of Au





# Relativistic effects in the bonding of Au



# Chain formation in transition metals

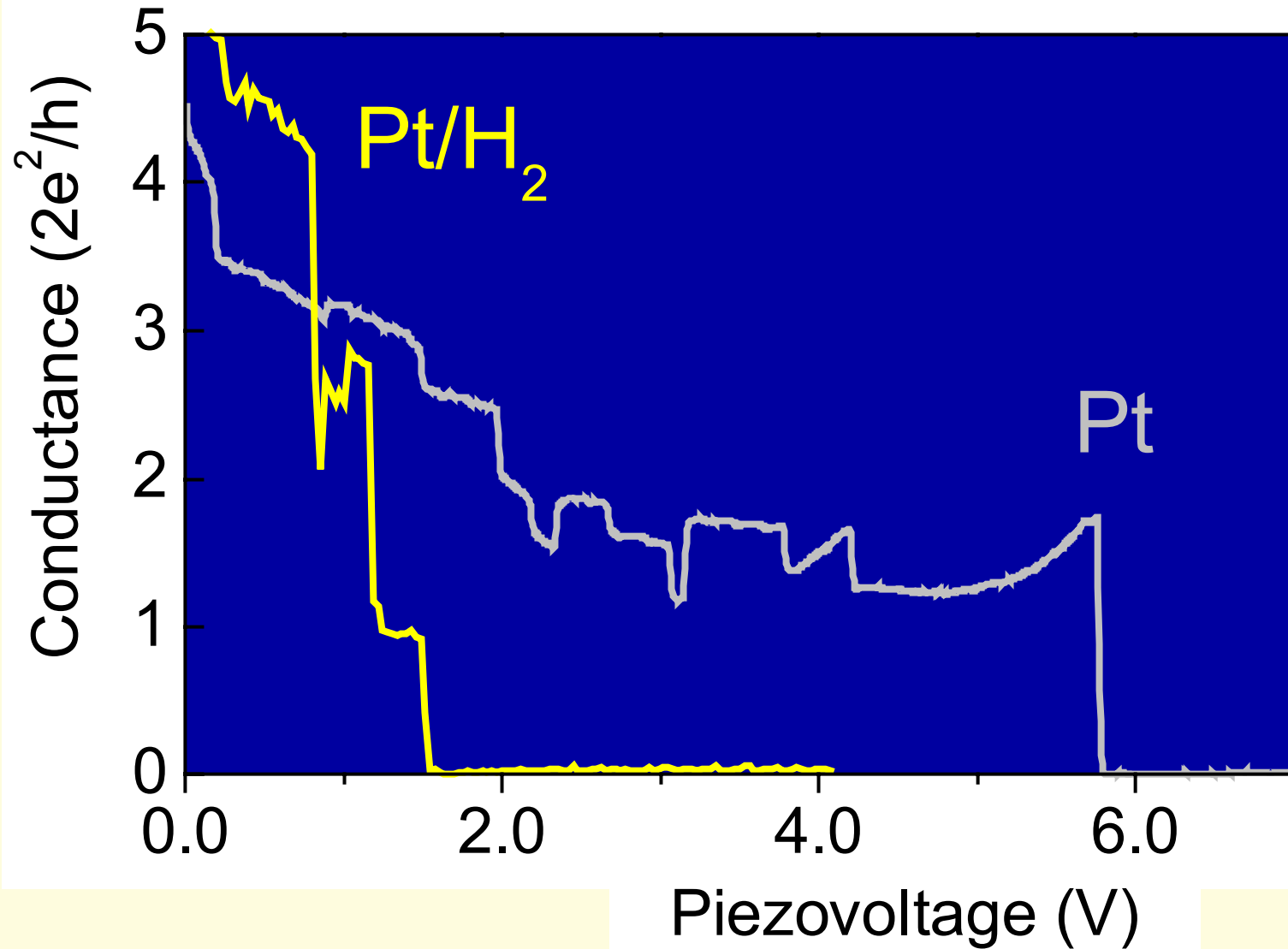
Fe	Co	Ni	Cu	Zn
Ru	Rh	Pd	Ag	Cd
Os	Ir	Pt	Au	Hg

