

# Electron Transport through Single Atoms and Molecules

J. Kröger, University of Kiel

# Acknowledgements

## Experiment

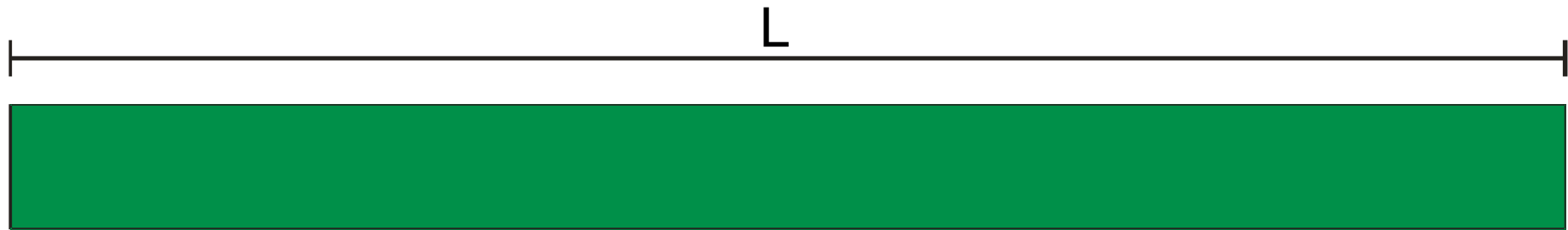
N. Néel, L. Limot, R. Berndt

## Theory

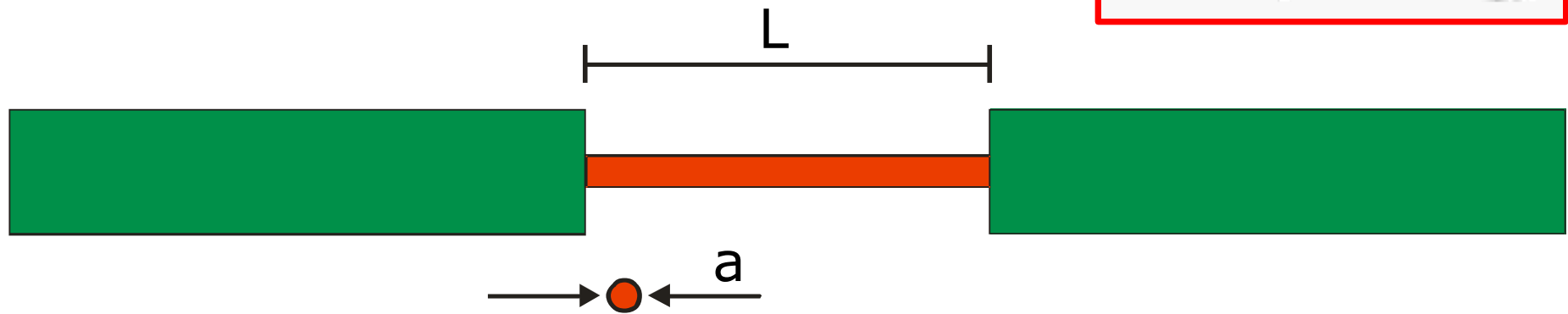
Th. Frederiksen, M. Brandbyge (Denmark)

