Tin-Phthalocyanine on Ag(111): A Molecular Switch & Single Molecule Contacts

J. Kröger, University of Kiel

Acknowledgements

Experiment

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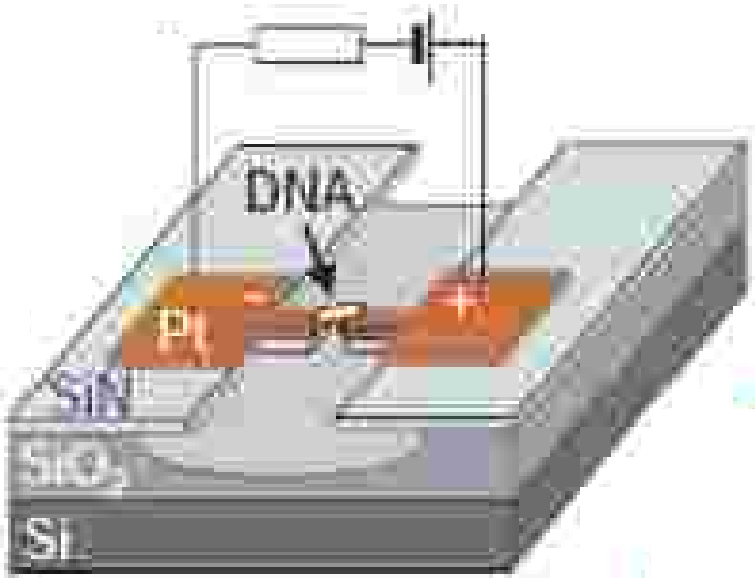
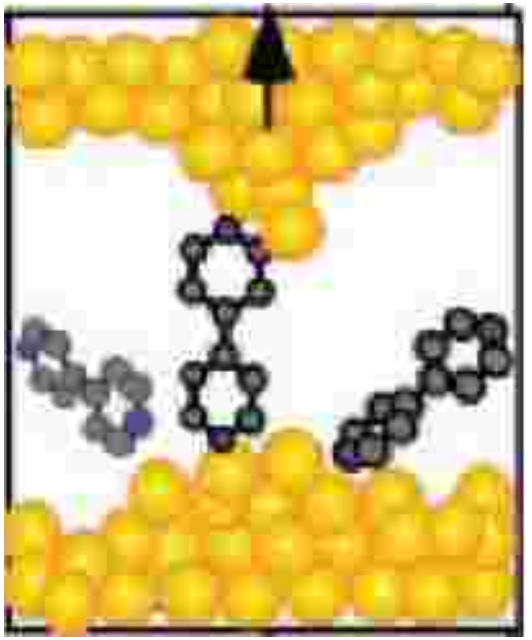
Theory

A. Garcia-Lekue, Th. Frederiksen (Spain)
M. Brandbyge (Denmark)
K. Palotas, W.A. Hofer (United Kingdom)

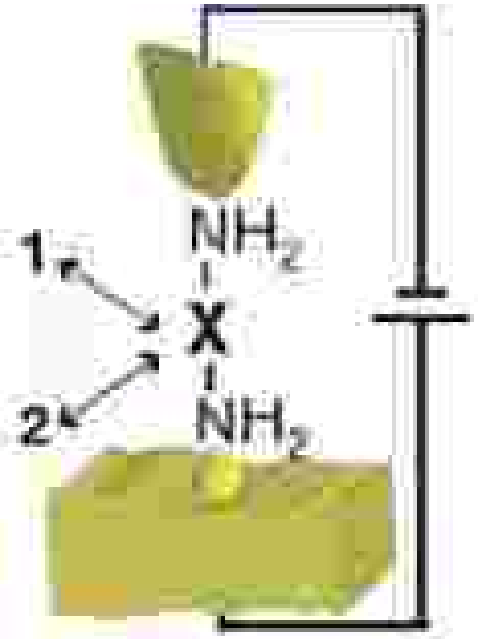
Probing the conductance of molecules



Porath *et al.*
Nature 2000



Xu and Tao
Science 2003



Venkataraman *et al.*
Nature 2006

Number of molecules in the junction?

Geometry of the junction?

Orientation of the molecule?

Single-Atom and Single-Molecule Contact using STM

2008: Temirov *et al.*, Nanotechnology **19**, 065401 (PTCDA)
Schulze, Franke *et al.*, PRL **100**, 136801 (C_{60})

2007: Néel, Kröger *et al.*, PRL **98**, 065502 (C_{60})

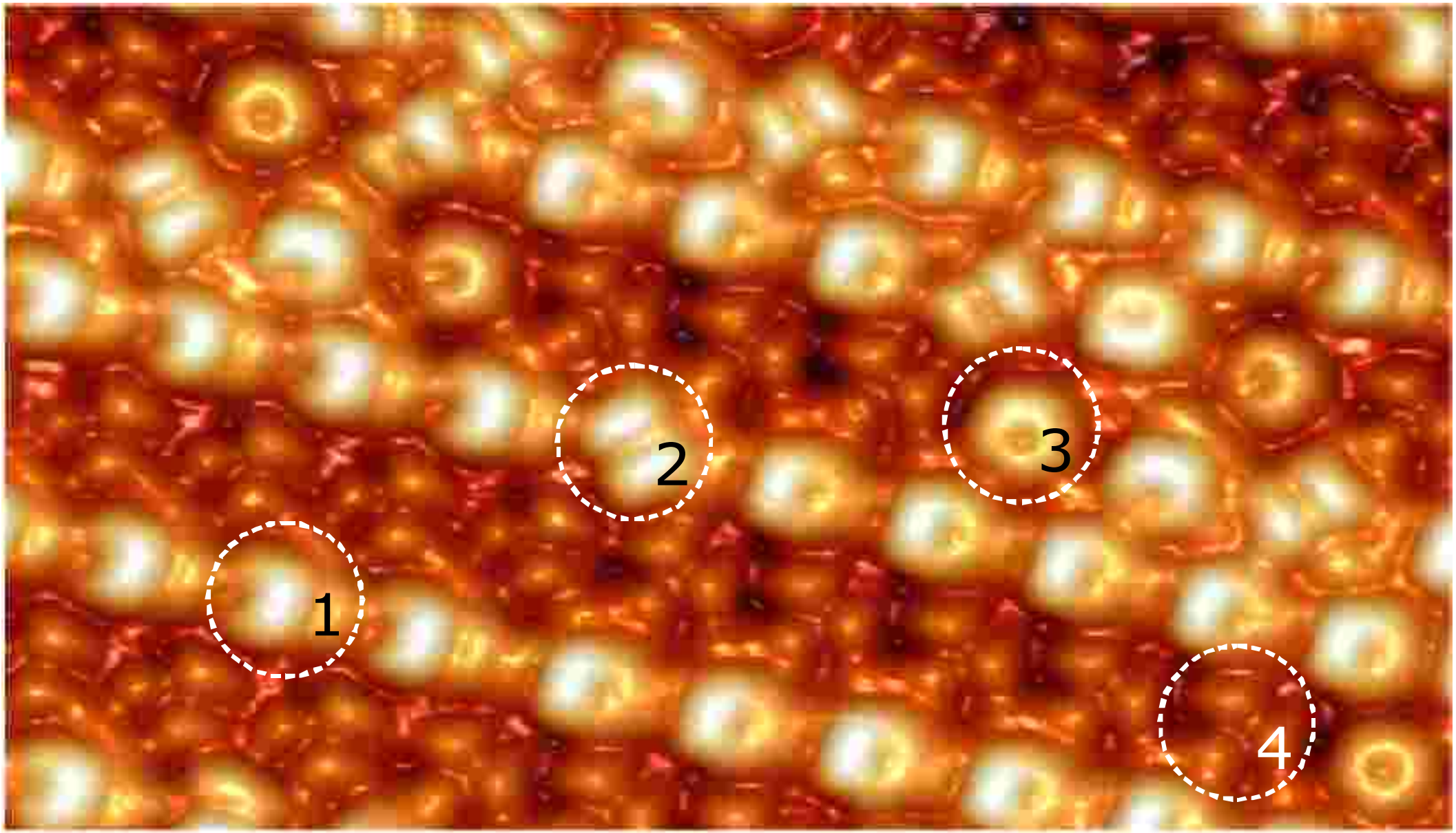
2005: Limot, Kröger *et al.*, PRL **94**, 126102 (Ag, Cu atoms)

