

Stepped Silicon Templates for Quantum Wire Structures

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Outline

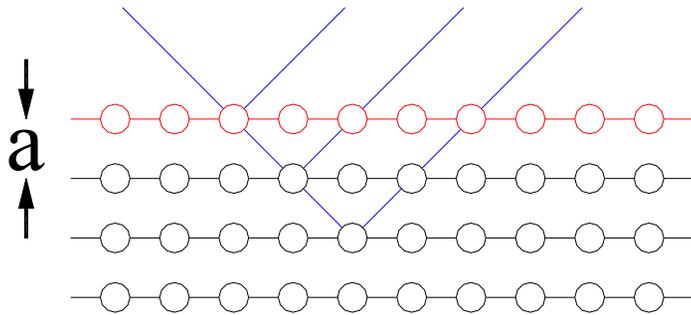
- Surface X-ray Diffraction
- Crystal Truncation Rods
- Quantum Wires
- Si(557) as a Facetted Template
- Au/Si(557) Structure

Measurements made at beamline X16A of the
National Synchrotron Light Source

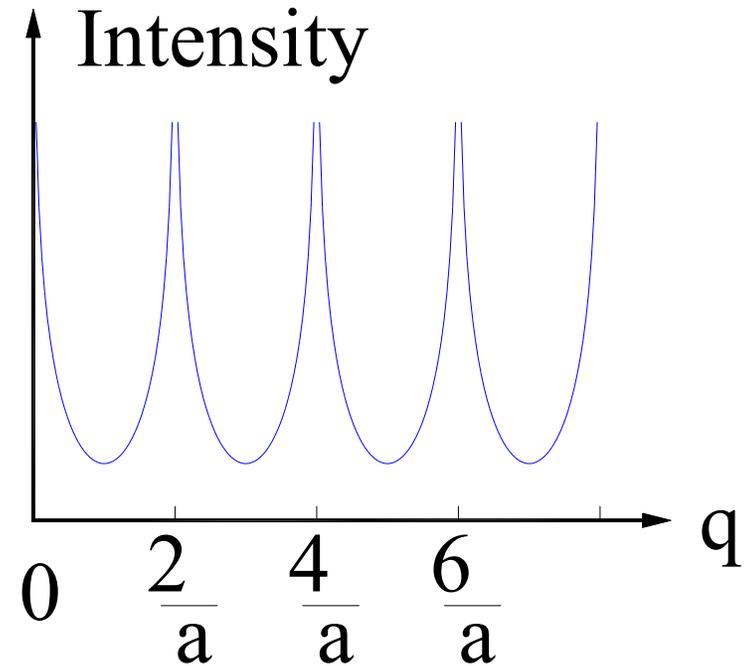
Surface X-ray Diffraction

- Surface sensitivity comes from *symmetry*
- Buried interfaces equally accessible
- Kinematical diffraction is quantitative
- Ordered superstructure or “ 1×1 ”
- Direct methods under development