Smit et al., PRL **87**, 266102 (2001)

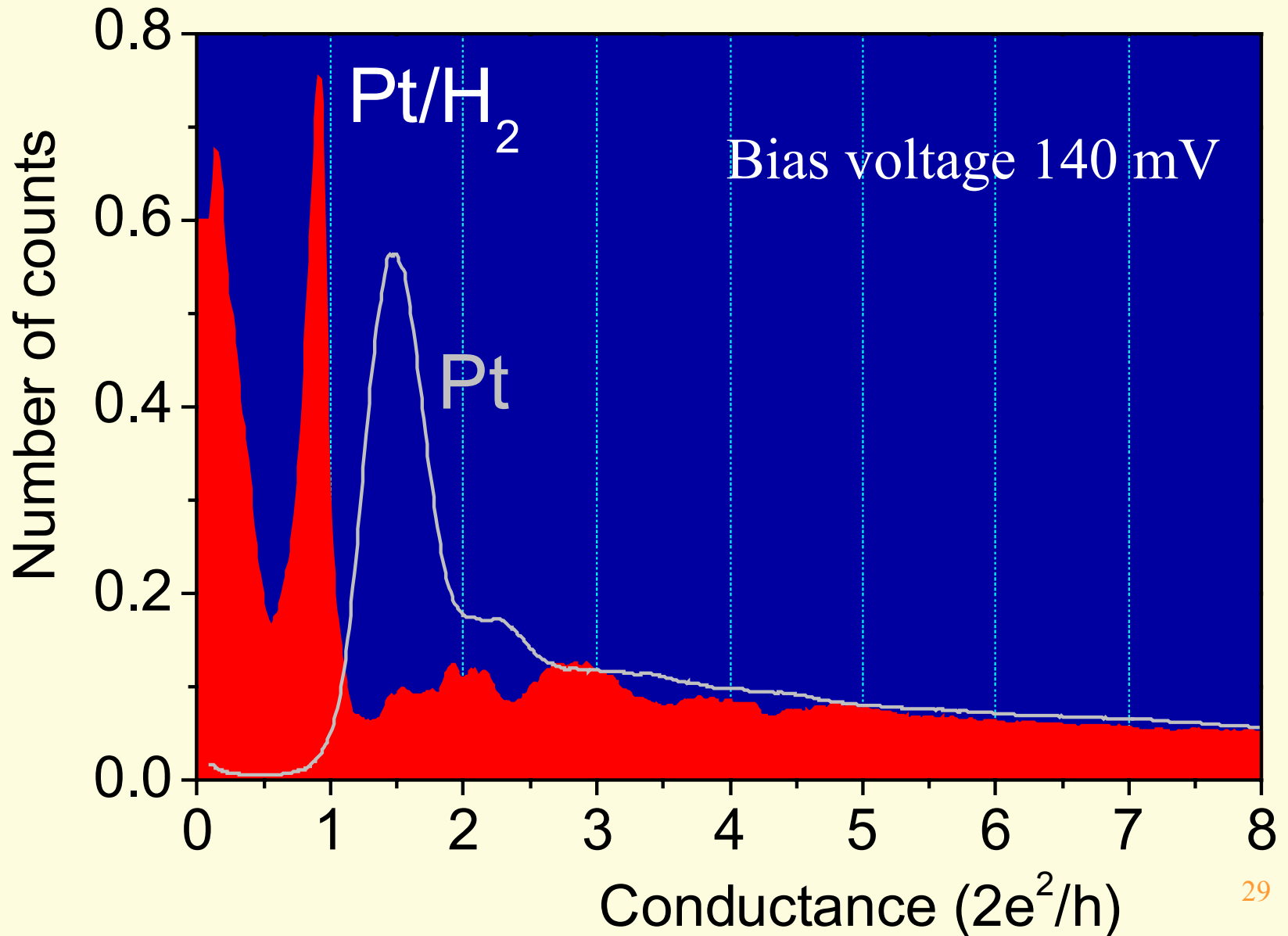
Bahn and Jacobsen, *ibid.*, 266101