2001: Moresco *et al.*, PRL **86**, 672 (Cu-TBPP)

1999: Bürgi, PhD Thesis, EPFL, Switzerland (Mn, Gd atoms)

1996: Yazdani *et al.*, Science **272**, 1921 (Xe atom)

1995: Joachim *et al.*, PRL **74**, 2102 (C_{60})



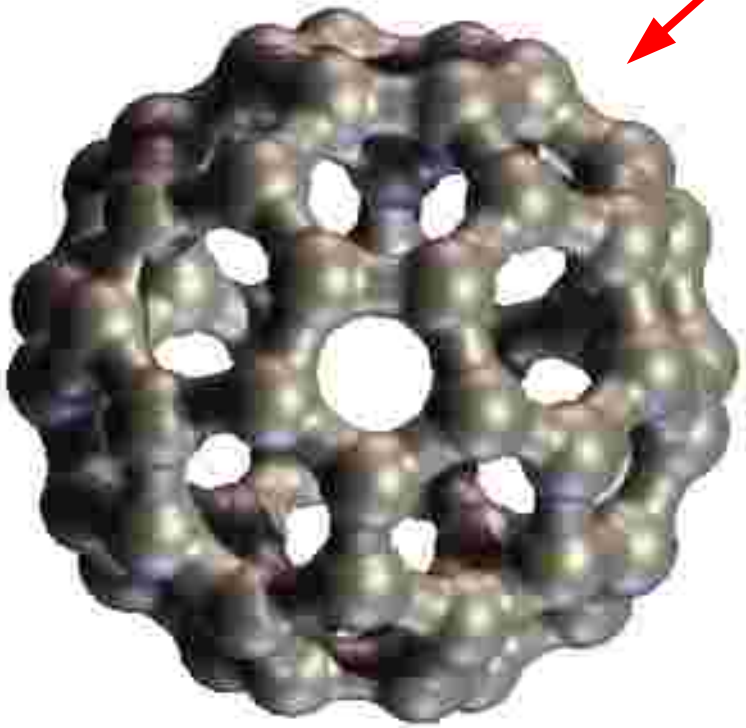
Cu(100) – C_{60}: 4 molecule orientations