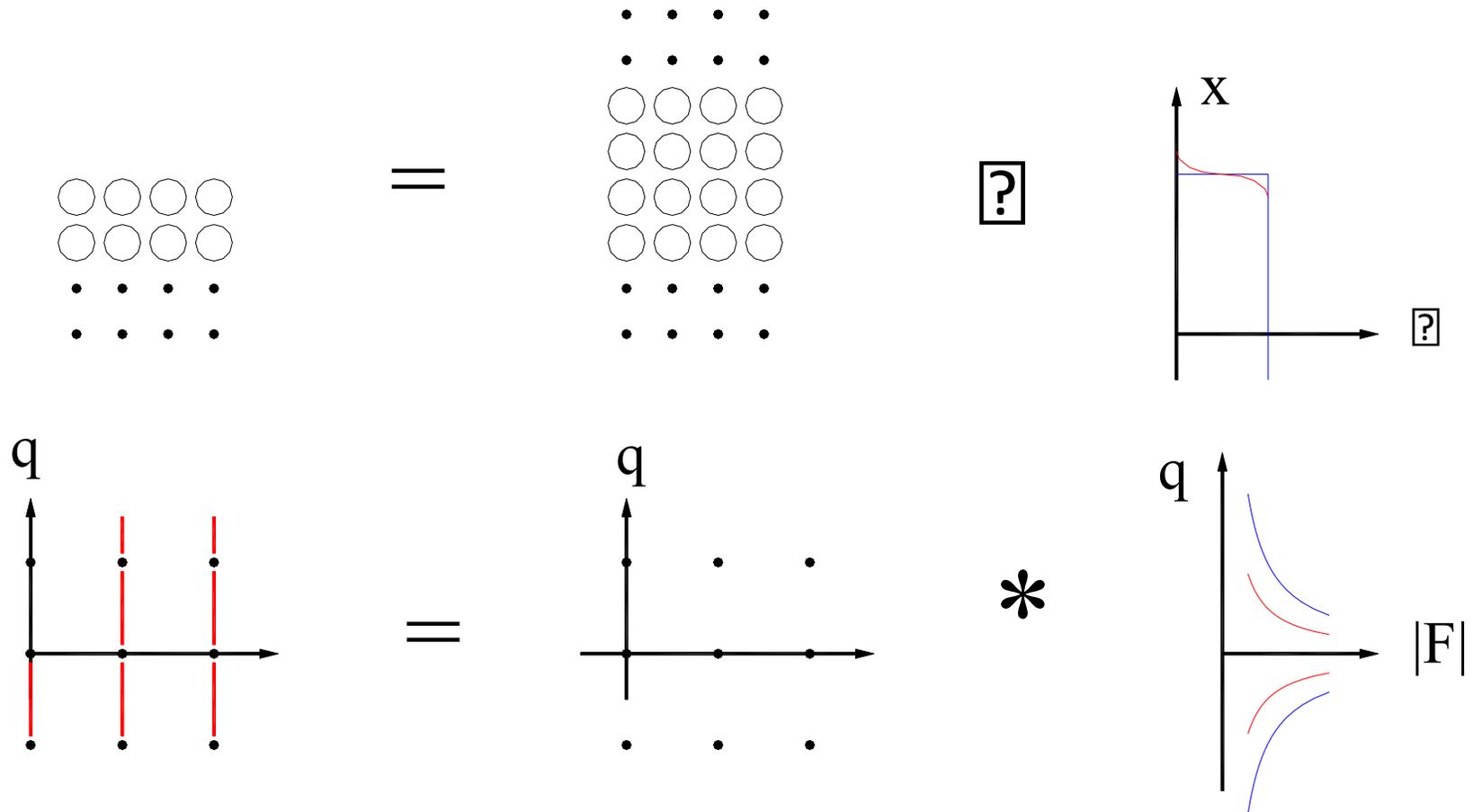
Origin of Truncation Rods



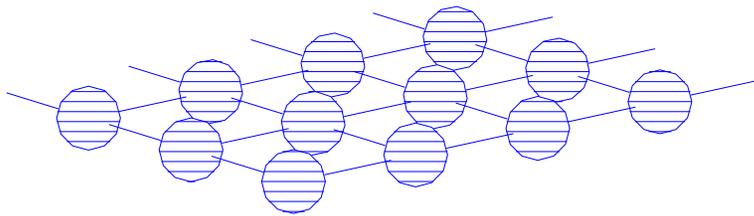
$$\begin{aligned} F_{CTR} &= \sum_{n=0}^{\infty} A_n \\ &= \sum_{n=0}^{\infty} f_L e^{inqa} \\ &= \frac{f_L}{1 - e^{iqa}} \end{aligned}$$