# Conductance of a single hydrogen molecule

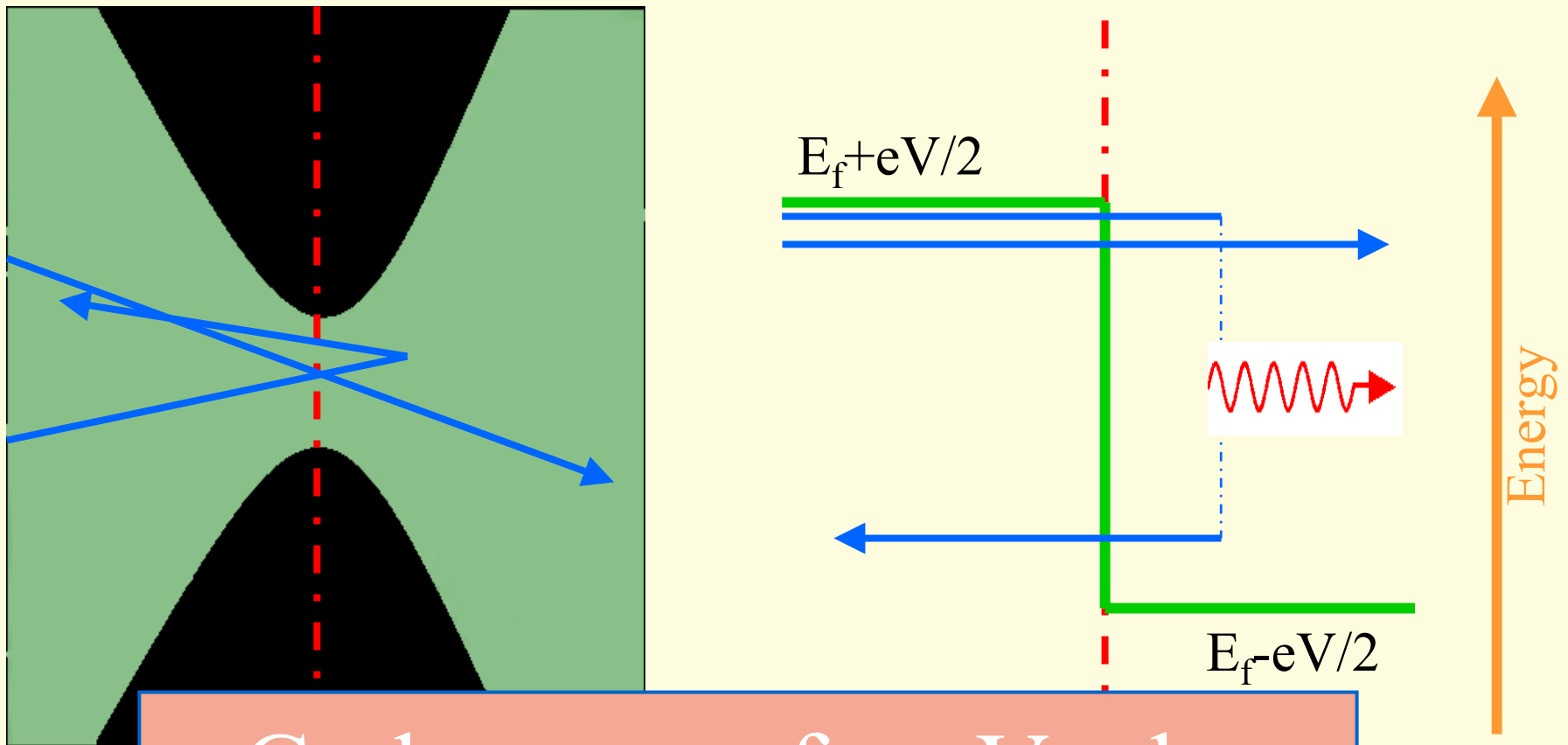
# Conductance curve for Pt/H<sub>2</sub>