1

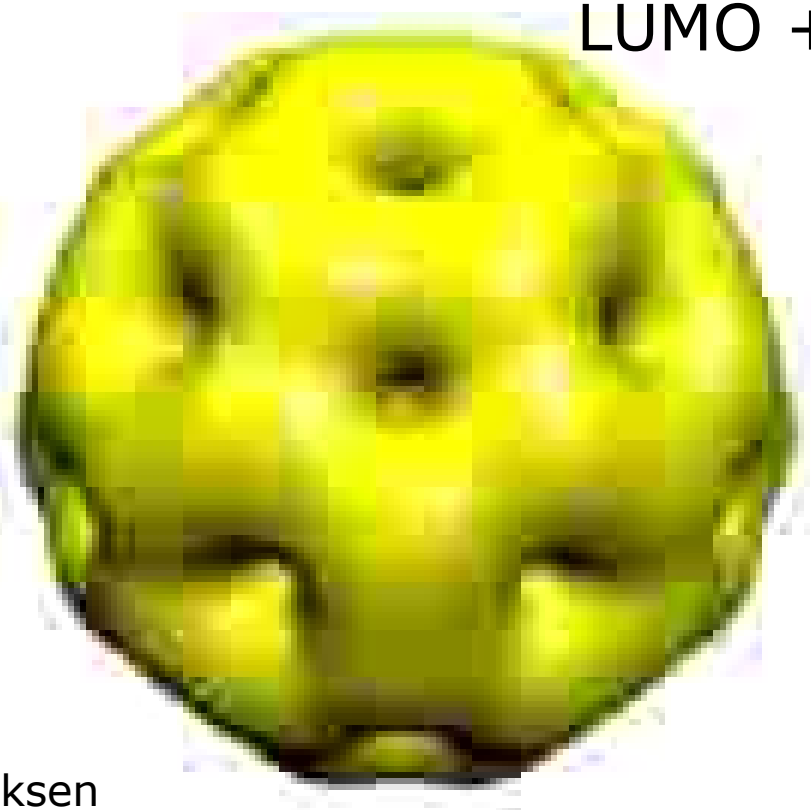

2


3


4

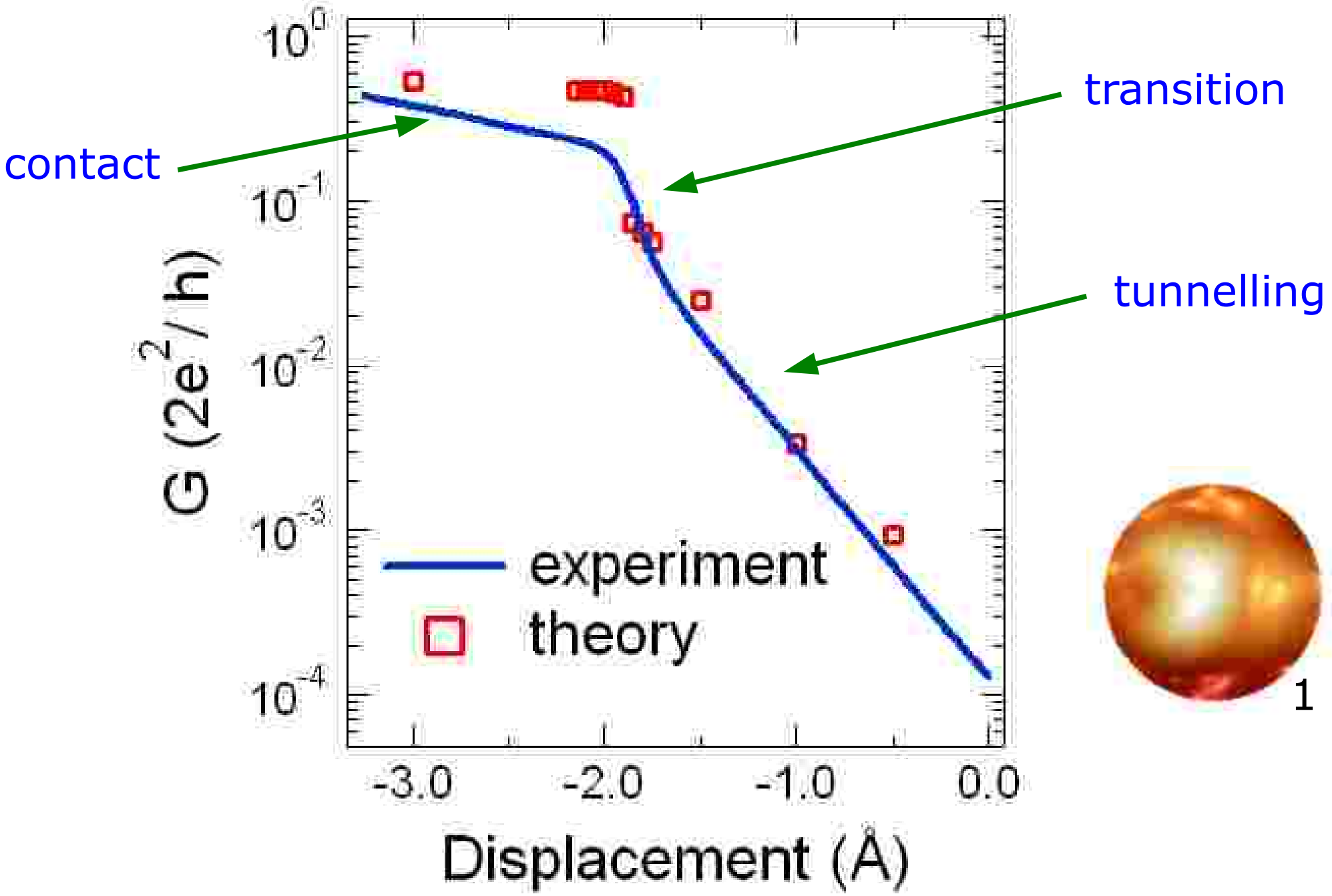


LUMO + 1



Th. Frederiksen
PhD Thesis (Technical University of Denmark, 2007).

Tip – Molecule Contact



1

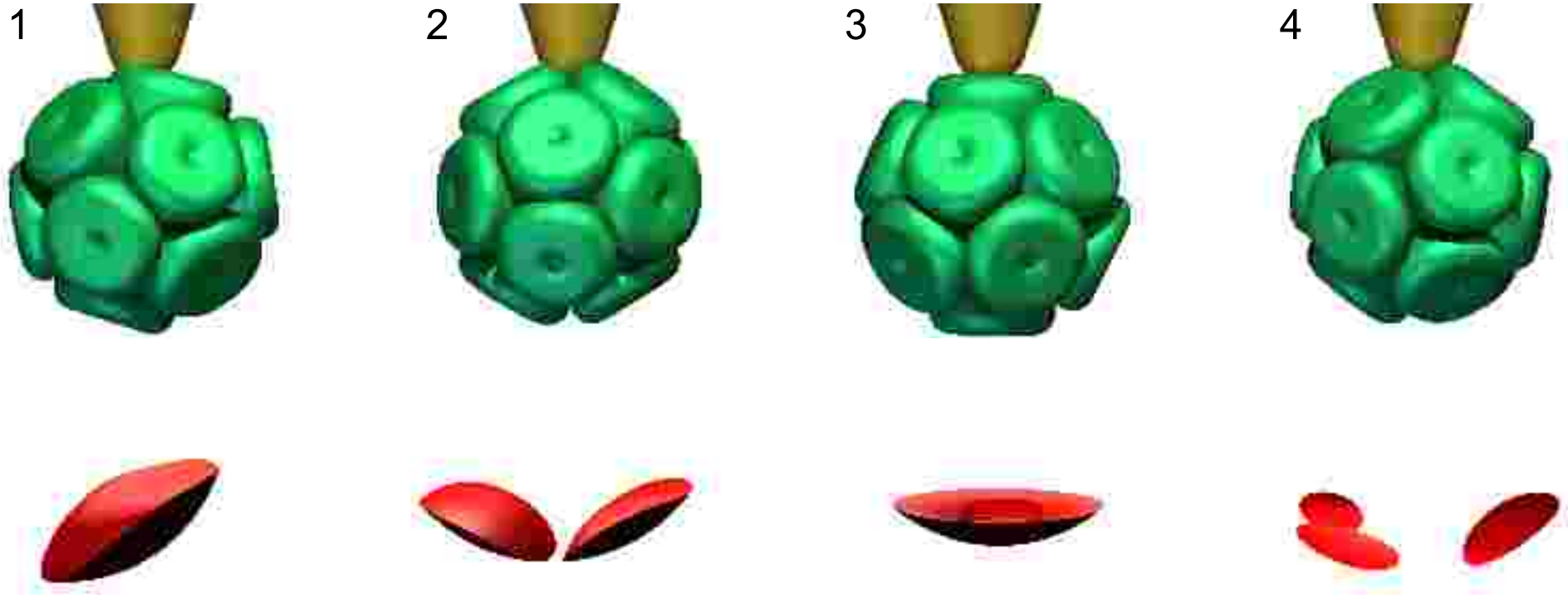
Néel, Kröger, Limot, Frederiksen, Brandbyge, Berndt, PRL **98**, 065502 (2007).