K. Palotas, A. Garcia-Lekue, W.A. Hofer (United Kingdom)

# Conductance

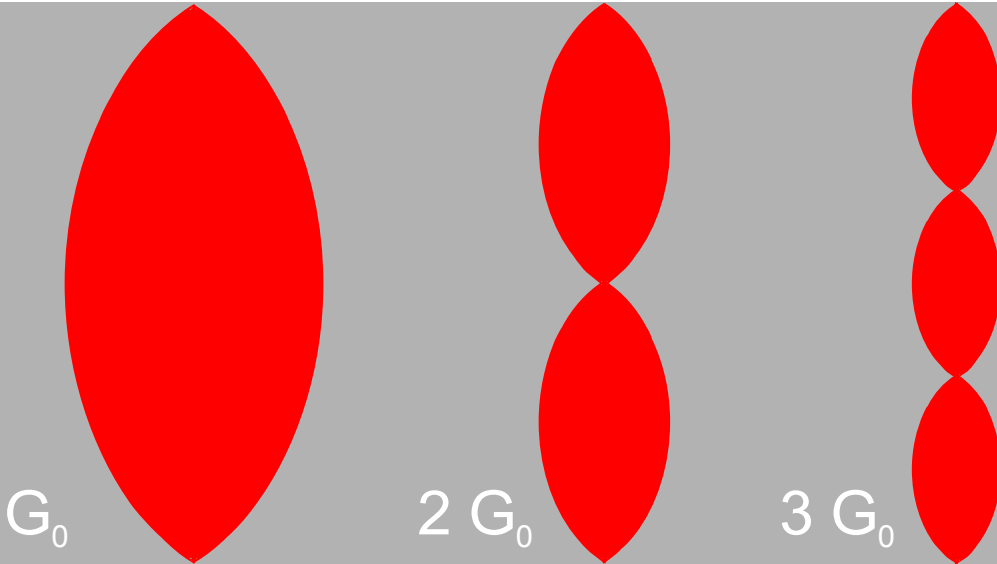


$$G = \frac{I}{V} = \sigma \frac{A}{L}$$

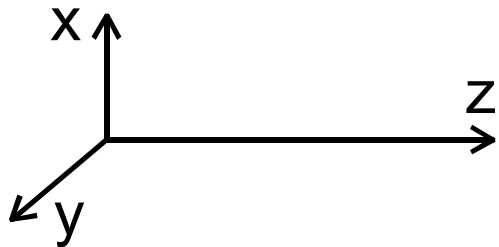


$$L < l, \quad a \ll l: \quad G = \frac{2e^2}{h} T$$

constriction: atom, cluster, molecule



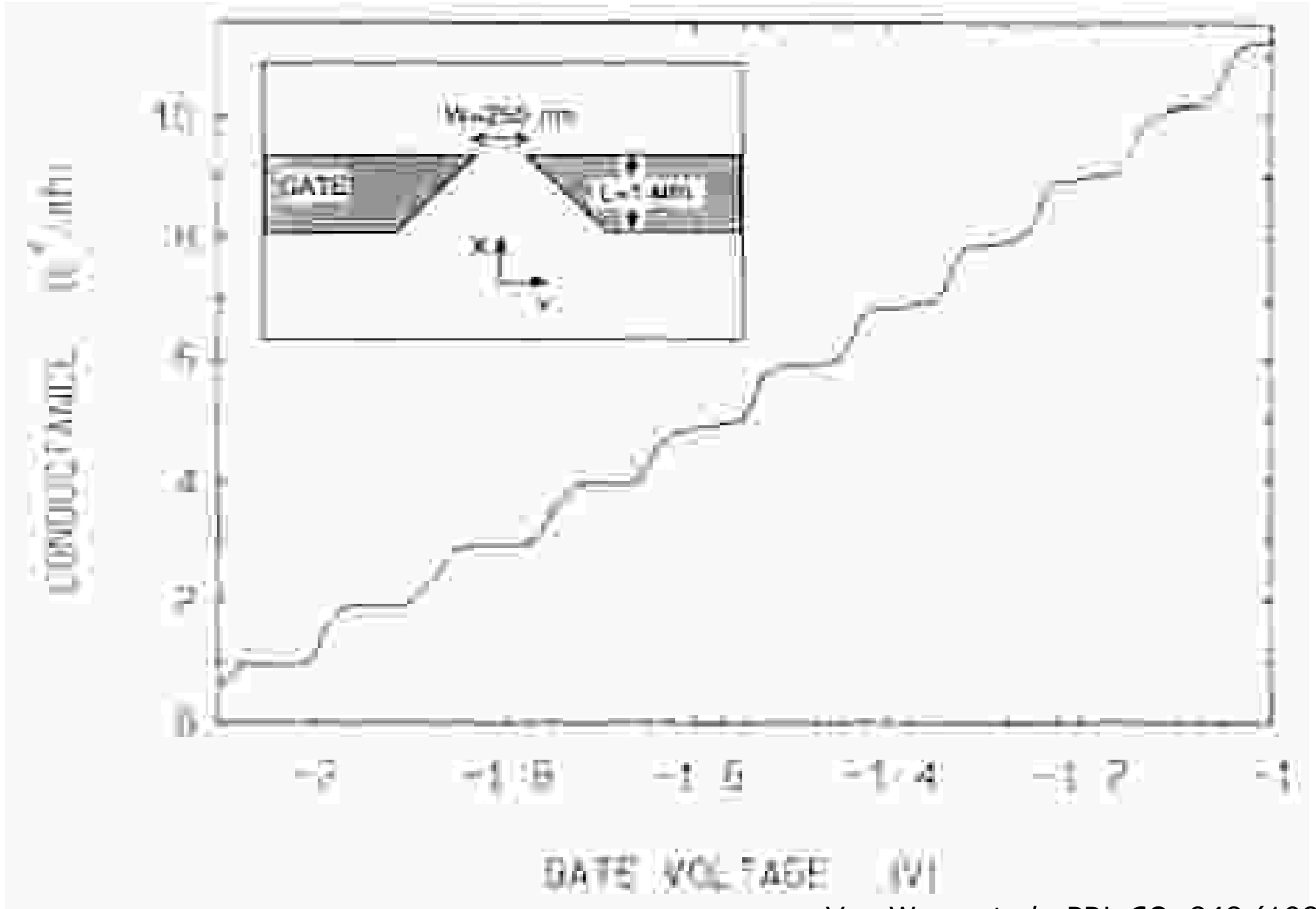
tip



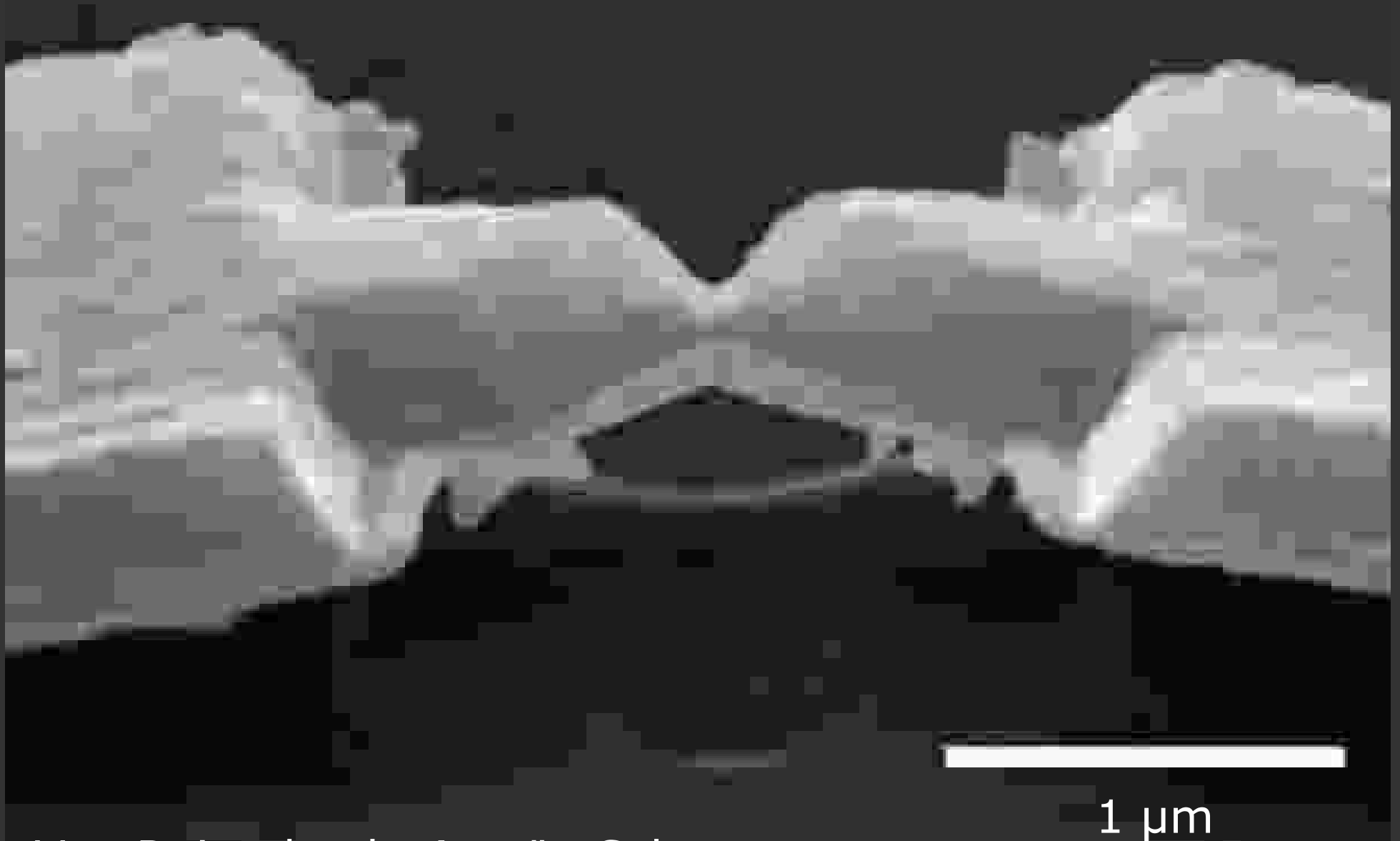
sample

$$G = \frac{2e^2}{h} \sum_{i=1}^N \tau_i$$

# Conductance quantization in experiments



# Mechanically controlled break junctions



Van Ruitenbeek, Agrait, Scheer

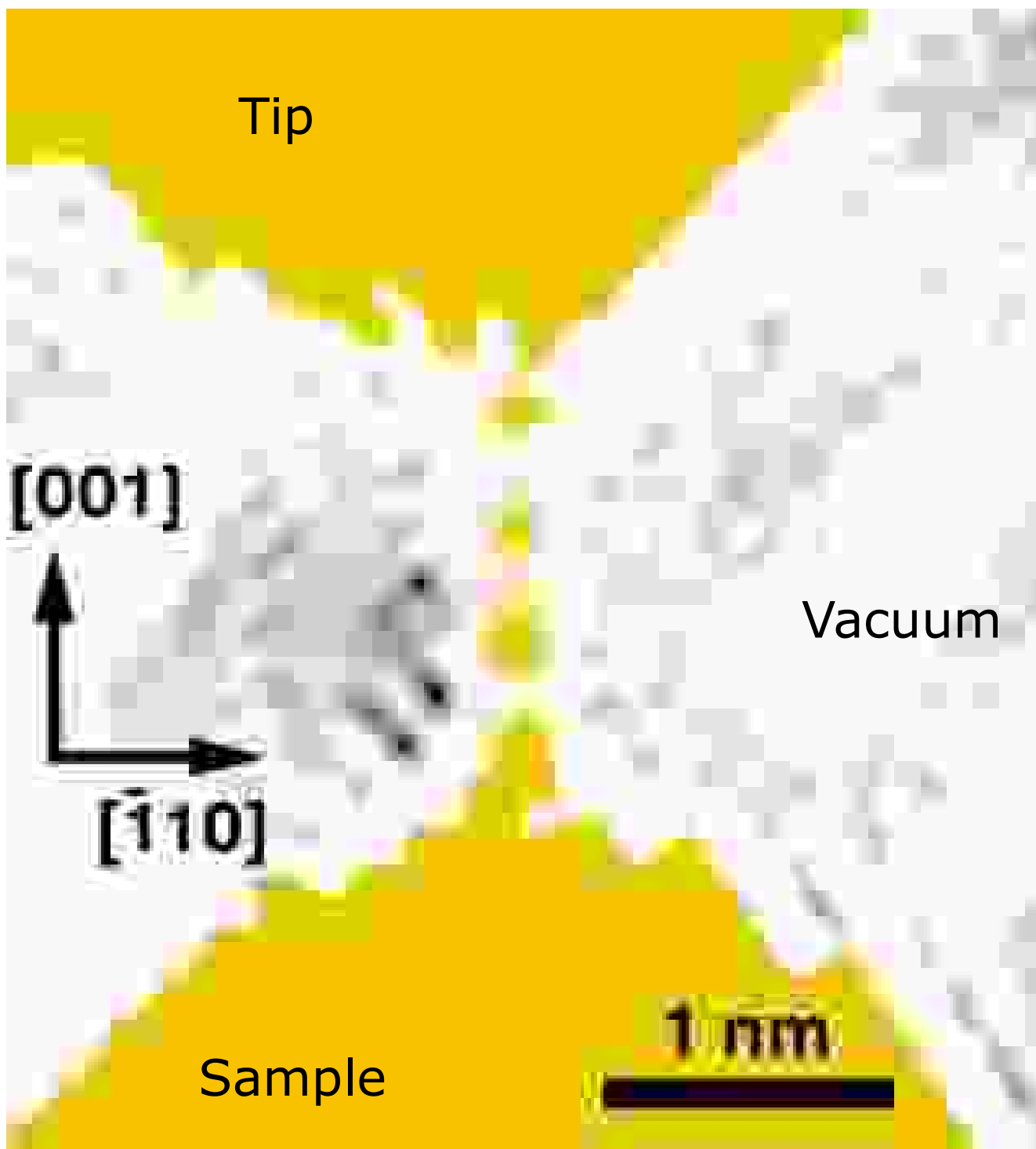
Number of conductance channels

=

Number of valence orbitals

Scheer *et al.*, Nature **394**, 154 (1998)

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



Ohnishi *et al.*, Nature **395**, 780 (1998)

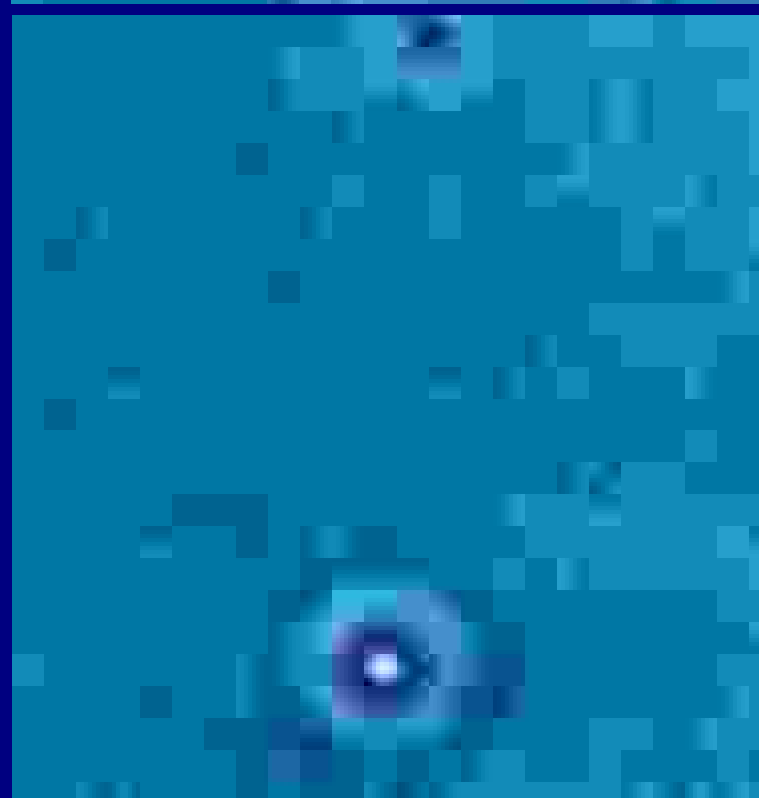
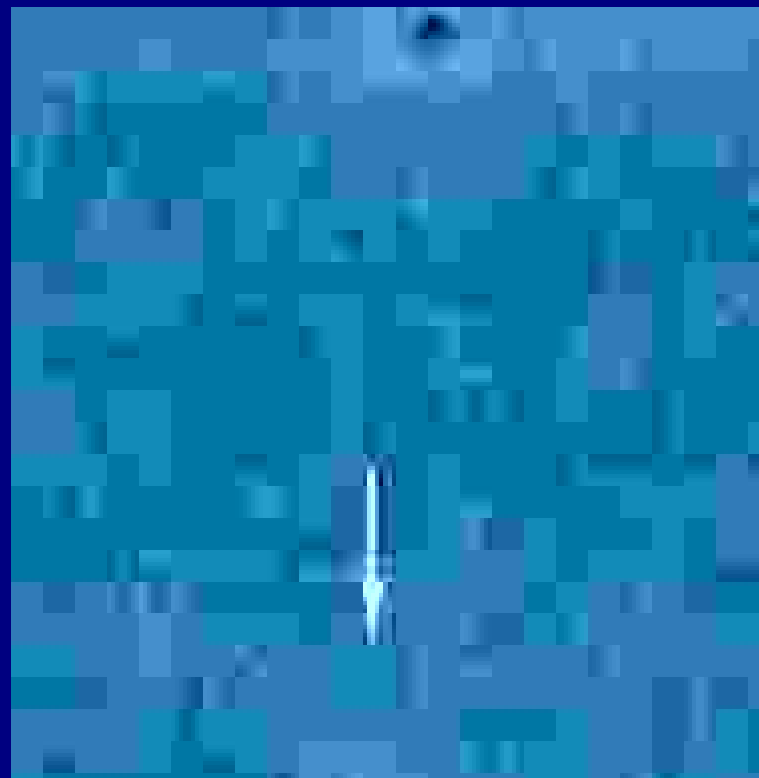
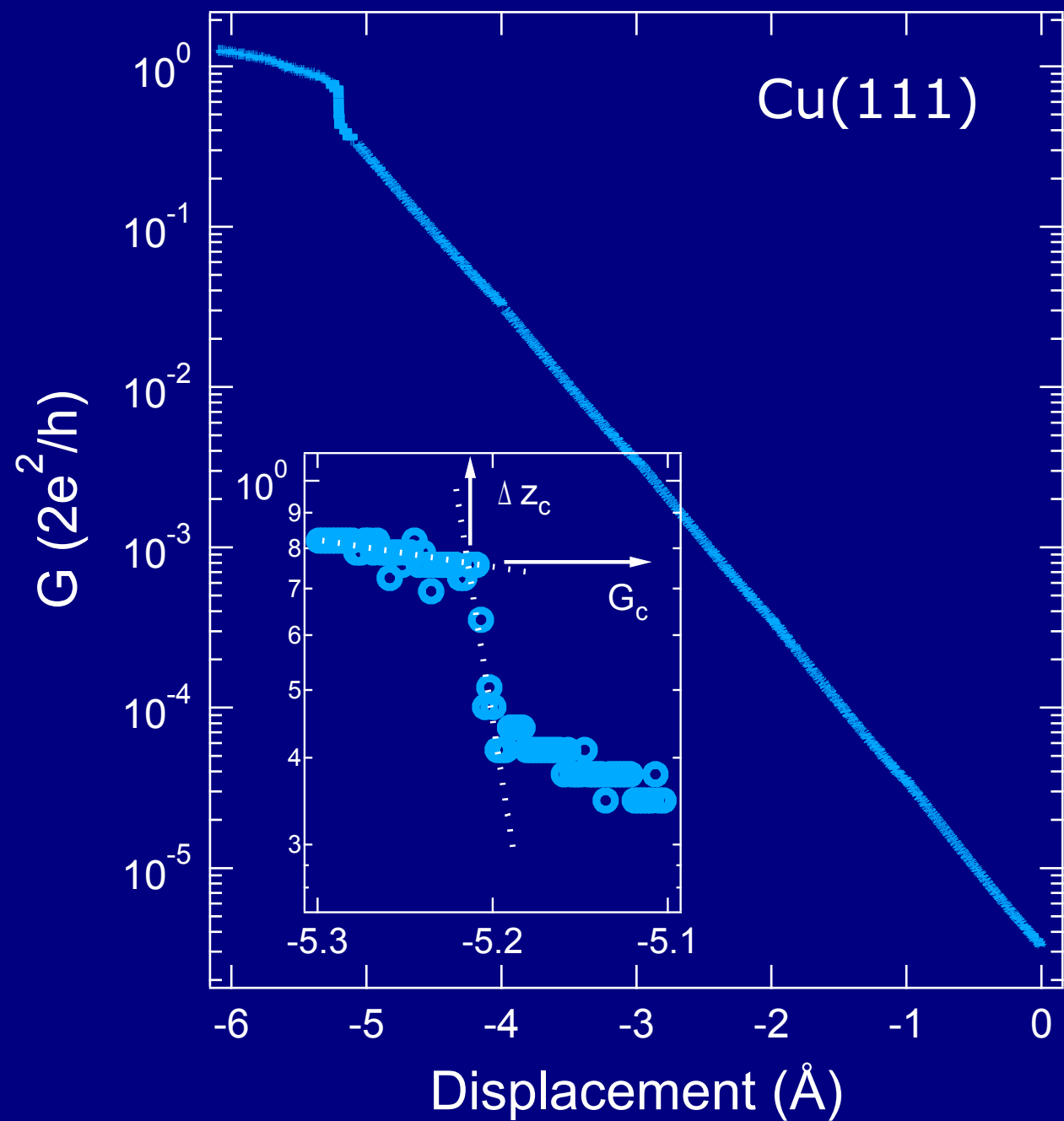