# Conductance histogram for Pt/H<sub>2</sub>

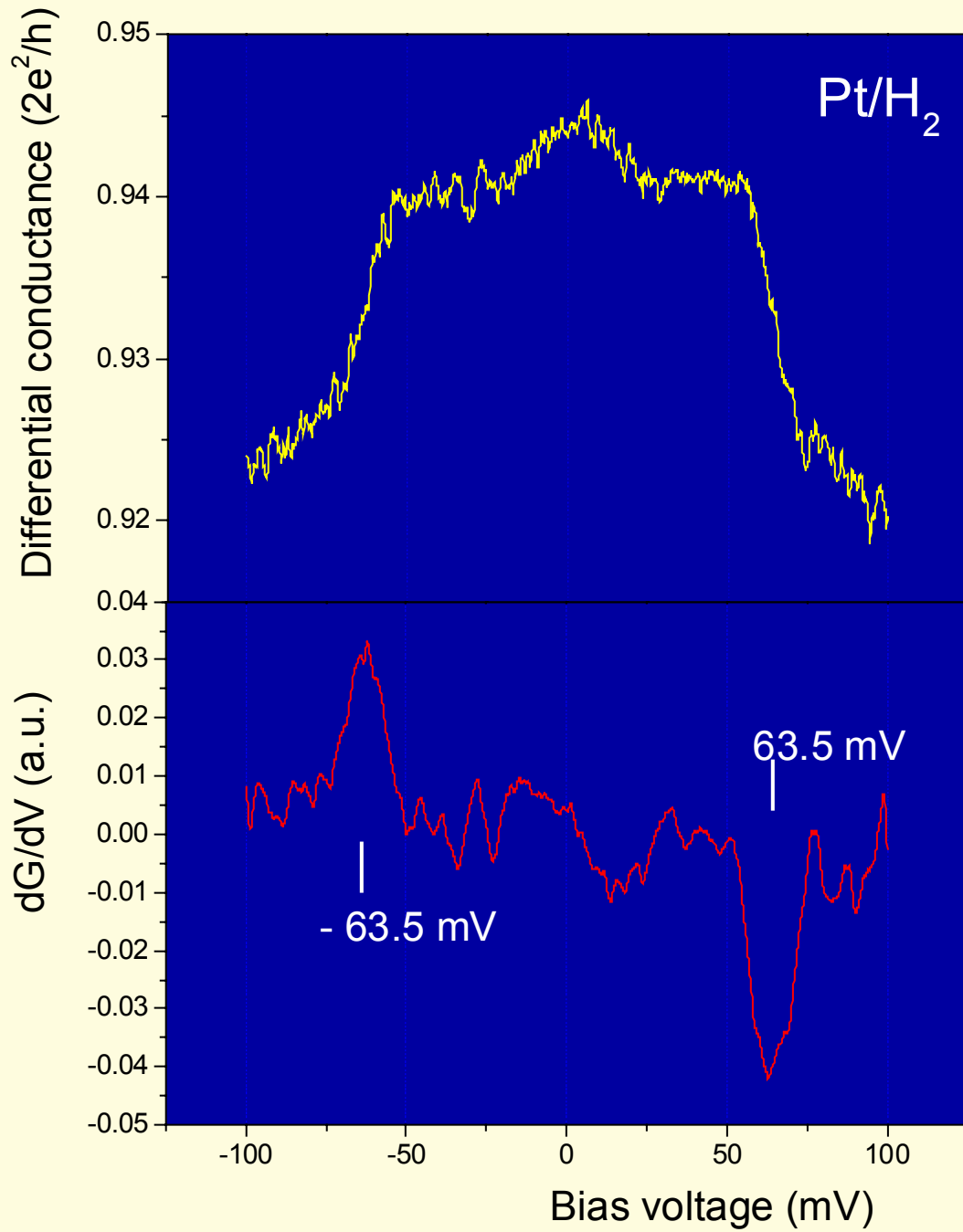


# Principle of point contact spectroscopy