Orientation Dependence

0.26 G_0 0.25 G_0 0.26 G_0 0.17 G_0

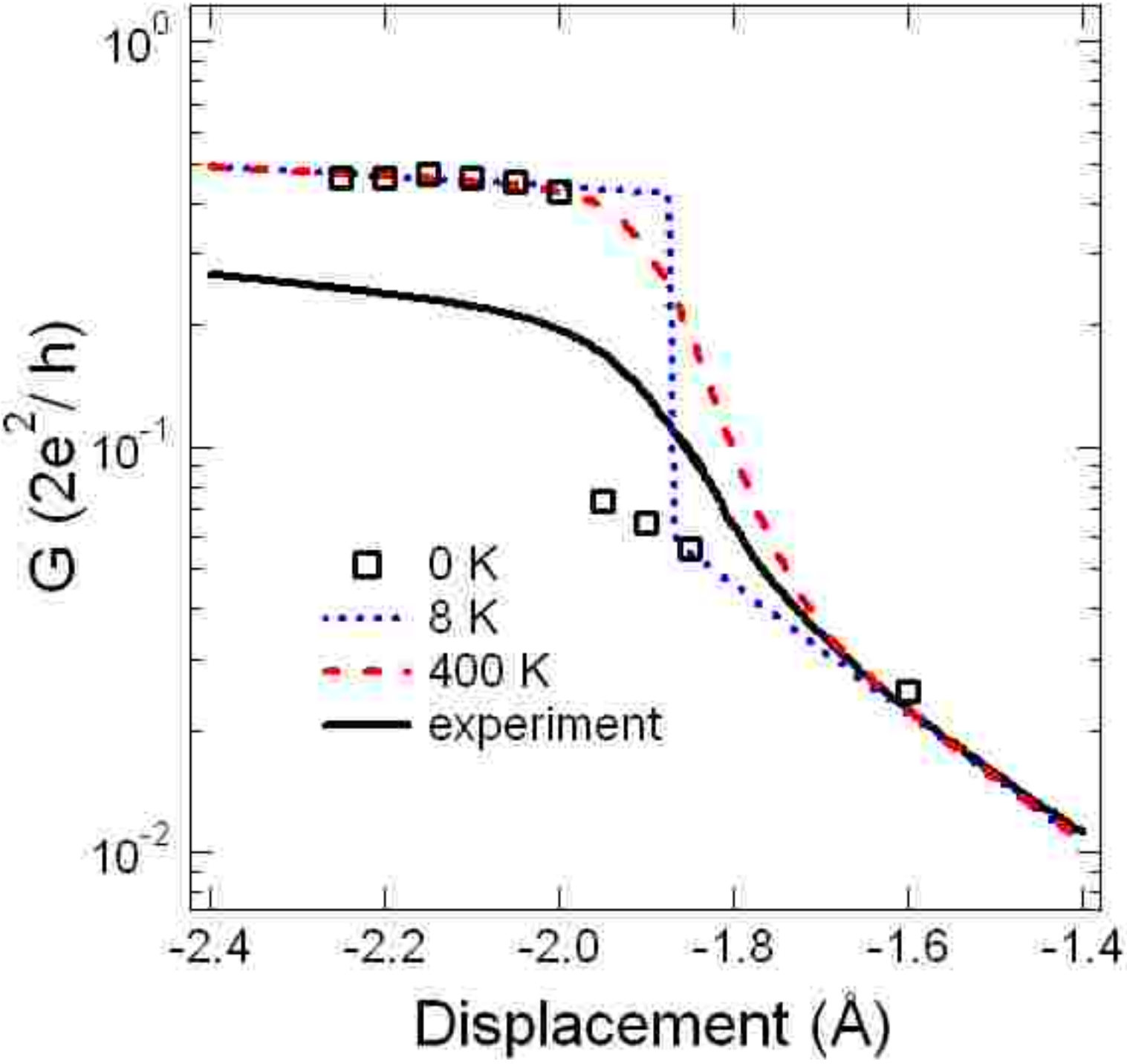
Néel, Kröger, Limot, Berndt, Nano Letters **8**, 1291 (2008).