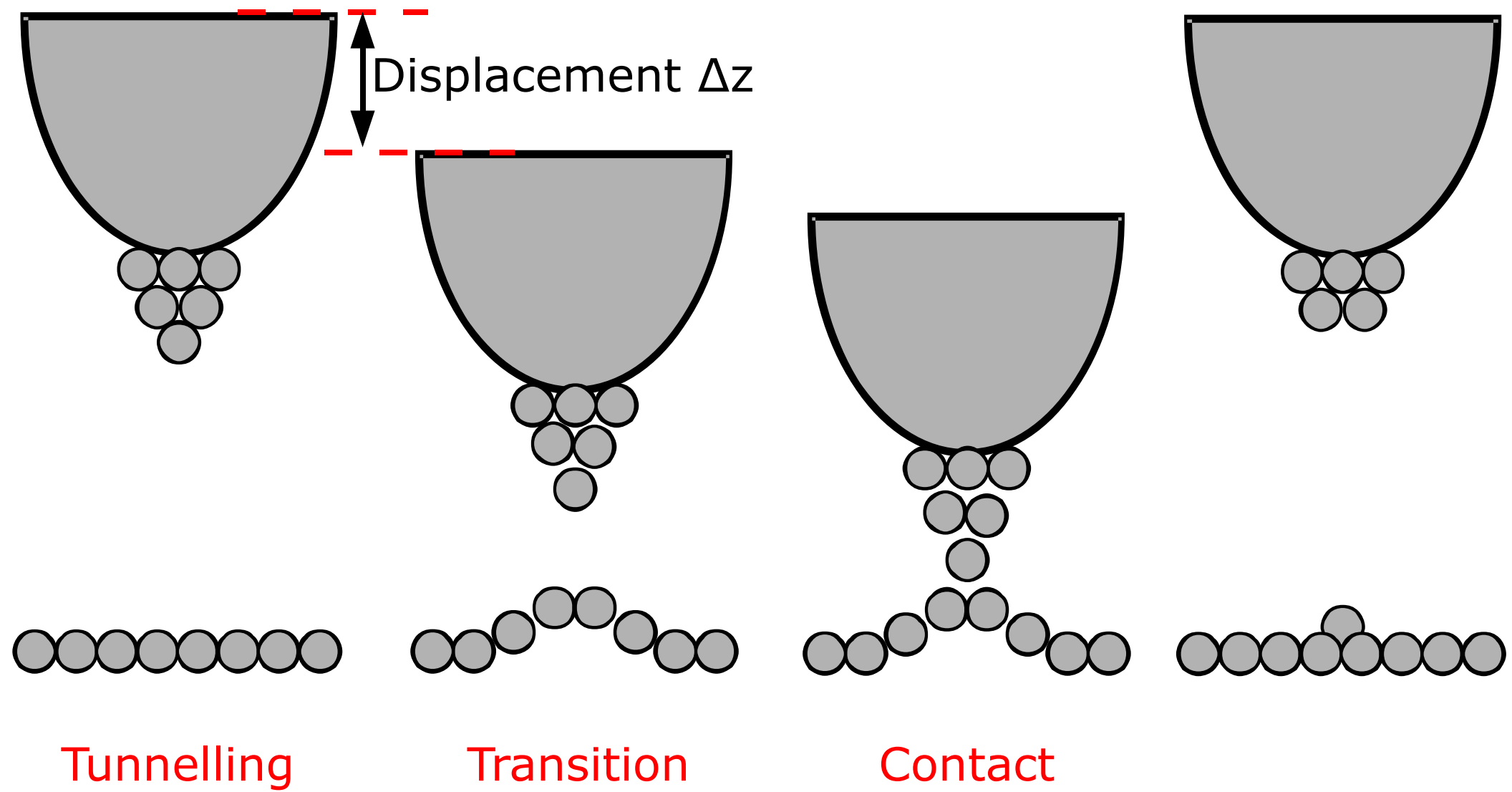


UHV, 7 K

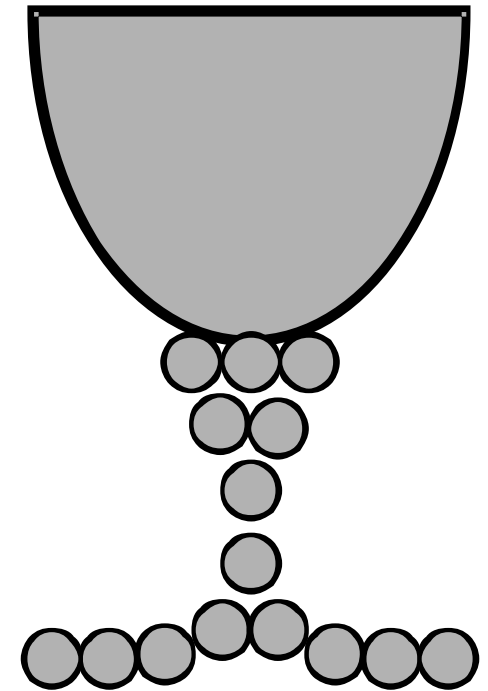
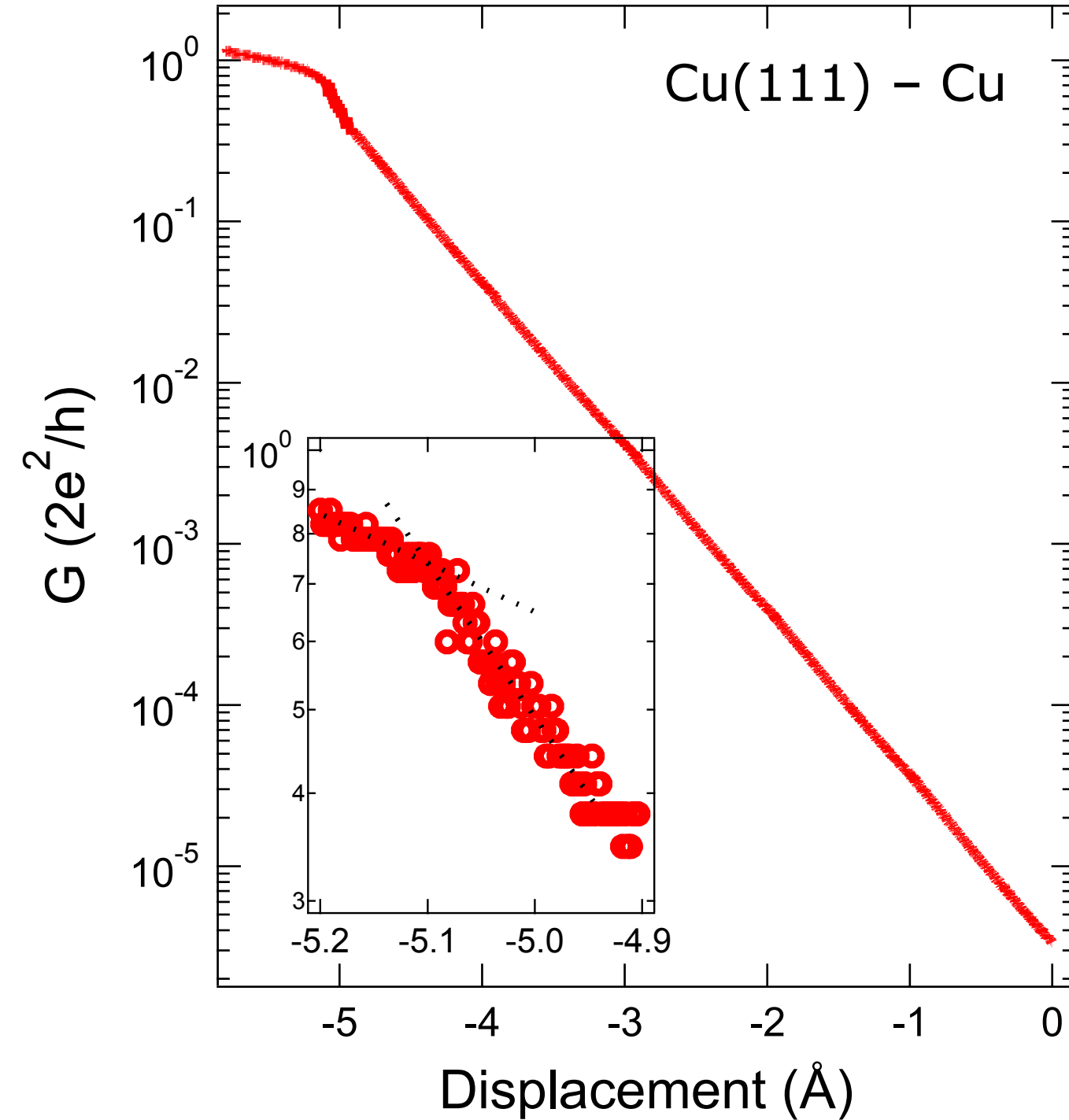
# Tip-surface contact

Limot, Kröger, Berndt, Garcia-Lekue, Hofer  
PRL **94**, 126102 (2005)





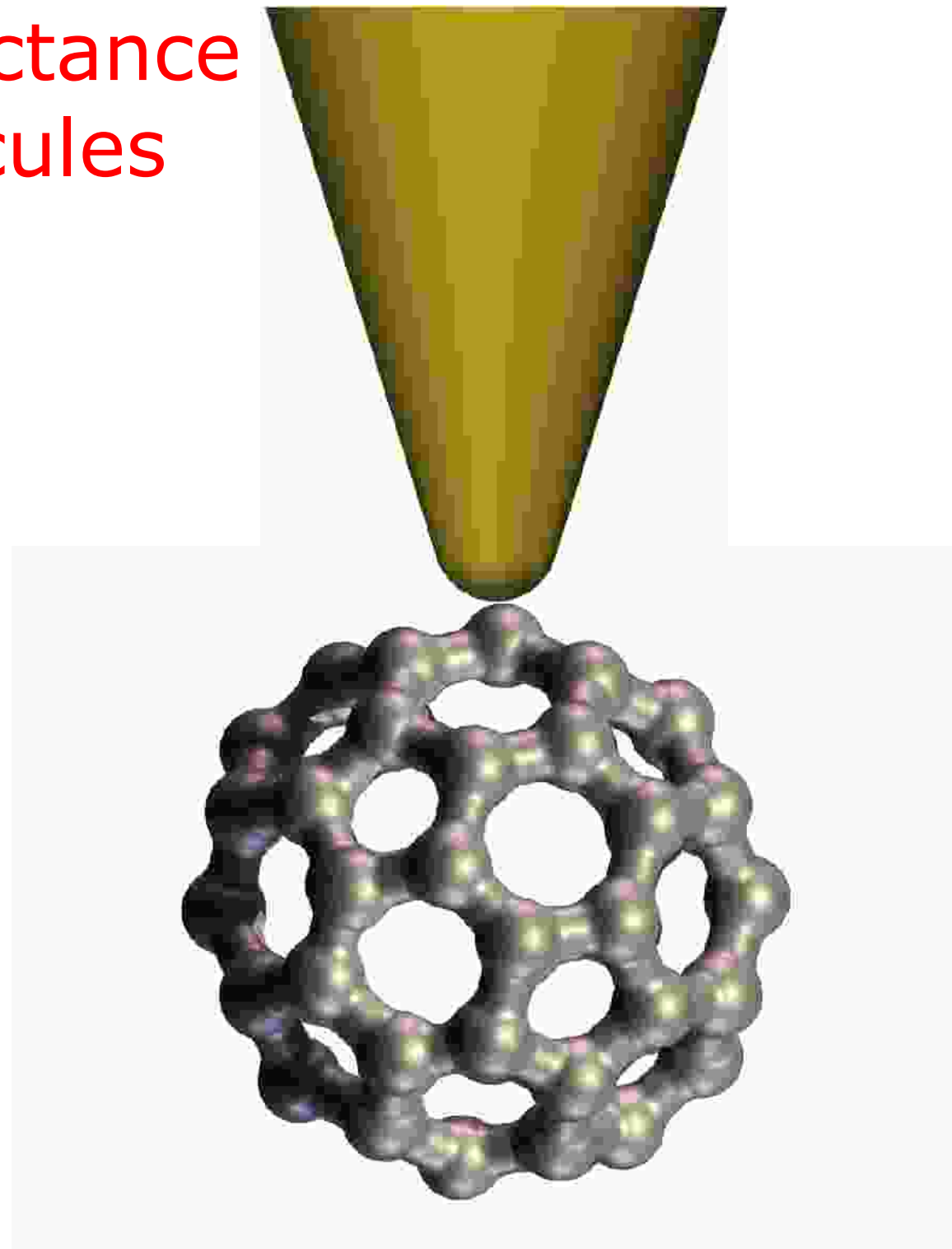
# Tip-adatom contact

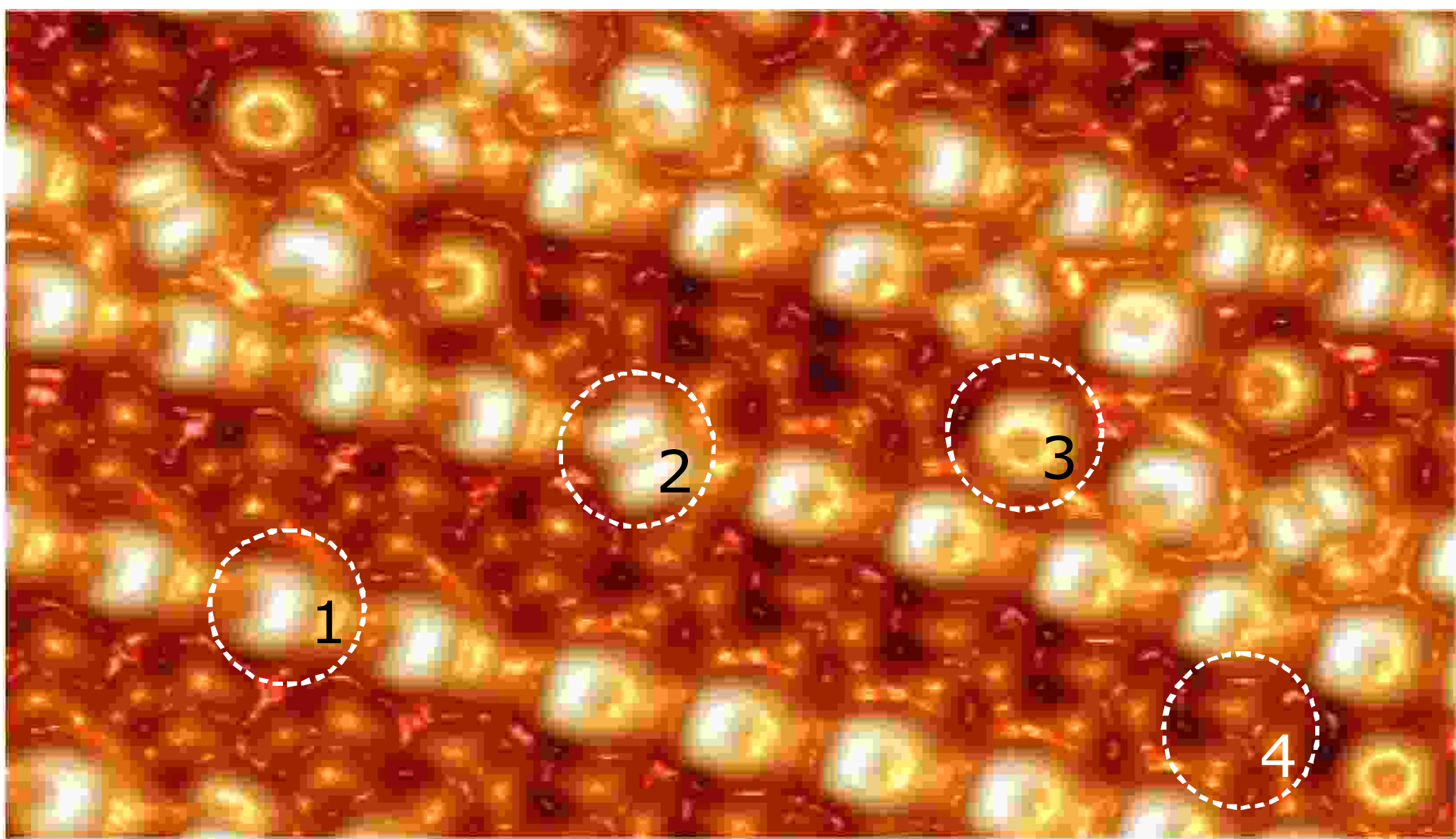


Ag(111)  
PRL **94**, 126102 (2005)