$G$  decreases for  $eV > h\nu$

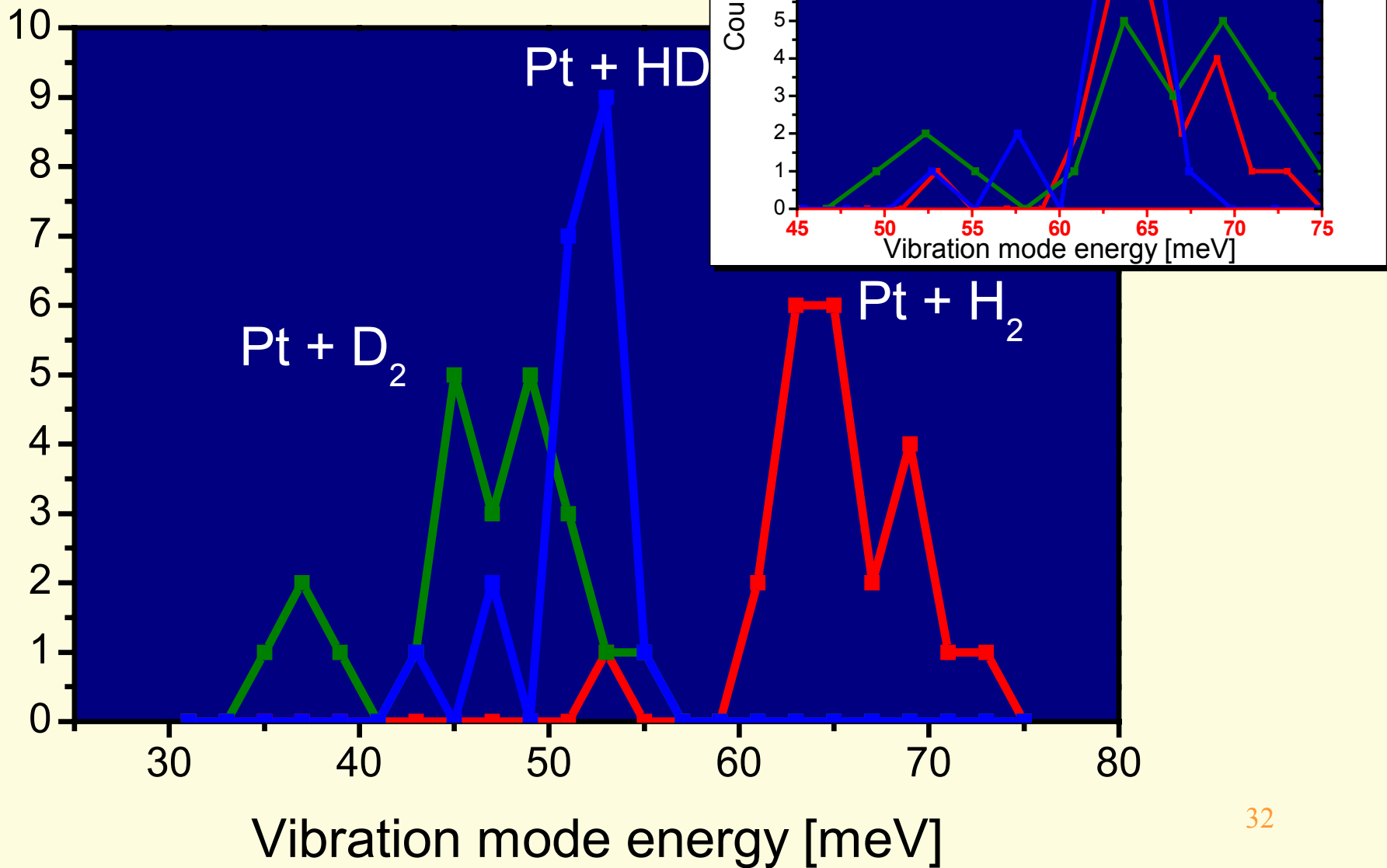
# Point contact spectrum for Pt/H<sub>2</sub>