Overlap of orbitals

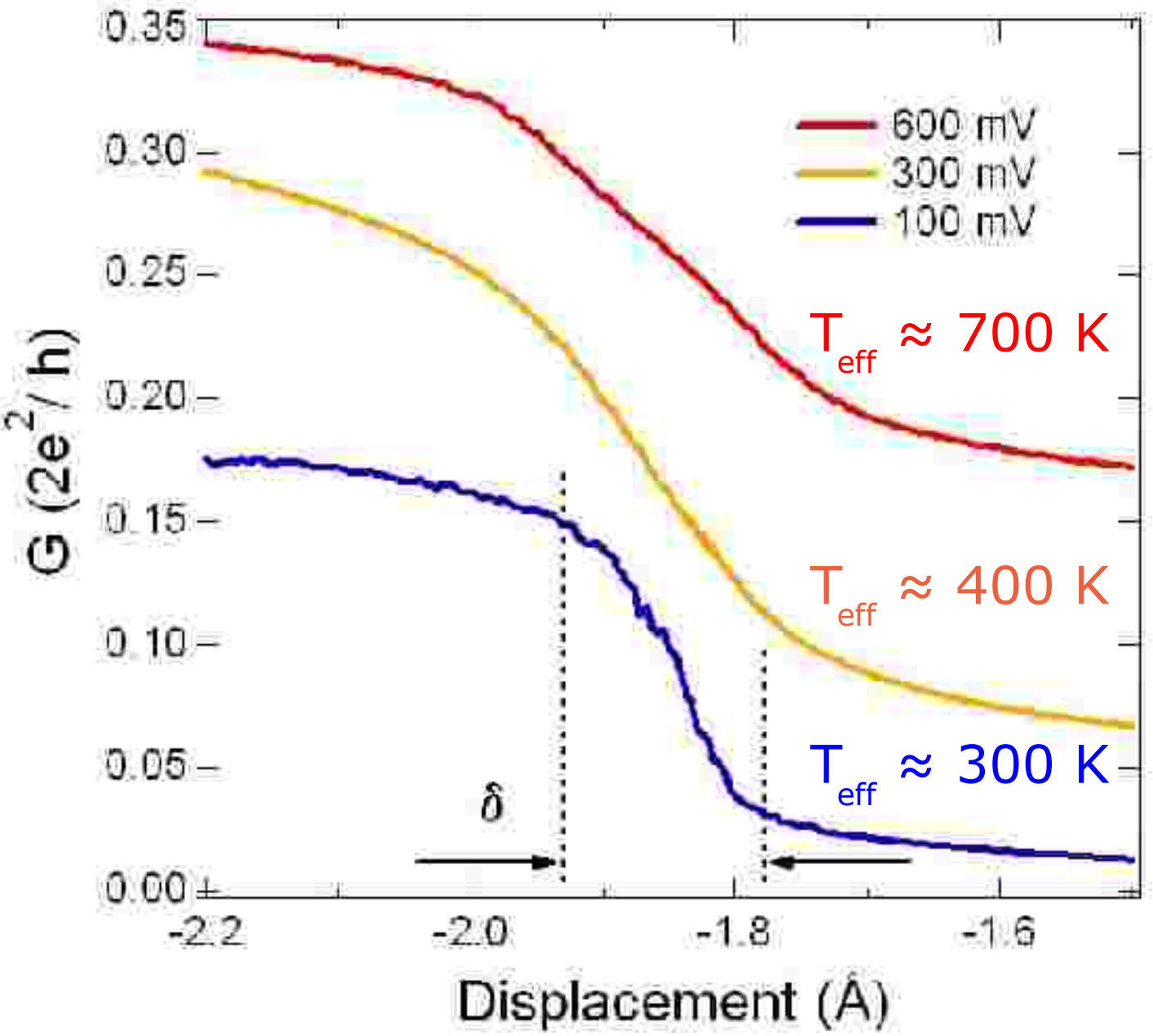


Conducting strongly → Conducting weakly

Local Heating

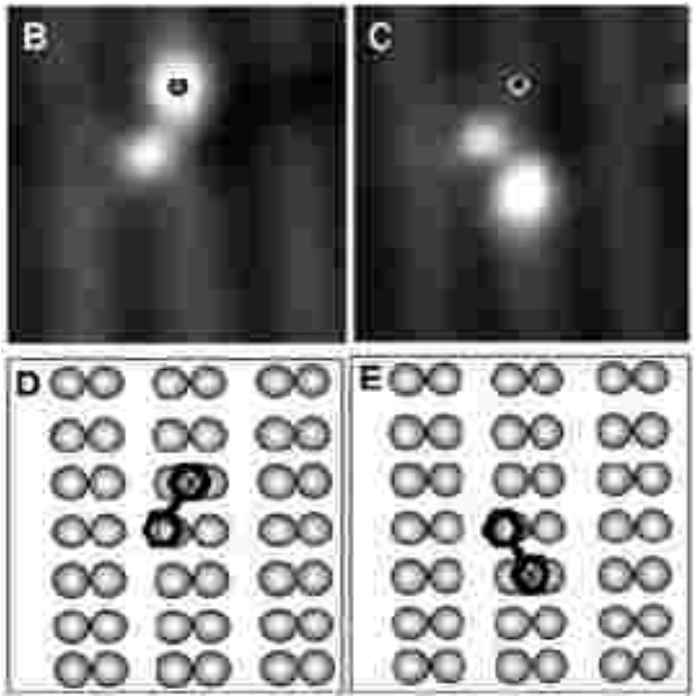


More power – more heating

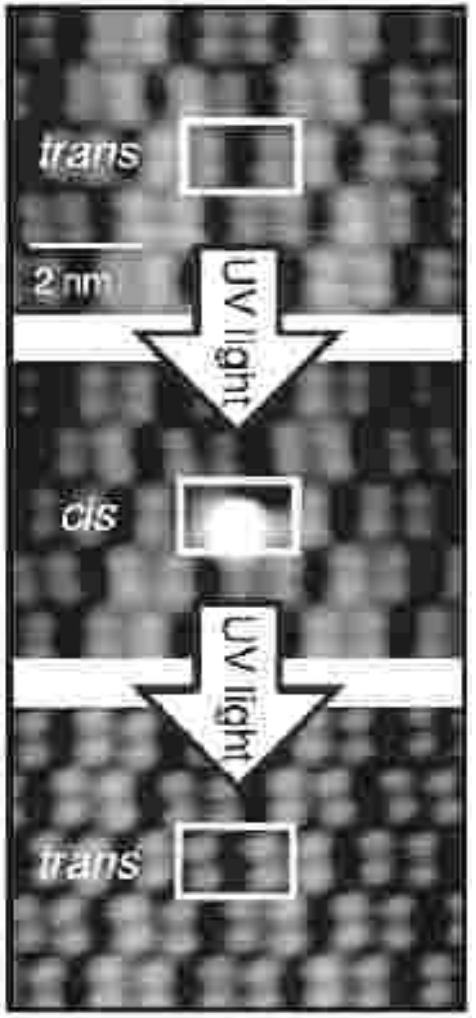


Kröger, Néel, Limot, J. Phys.: Condens. Matter **20**, 223001 (2008).

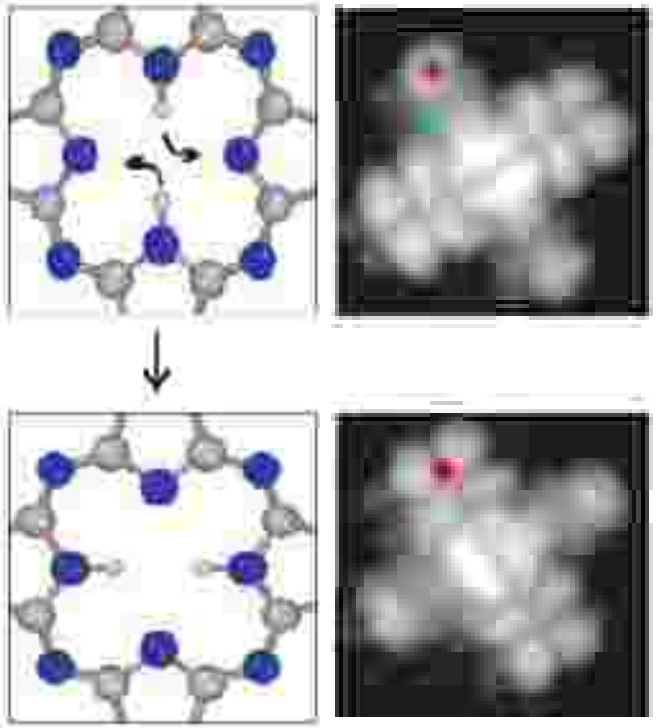
Some Molecular Switches



Lastapis et al.,
Science **308**, 1000 (2005).