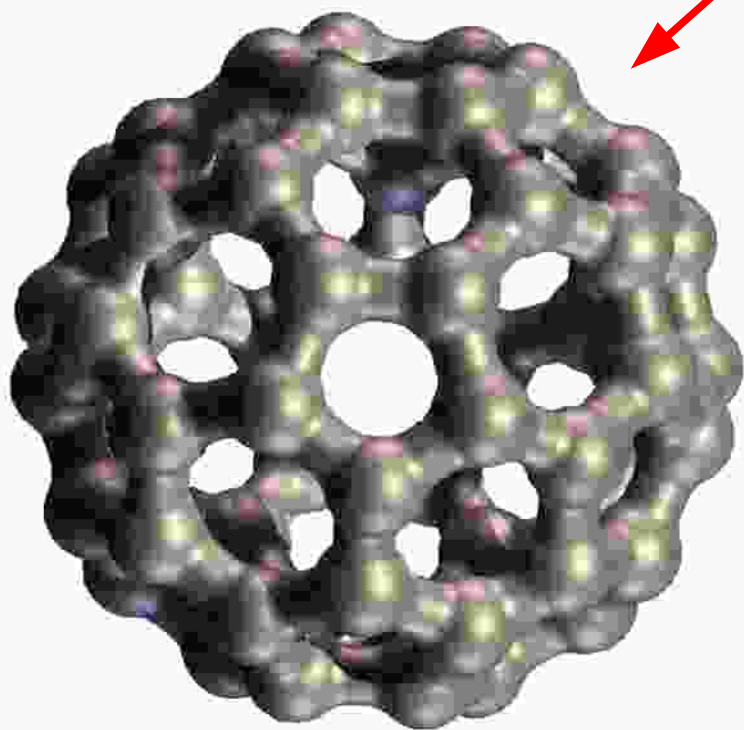
Au(111)  
New J. Phys. **9**, 153 (2007)