Modulation: 1 mV, 7 kHz  
Recording time: 10 s  
Temperature: 4.2 K

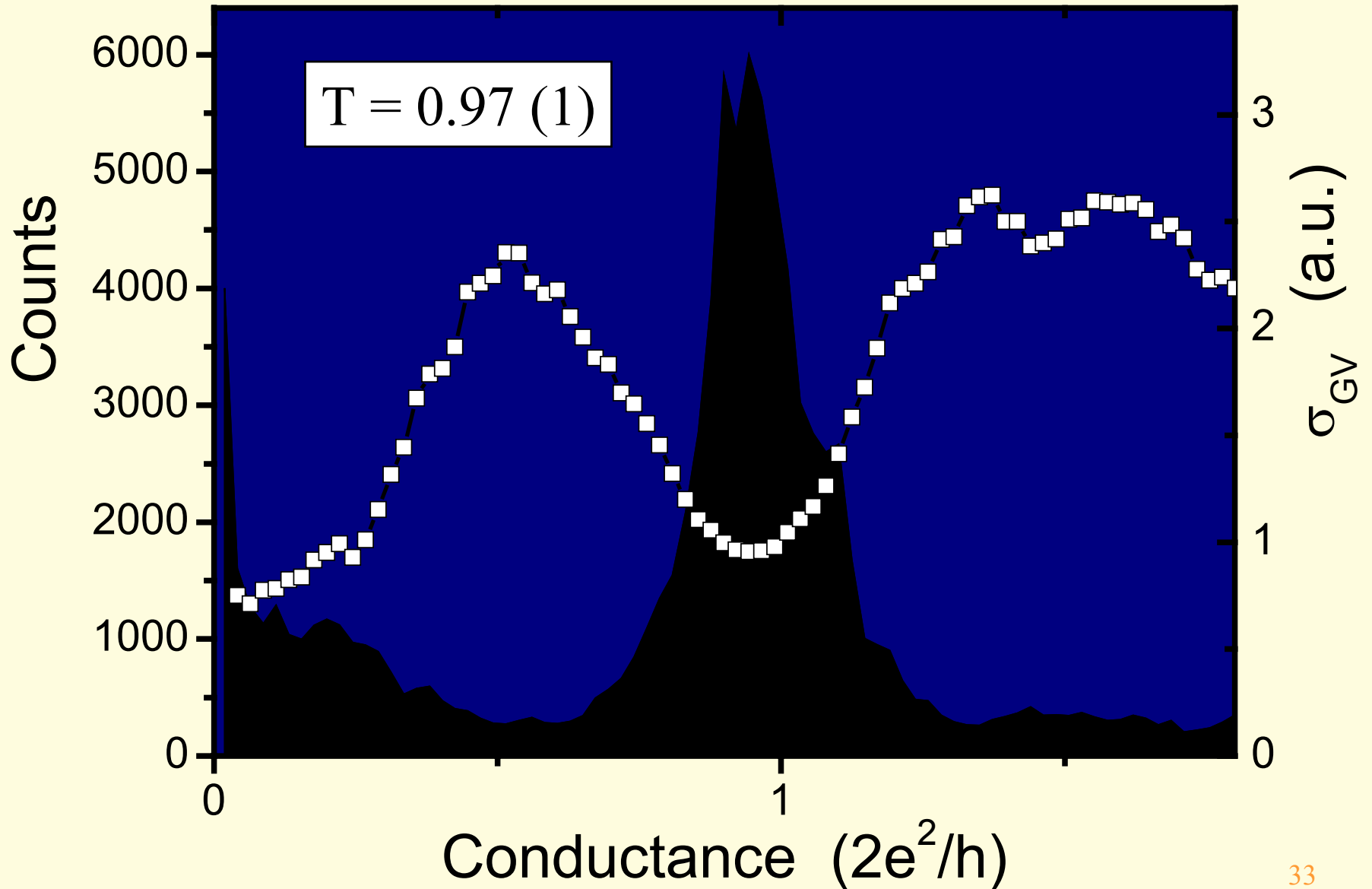
Numerical results for  
Pt-H-H-Pt  
Symm., longit.: 68 meV  
Asymm., longt.: 431 meV