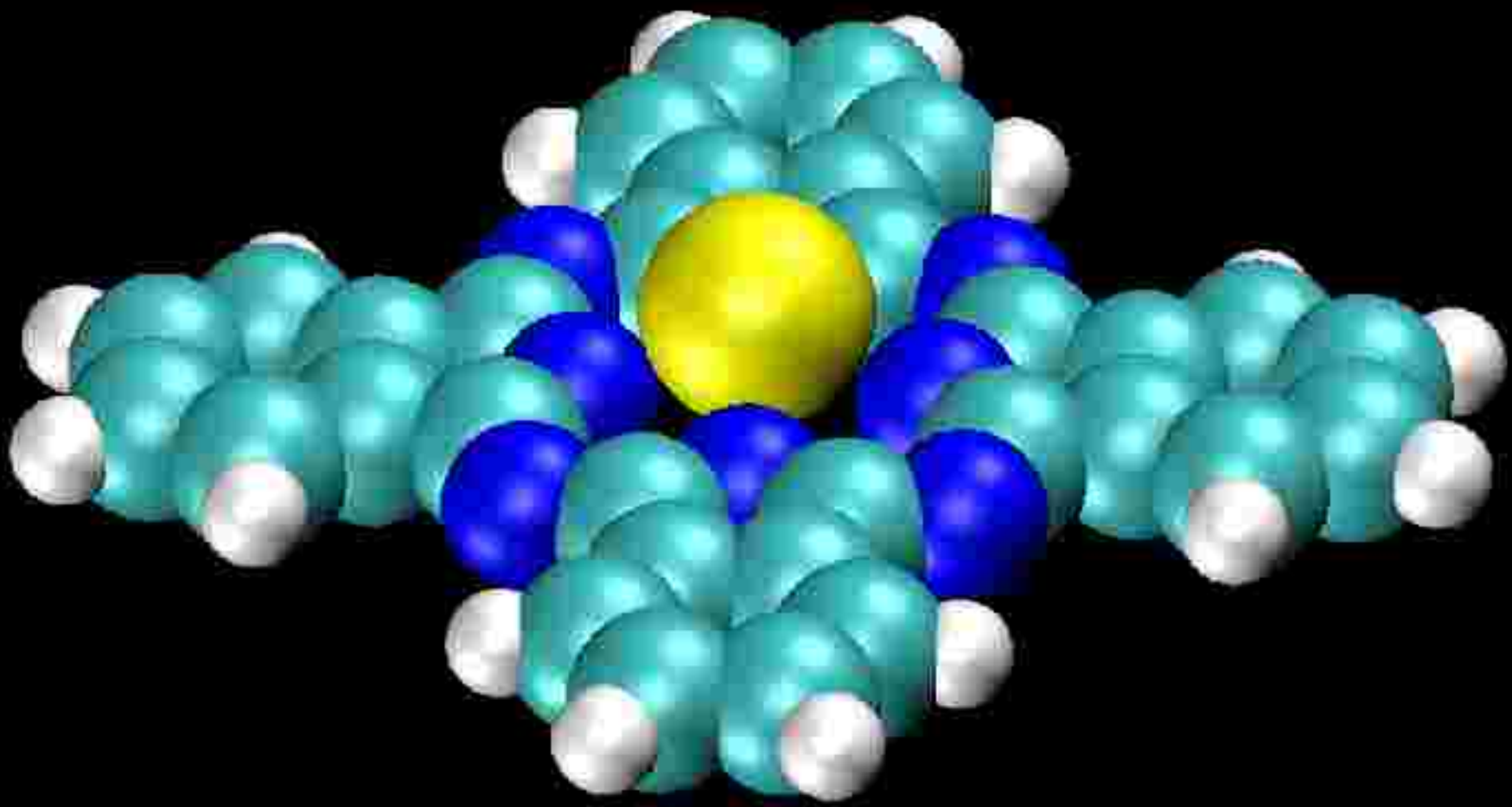


Comstock et al.,
Phys. Rev. Lett. **99**, 038301 (2007).



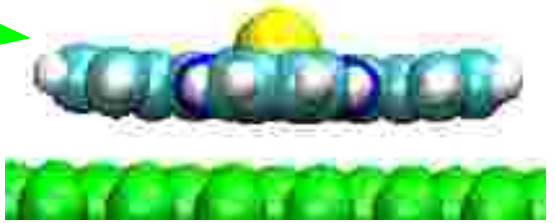
Liljeroth et al.,
Science **317**, 1203 (2007).

Tin Phthalocyanine



Adsorption on Ag(111)