# Probing the conductance of individual molecules

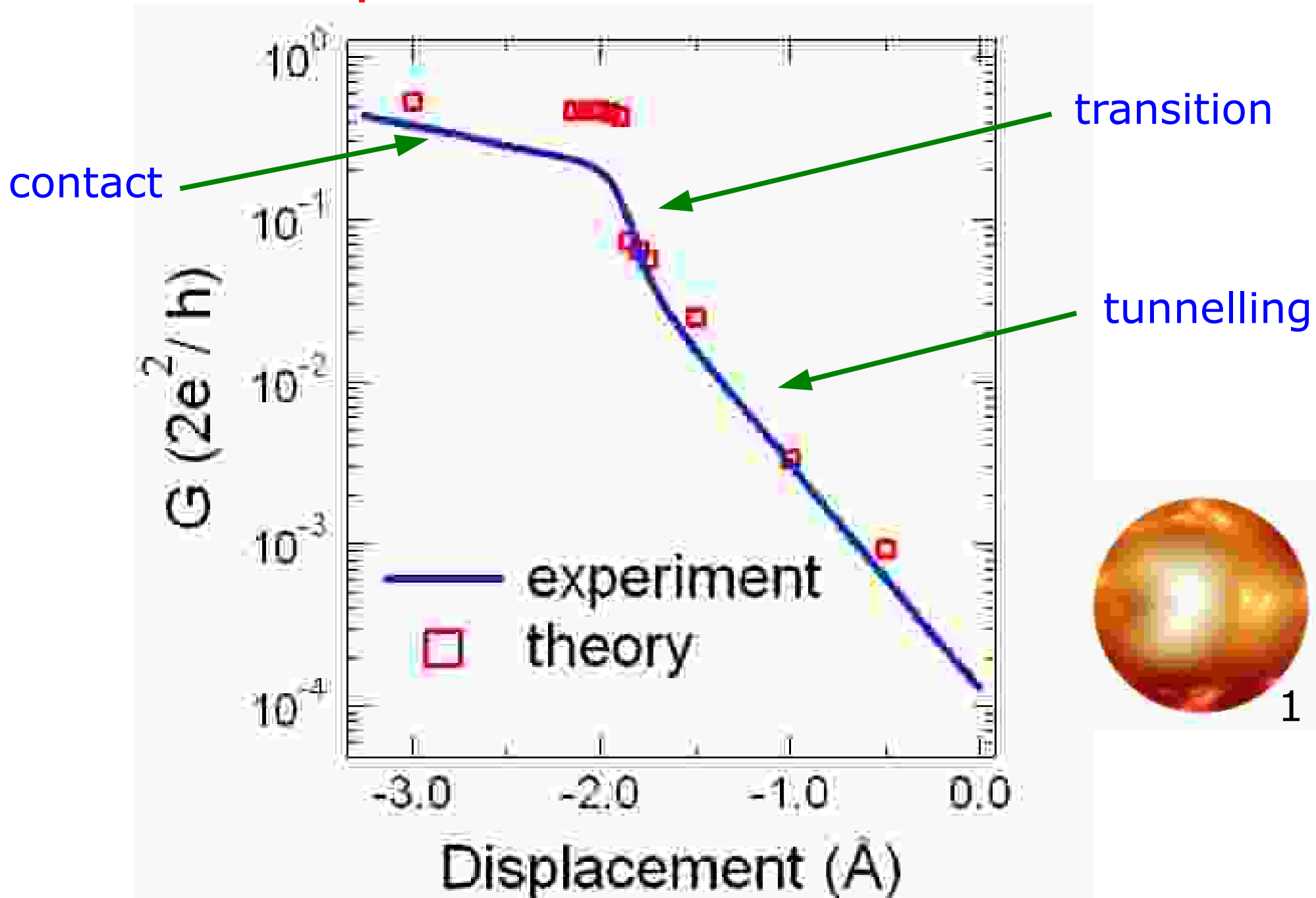




Cu(100) – C<sub>60</sub>: 4 molecule orientations

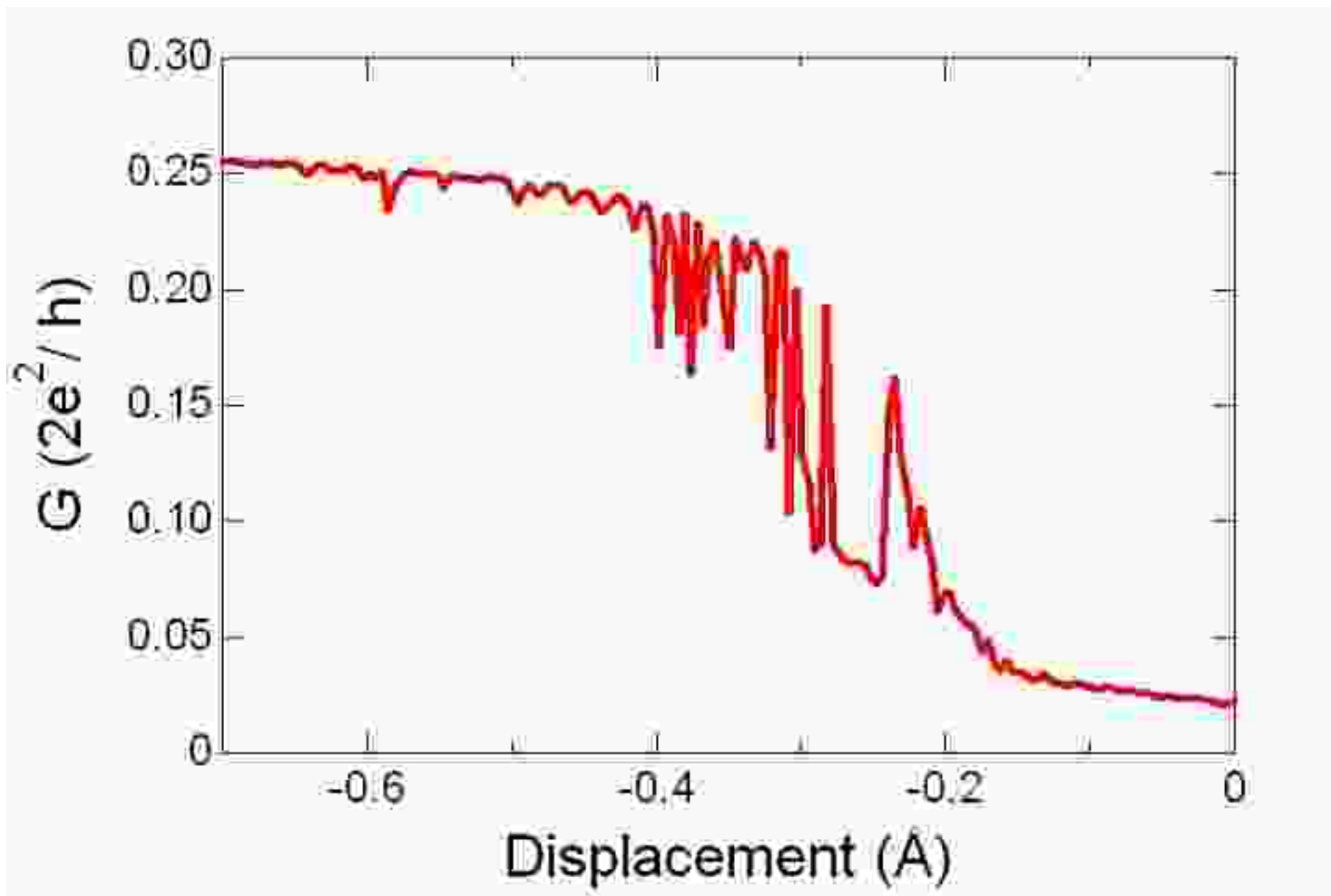


# Tip - Molecule Contact

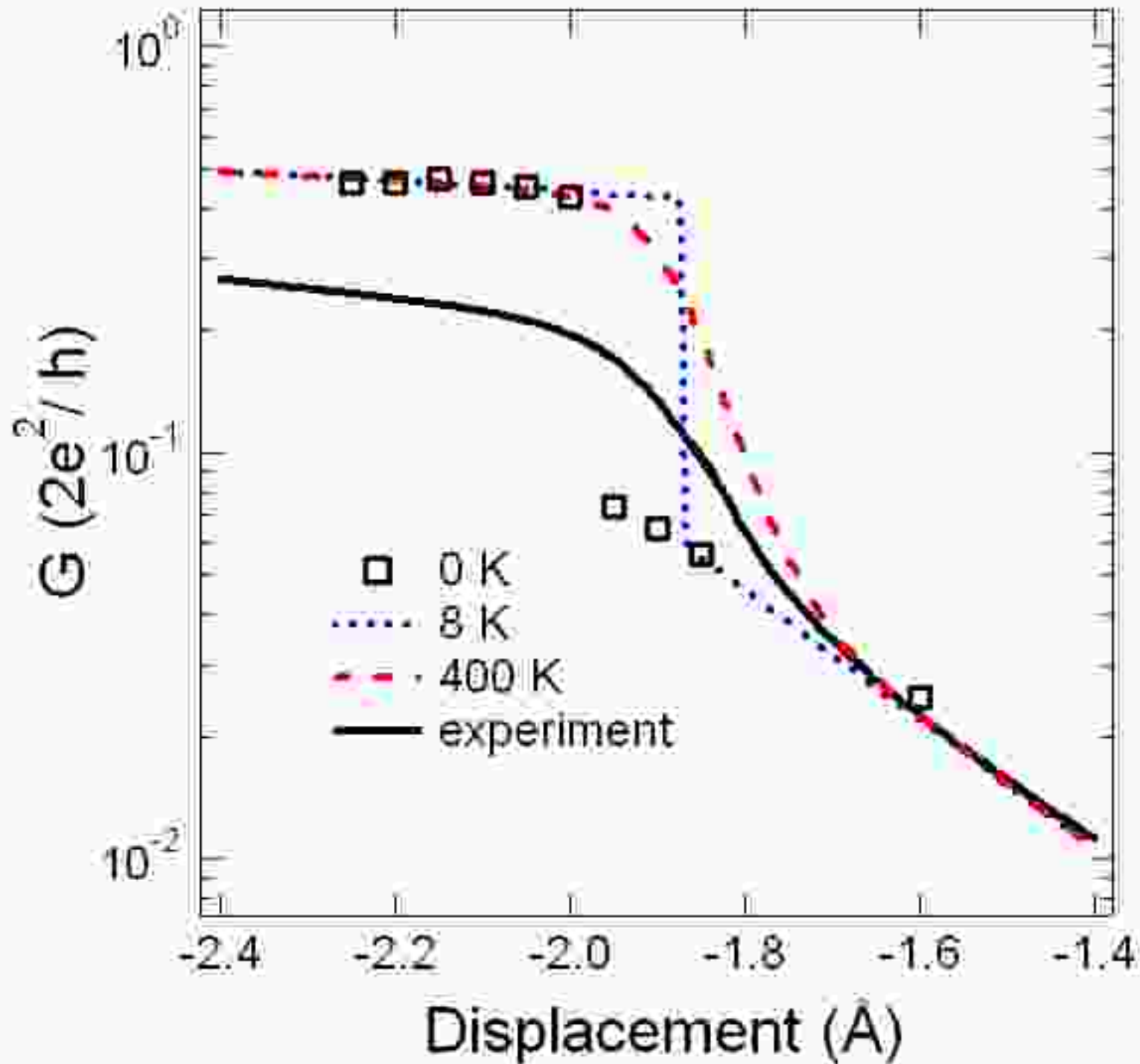




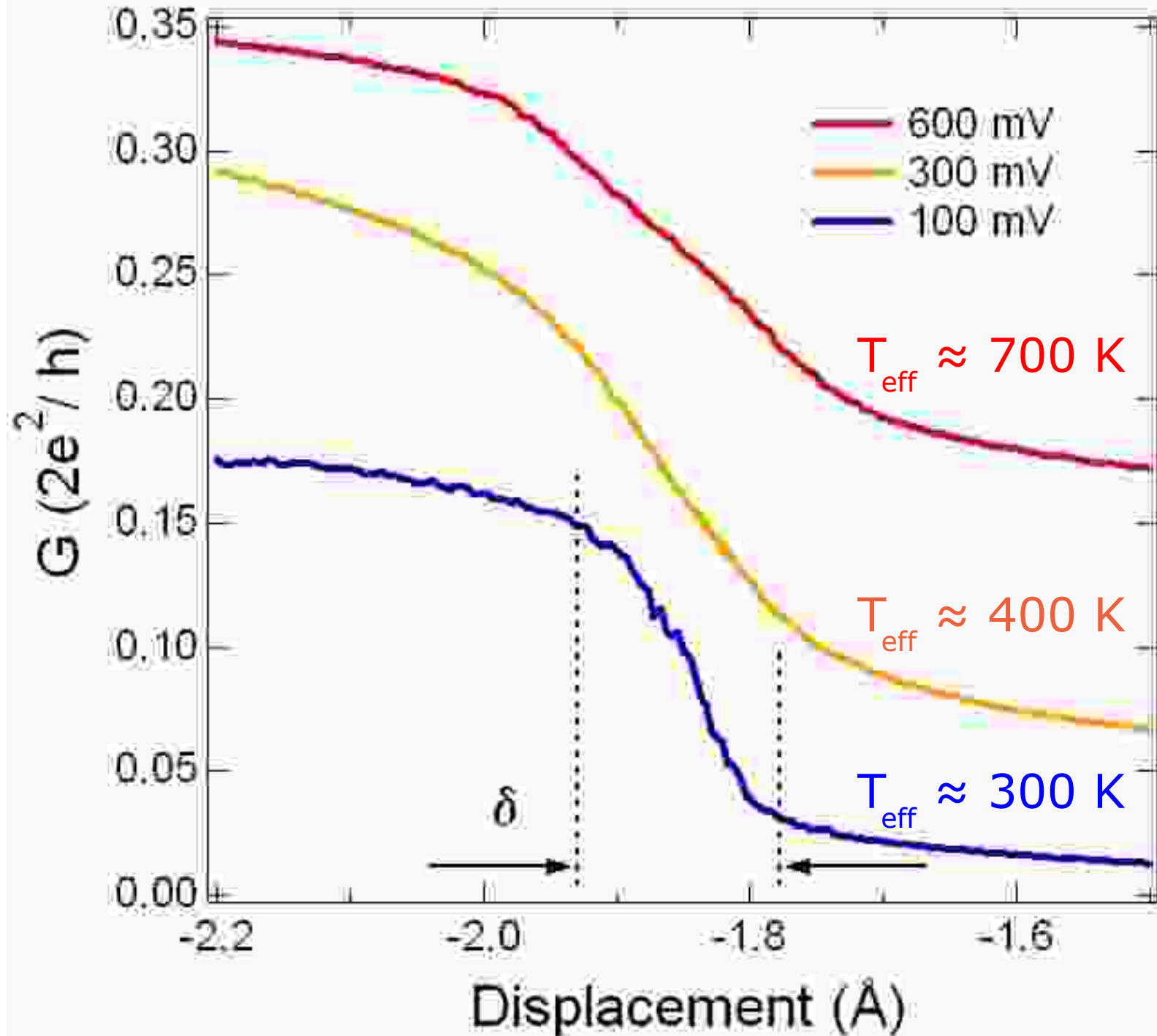
# Fluctuations in transition regime



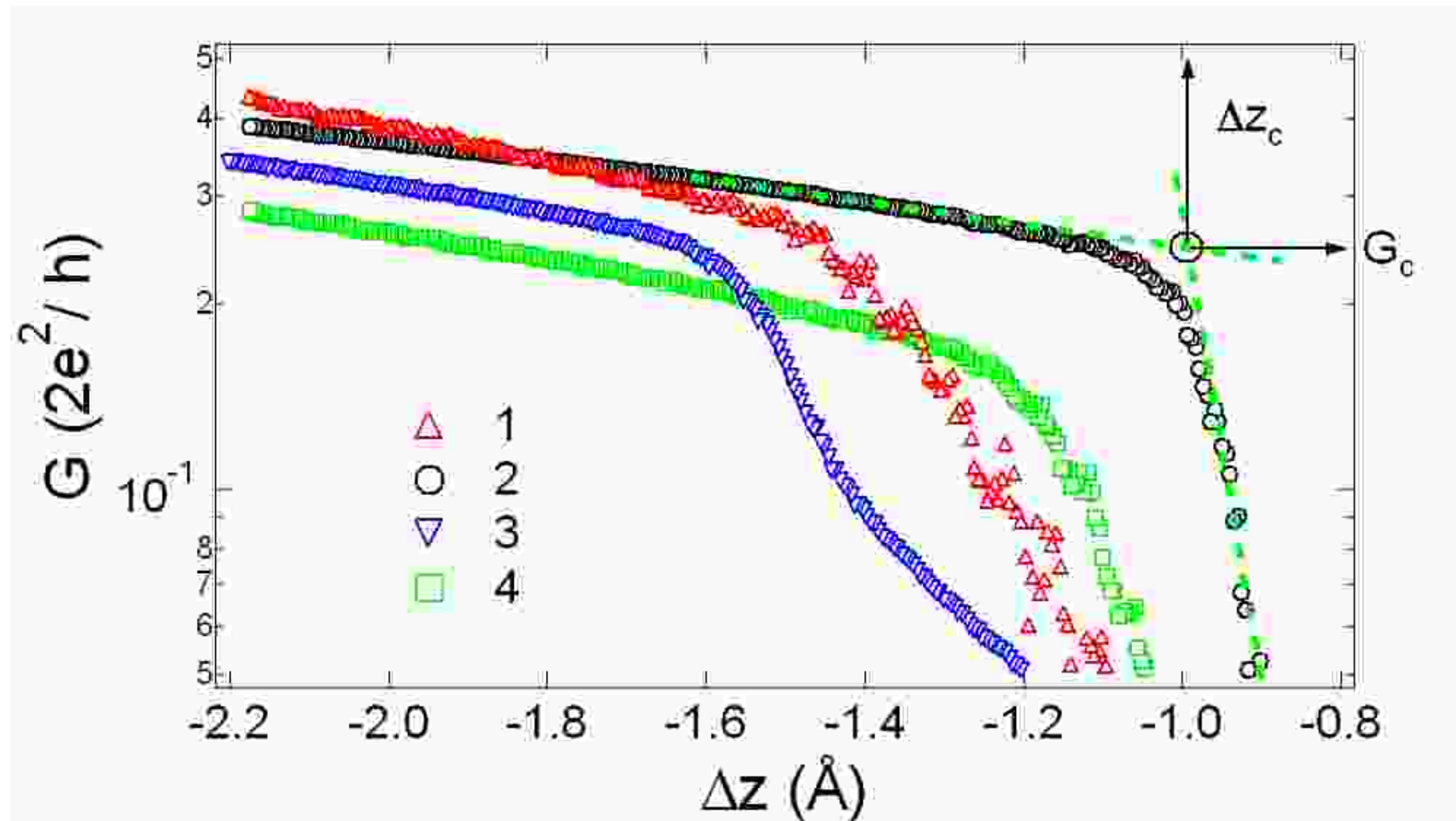