# Isotope shift

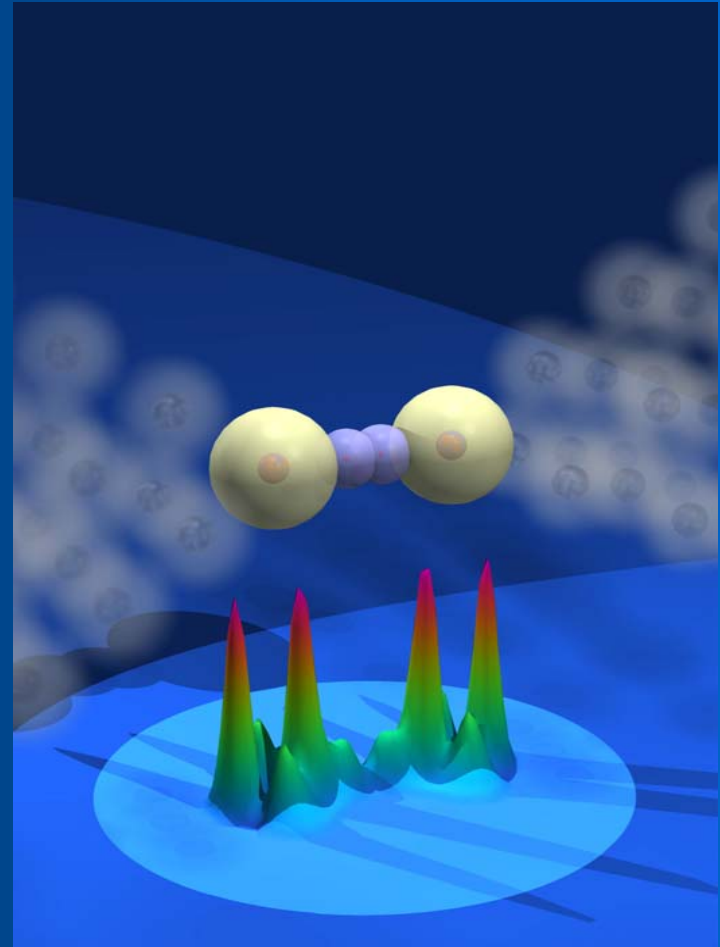
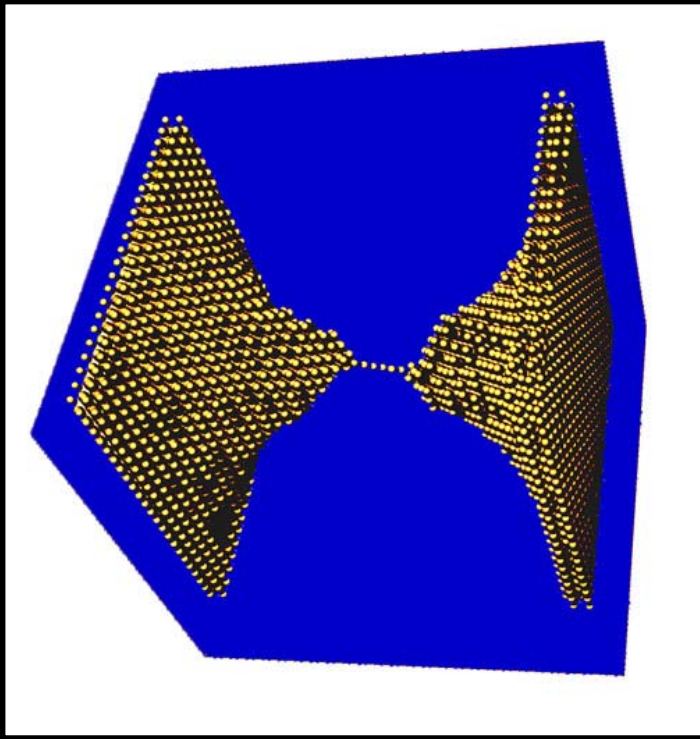




# Conductance fluctuations



# Conclusions



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