down

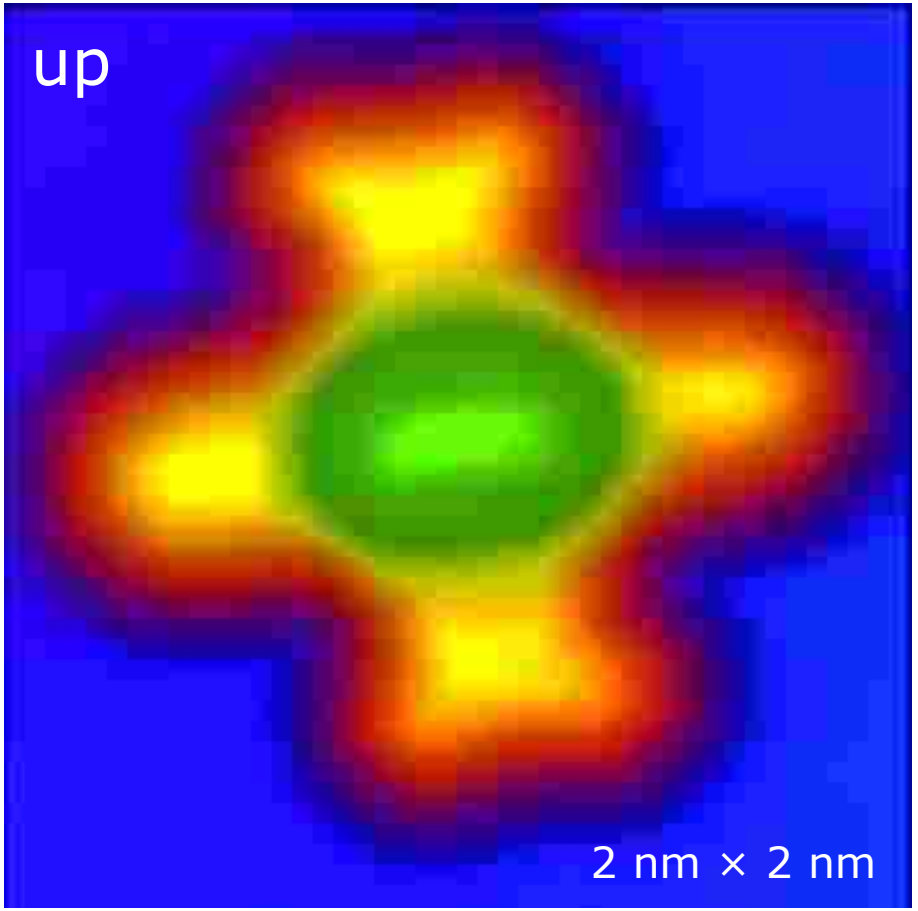


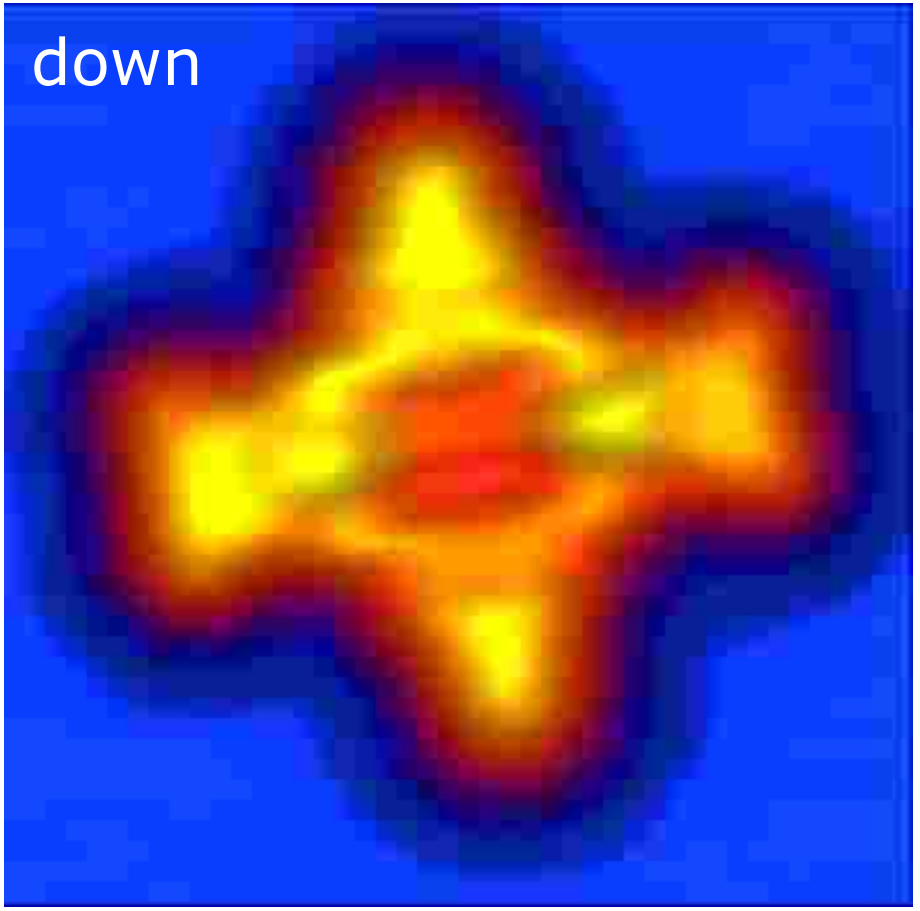
up

14 nm × 14 nm

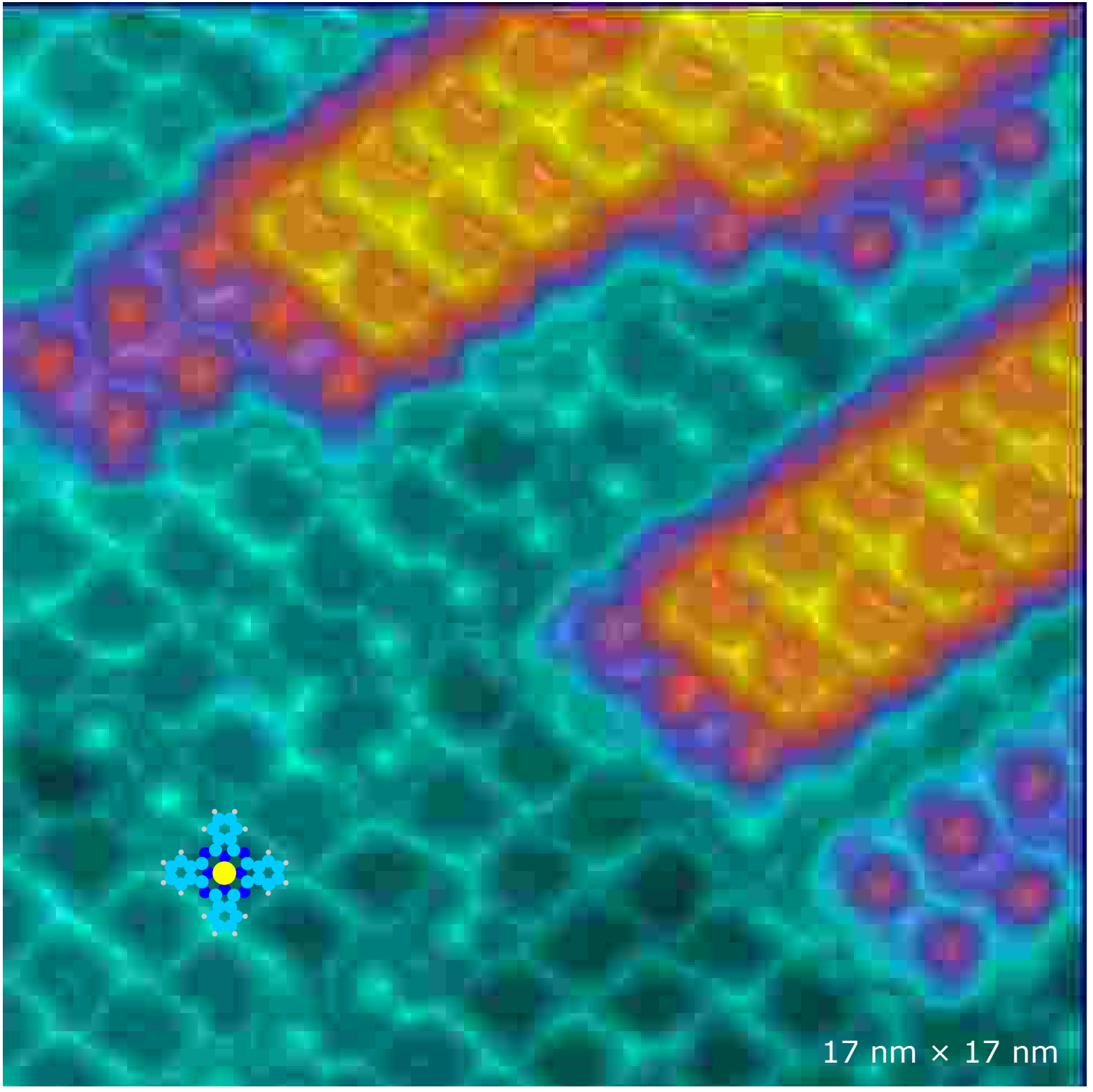
Wang, Kröger, Berndt, Hofer
Angew. Chem., submitted.