# Local heating

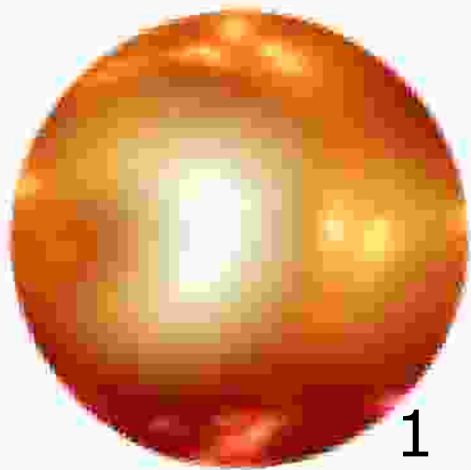


# More power – more heating



# Orientation-dependent conductance





1

$0.26 G_0$



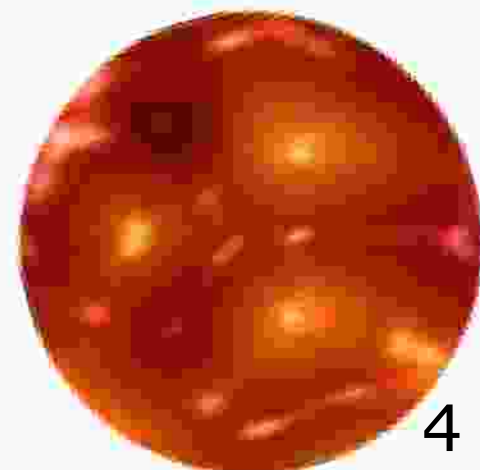
2

$0.25 G_0$



3

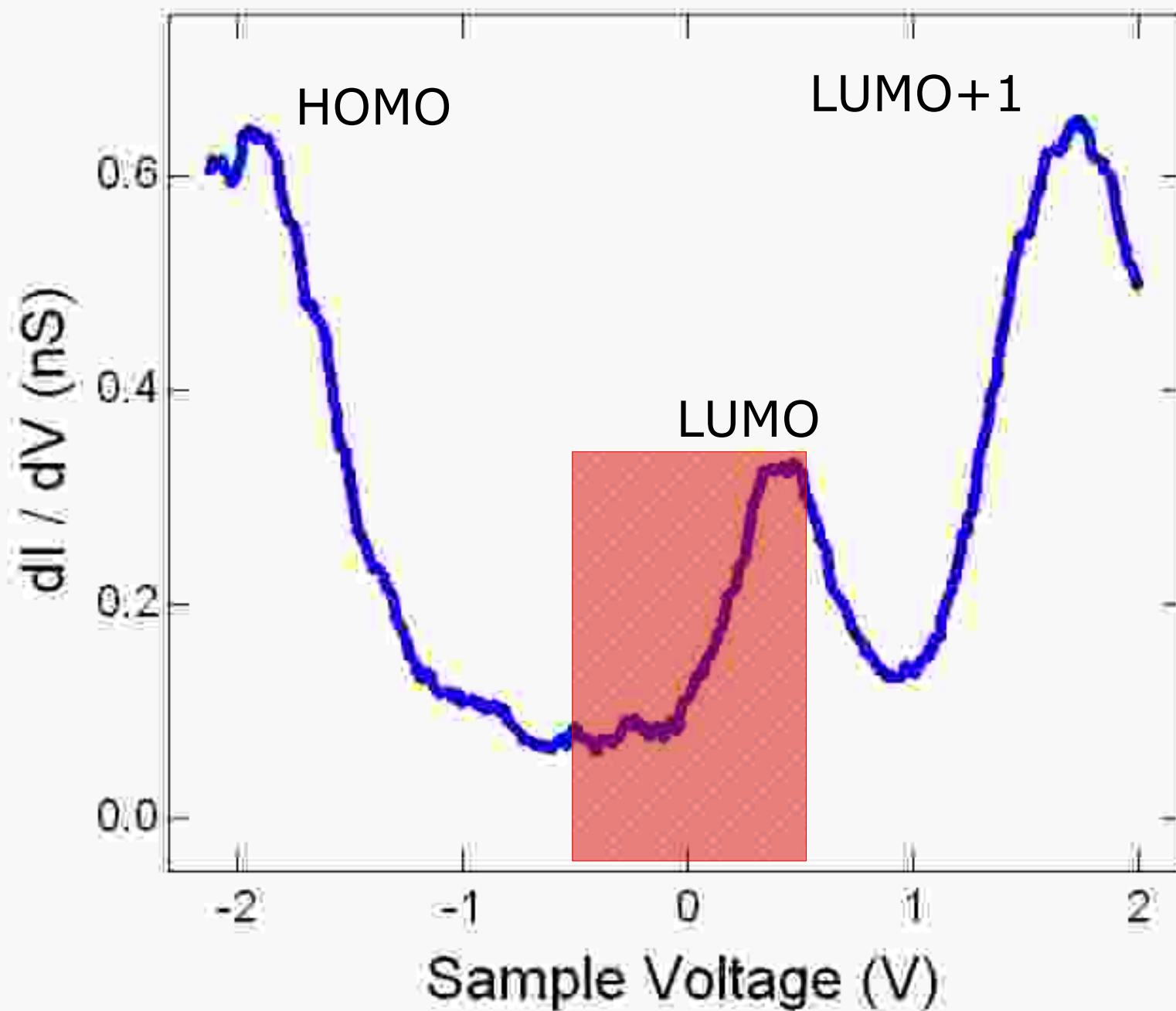
$0.26 G_0$



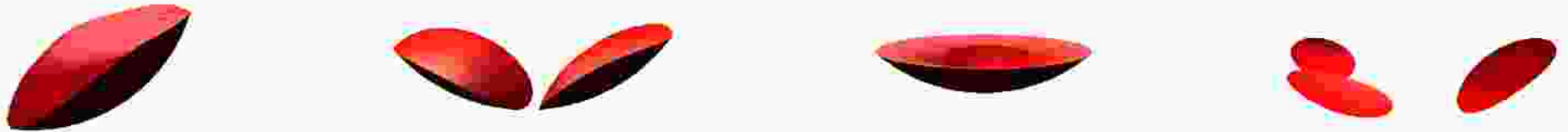
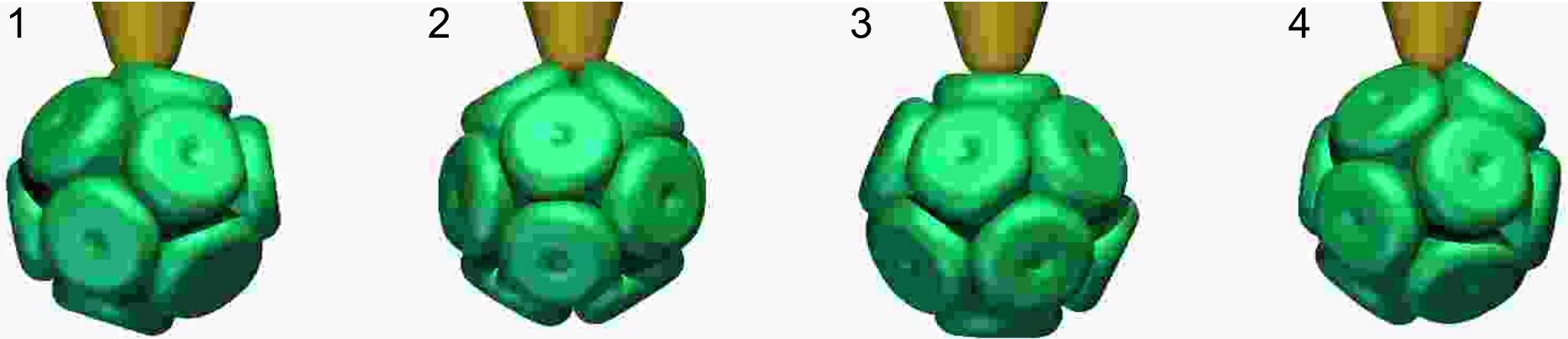
4

$0.17 G_0$

# Spectroscopy of molecular orbitals



# Overlap of orbitals

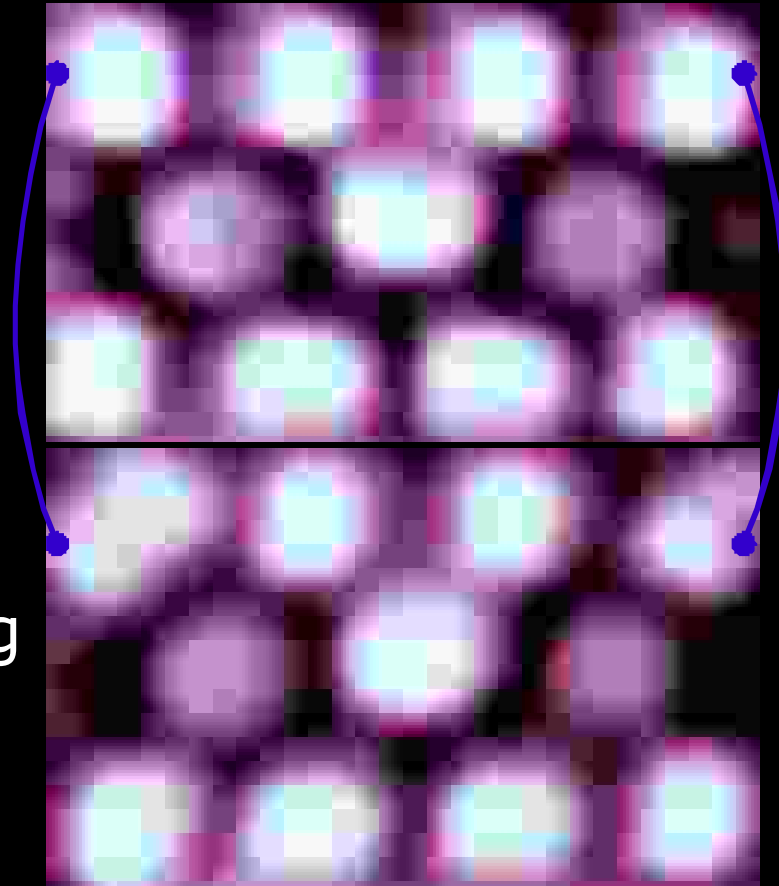


Conducting  
strongly



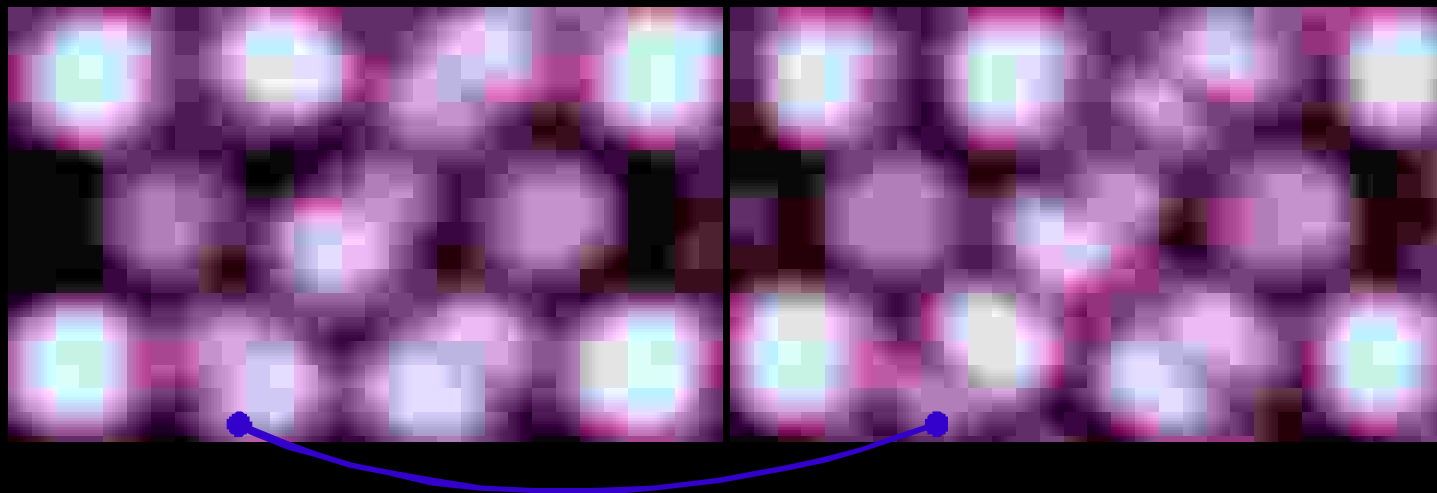
Conducting  
weakly

# Rotation in a single-molecule contact

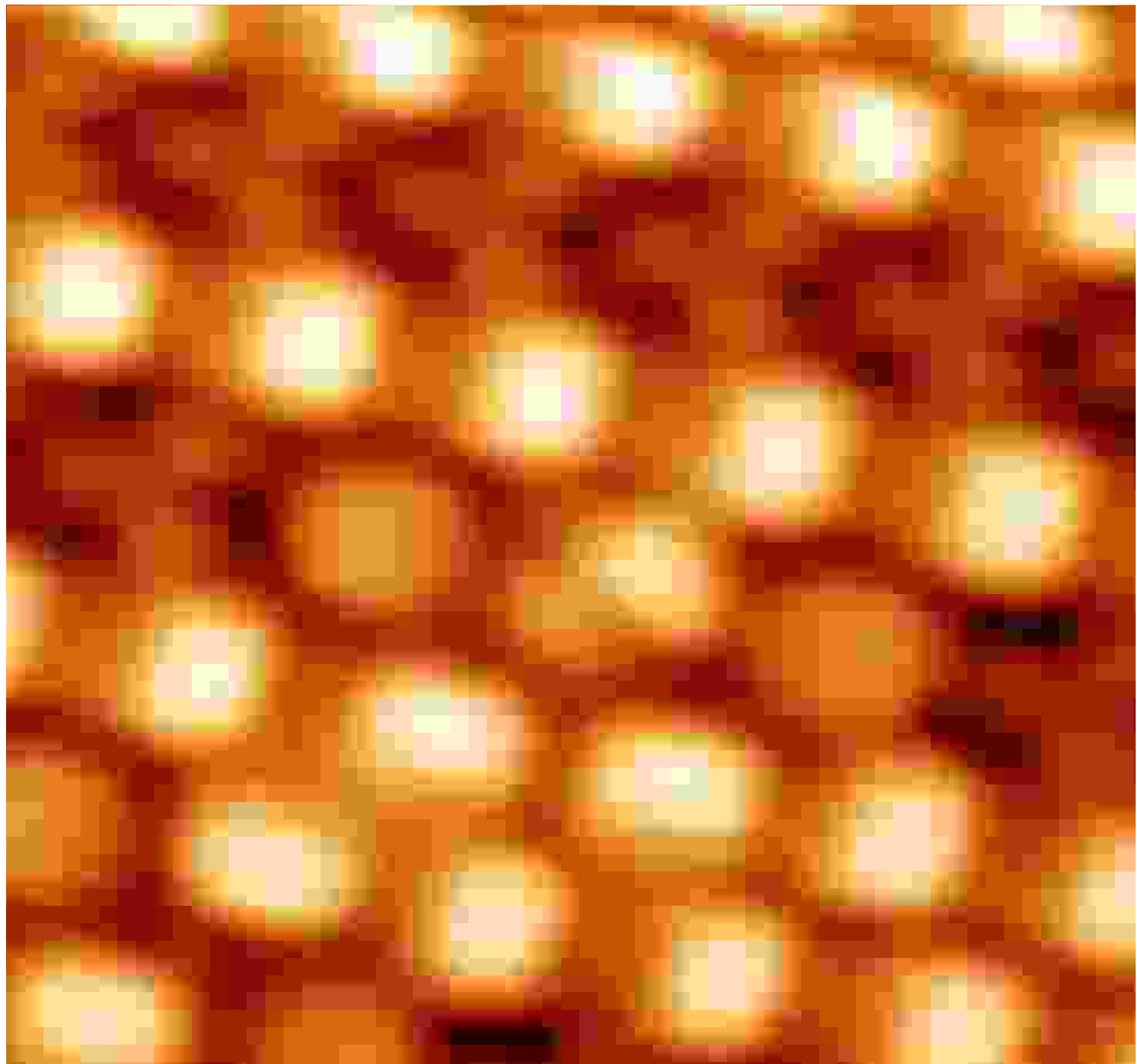


SFB 677:  
Function by Switching

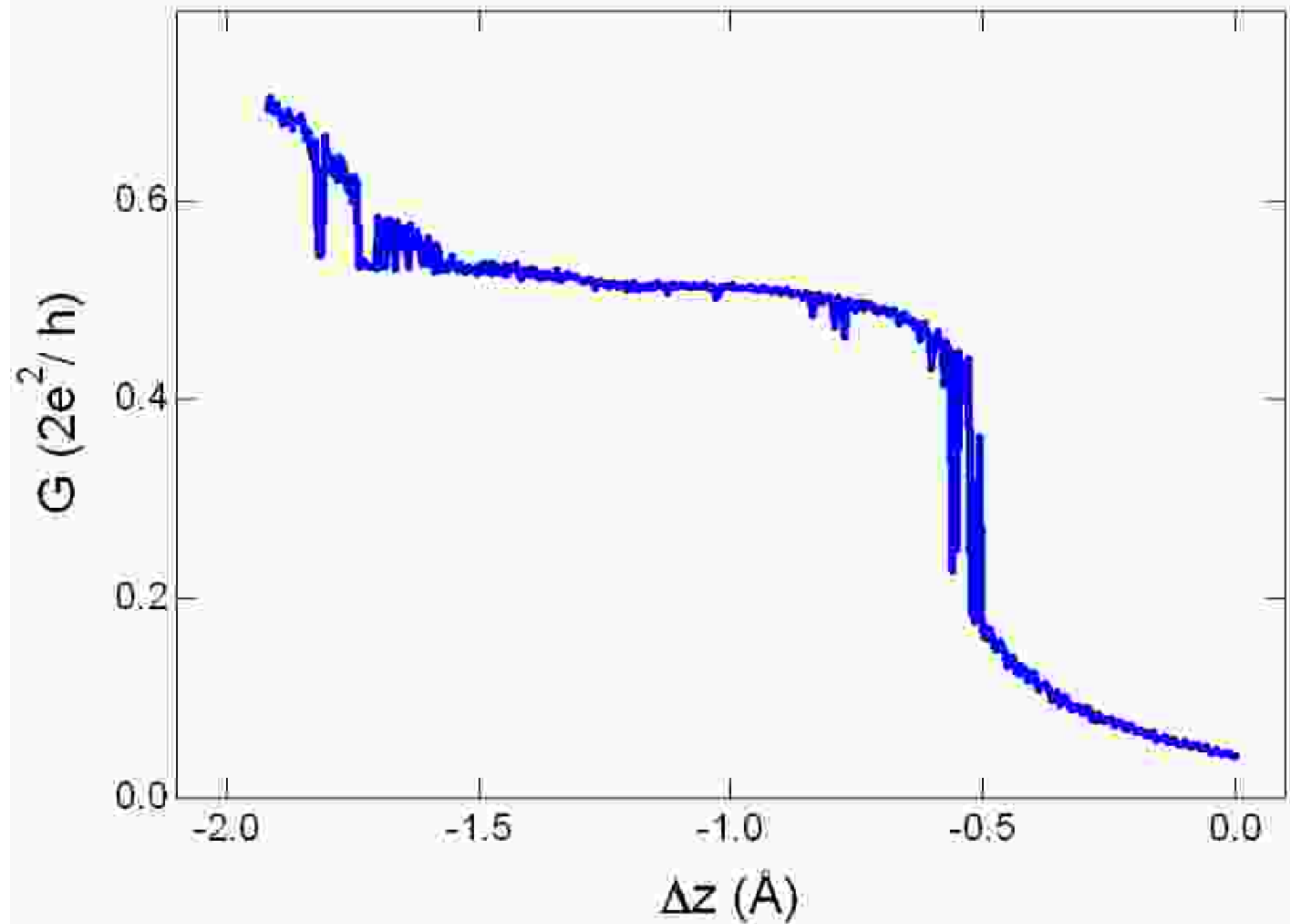
Néel, Limot, Kröger, Berndt  
PRB **77**, 125431 (2008)