Irreversible switch on metal surface

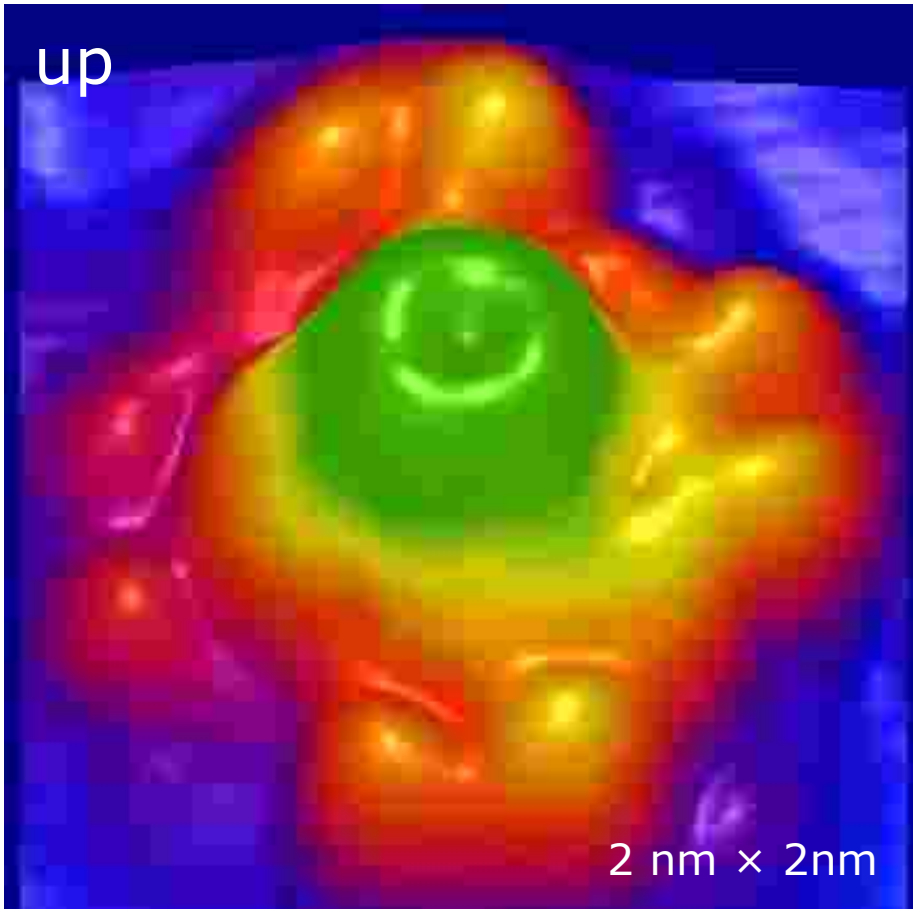


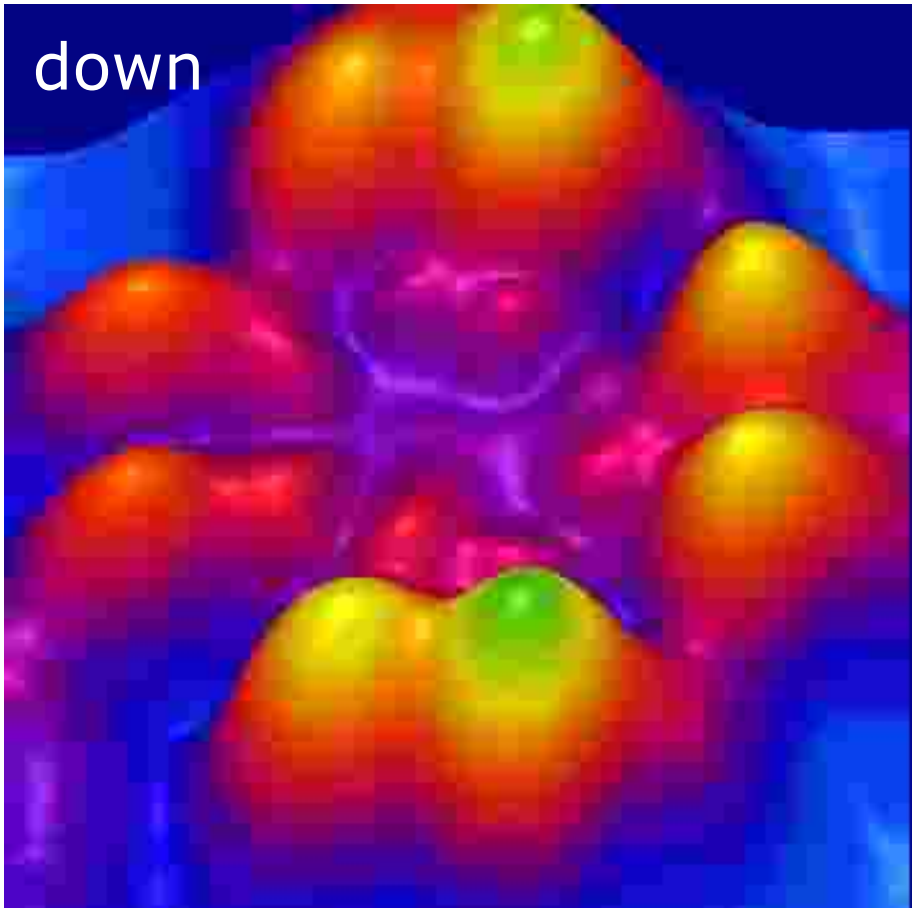


Resonant tunnelling out of HOMO-1
"hole attachment"

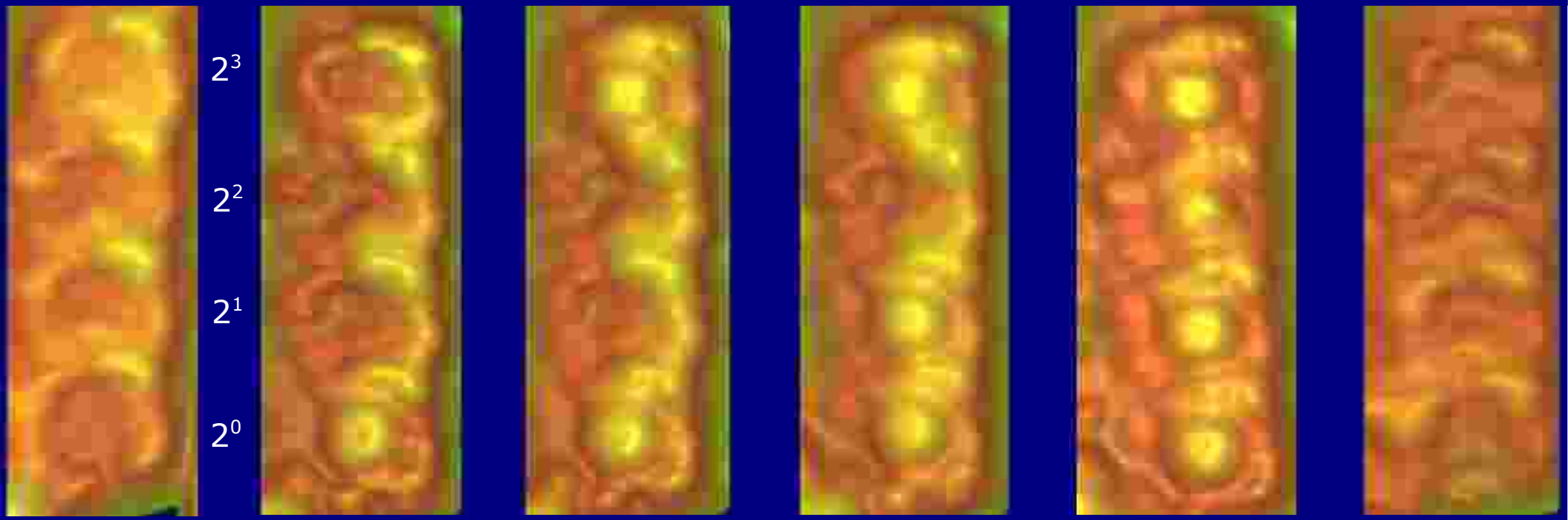

Buffer layer
17 nm × 17 nm

Reversible switch on buffer layer





Resonant tunnelling into LUMO+1
"electron attachment"



Engineering of an ordered array of molecular switches

Wang, Kröger, Berndt, Hofer,
J. Am. Chem. Soc., submitted.

Summary

Aspects of Molecular Electronics

- Controlled contact of molecules with electrodes
- Engineering of a molecular switch