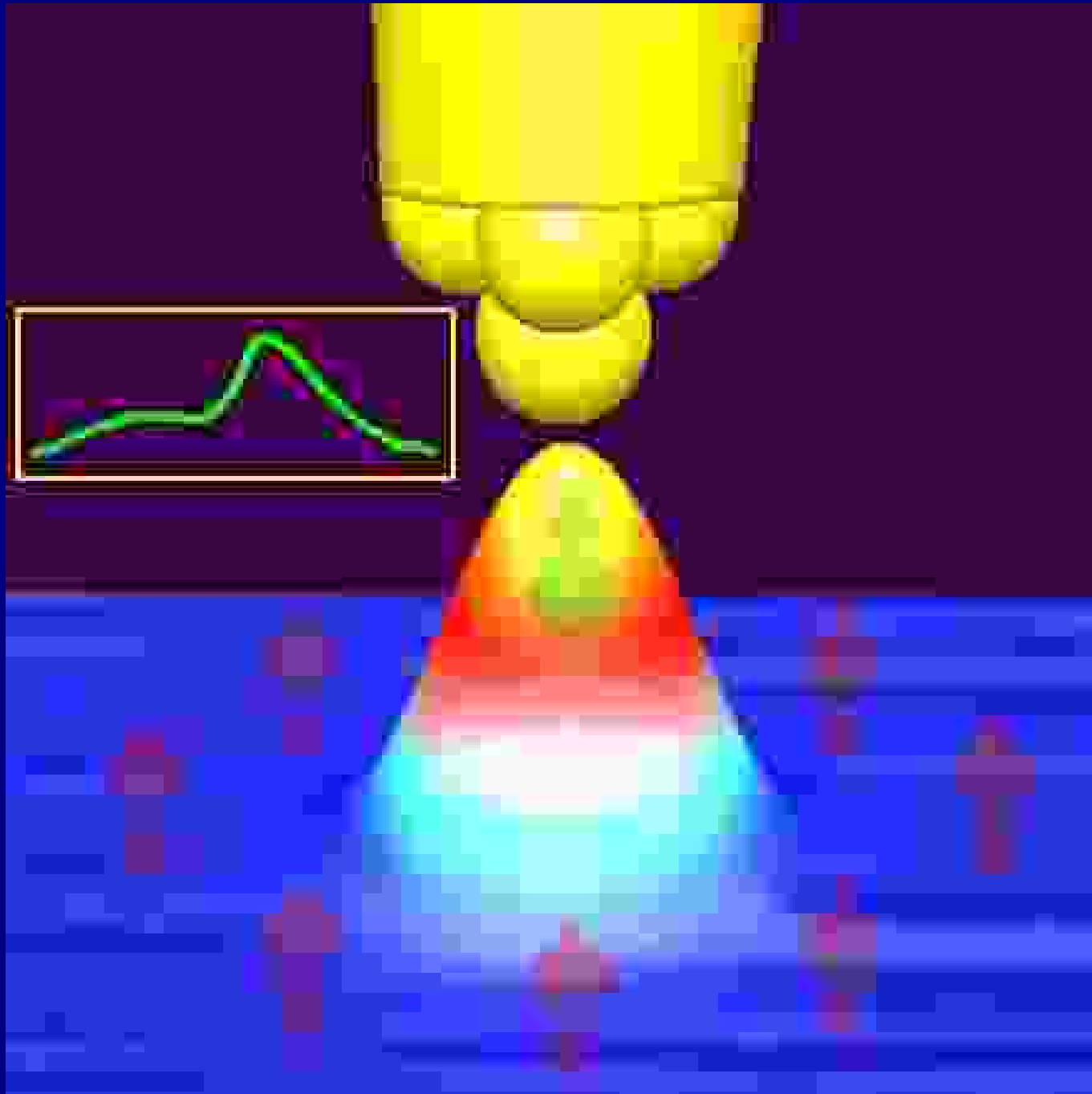
# Threshold behaviour



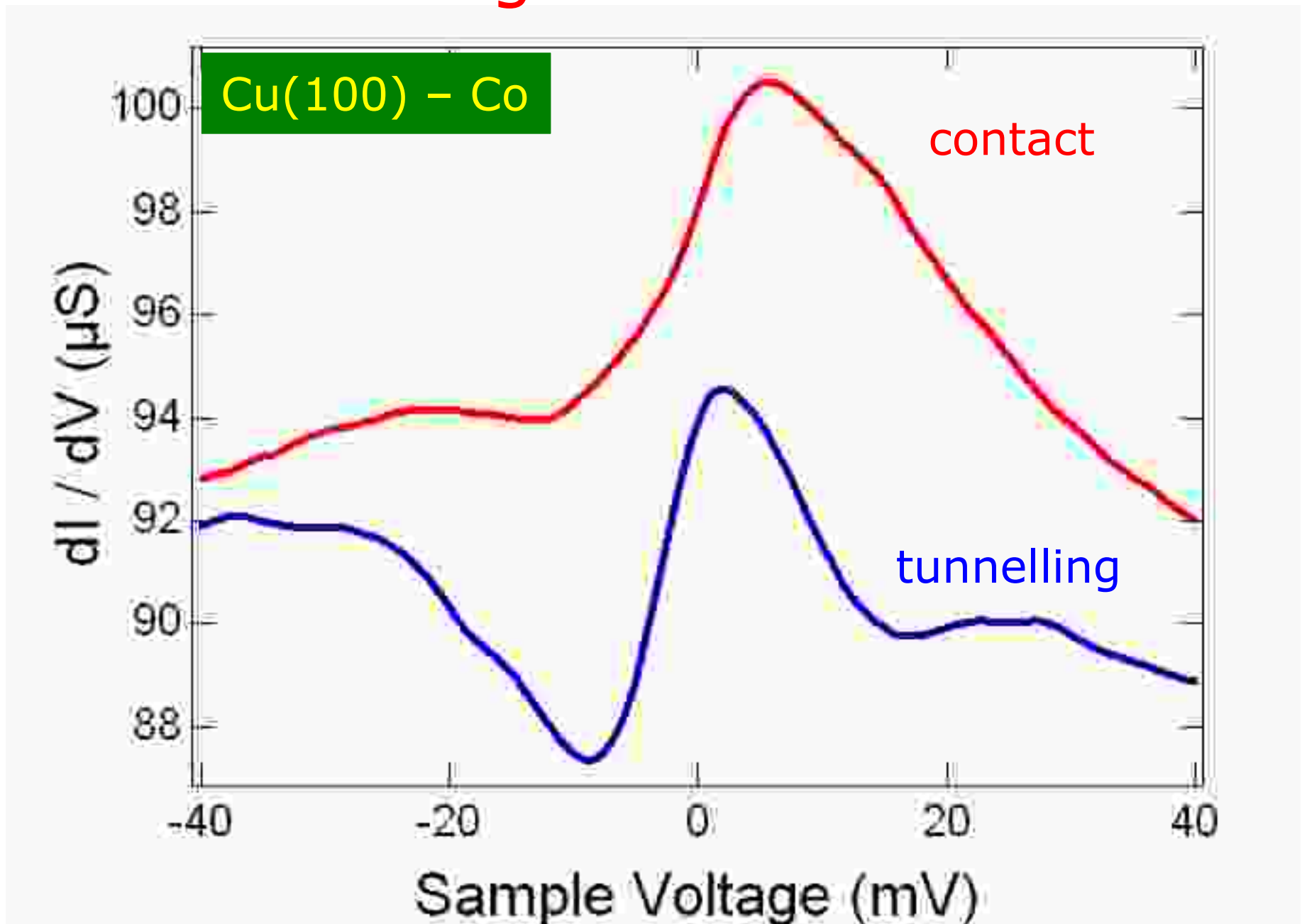
# Controlled contact to magnetic atoms

SFB 668: Magnetism from the single atom  
to the nanostructure

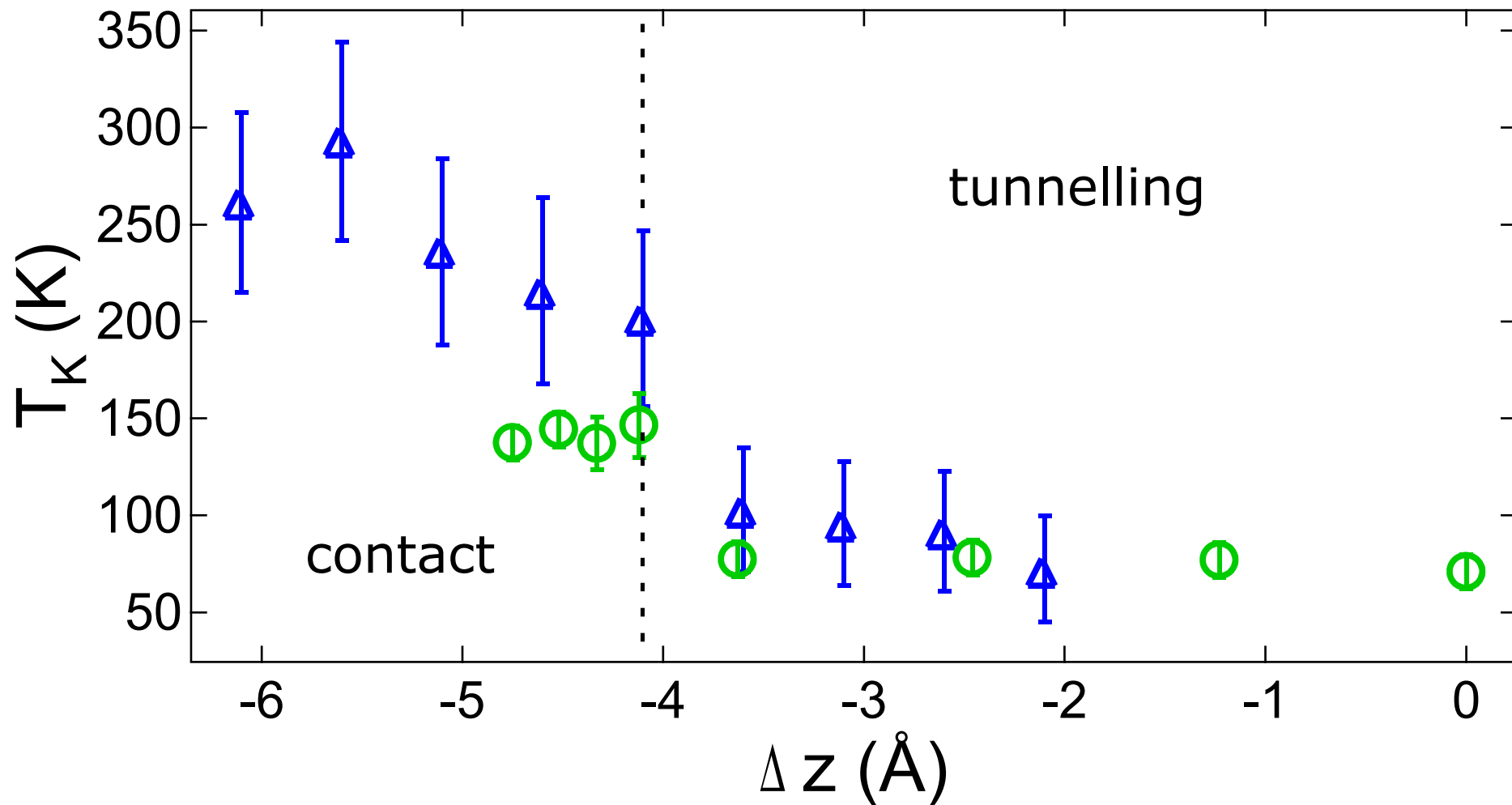
# Kondo effect of magnetic impurities

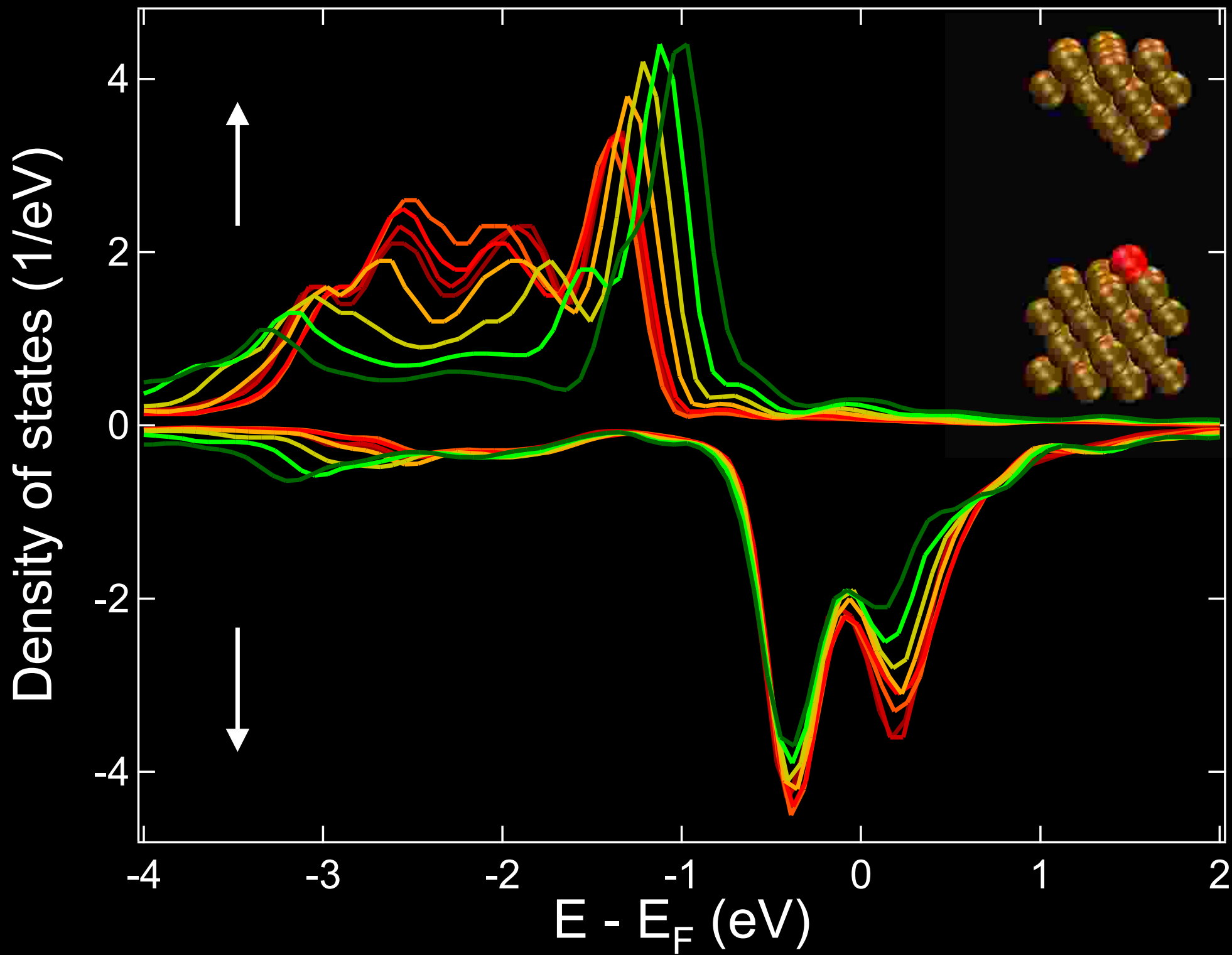


# Broadening of Kondo resonance



# Increase of Kondo temperature





## Spin-integrated transport

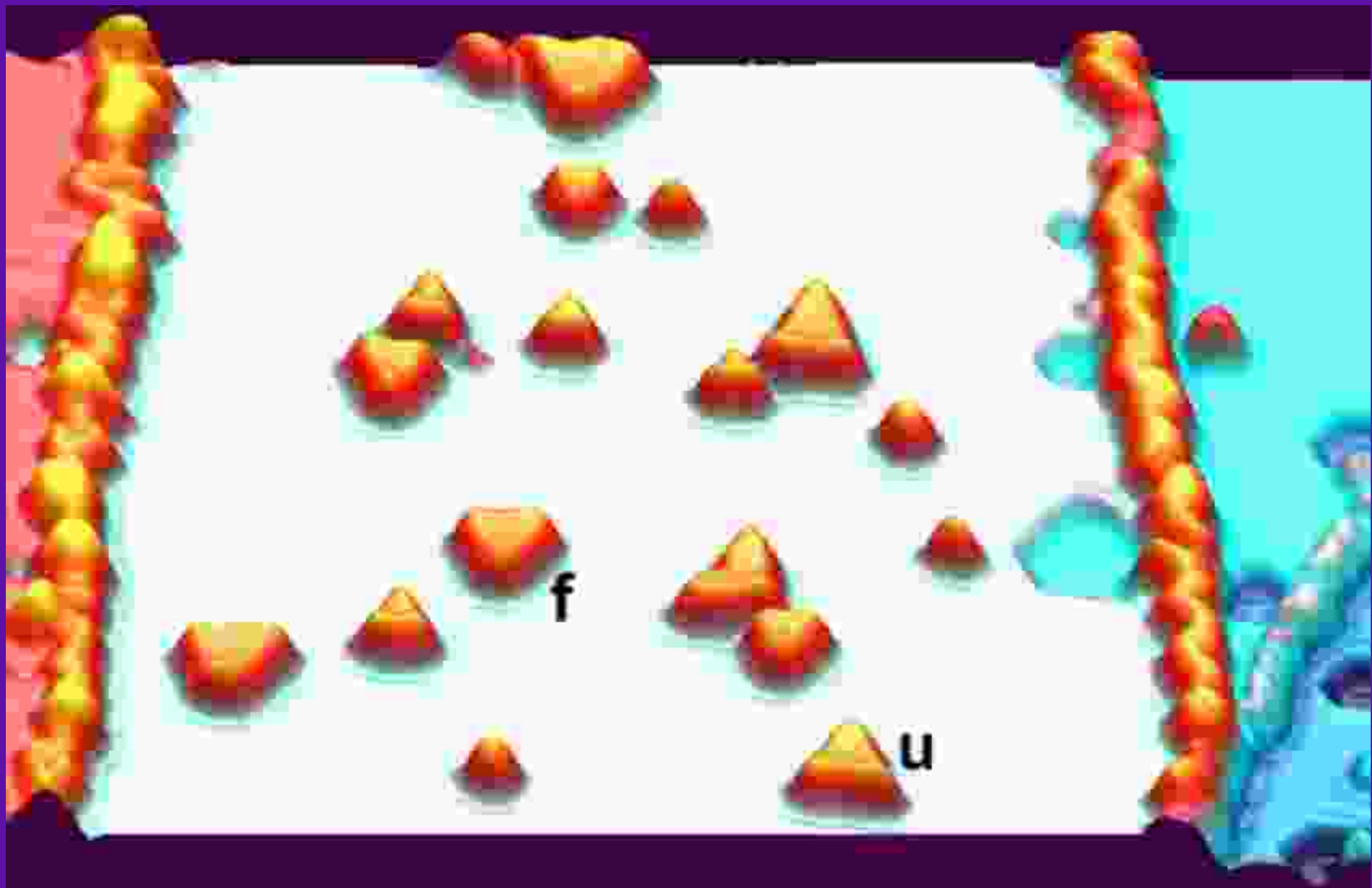
$$G = \frac{2e^2}{h} \sum_i \tau_i$$

## Spin-polarized transport

$$G = \frac{e^2}{h} \left( \sum_i \tau_i^\uparrow + \sum_i \tau_i^\downarrow \right)$$



# Cobalt islands on Cu(111)



# Electron transport through single magnetic atom

Co atom



Co island

Cu(111)



Electrode combinations:

Cu – Co – Cu

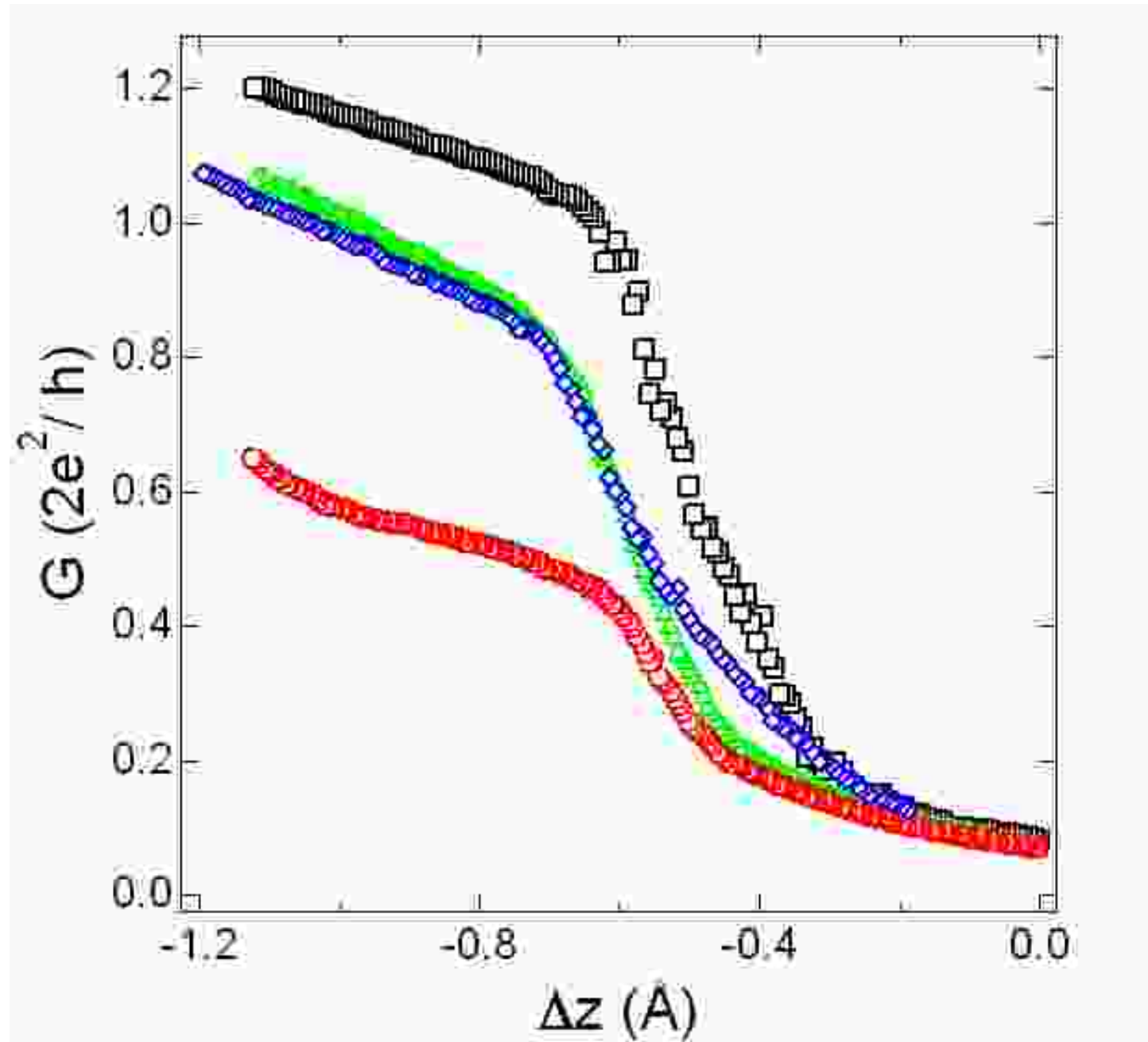
Cu – Co – Co

Ni – Co – Co

Cu - Co - Cu:  $\approx 1.0 G_0$

Cu - Co - Co:  
Ni - Co - Cu:  $\approx 0.8 G_0$

Ni - Co - Co:  $\approx 0.5 G_0$



# Summary

Kröger, Néel, Limot, J. Phys.: Condens. Matter, at press

## Outlook

- Extension to other molecules
- Time-resolved fluctuations
- Vibration spectroscopy
- Spin-polarized transport