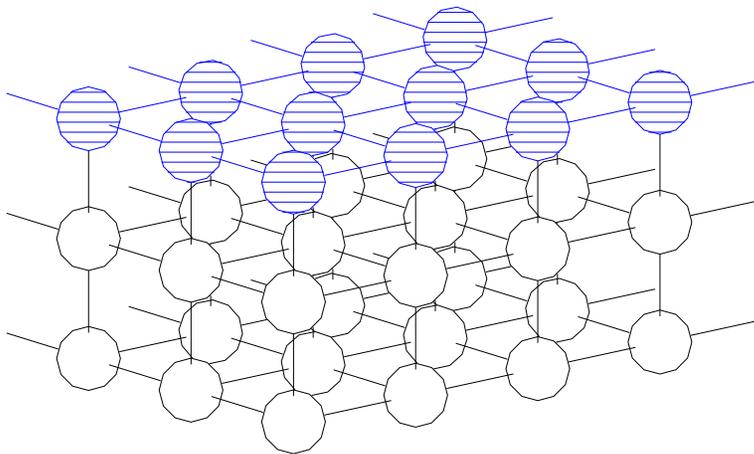
CTR as Convolution



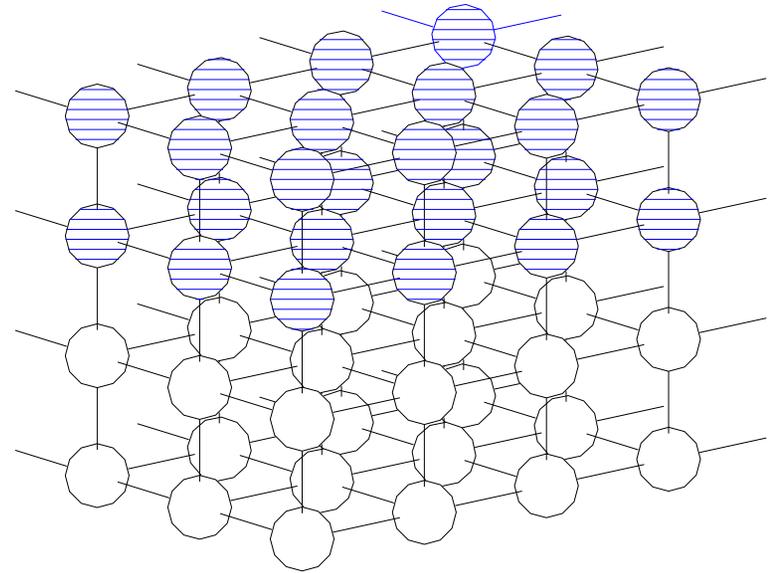
Surfaces and Interfaces



Isolated monolayer



Surface of Crystal

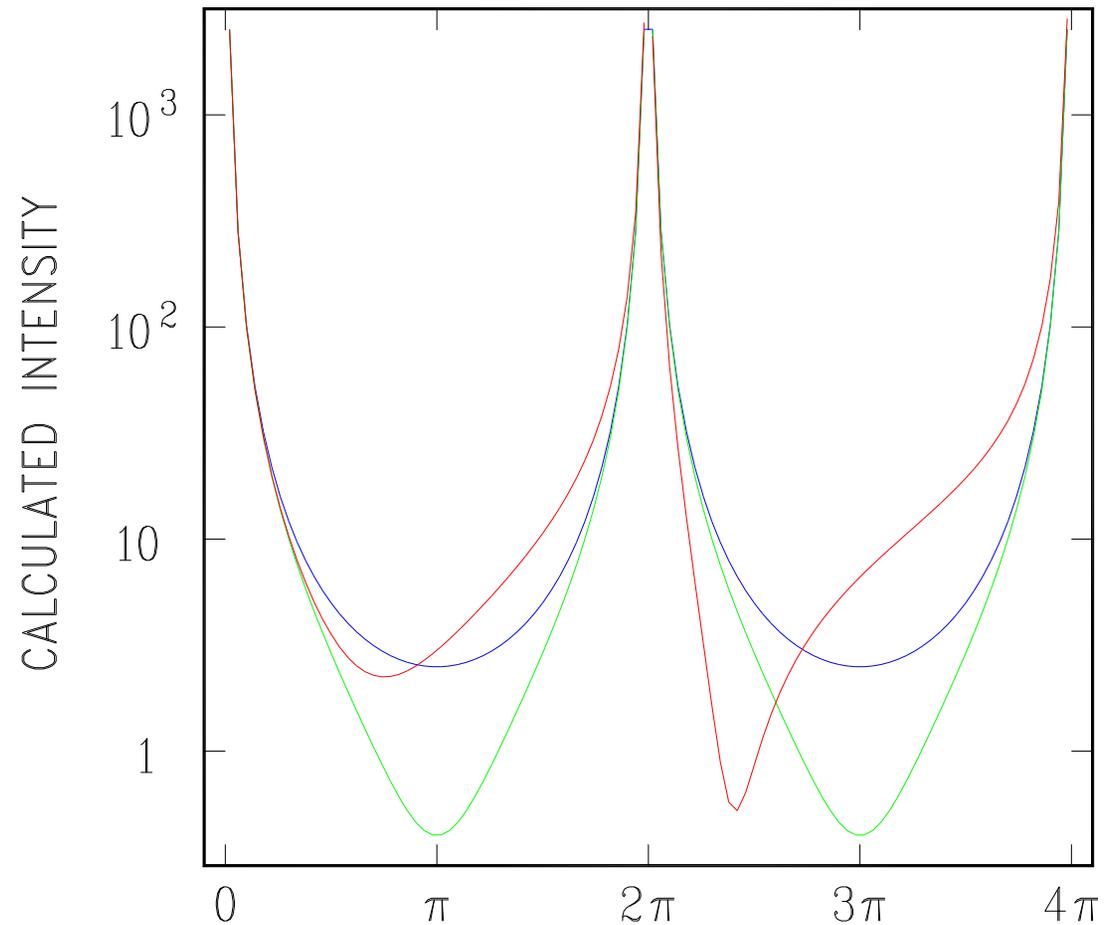
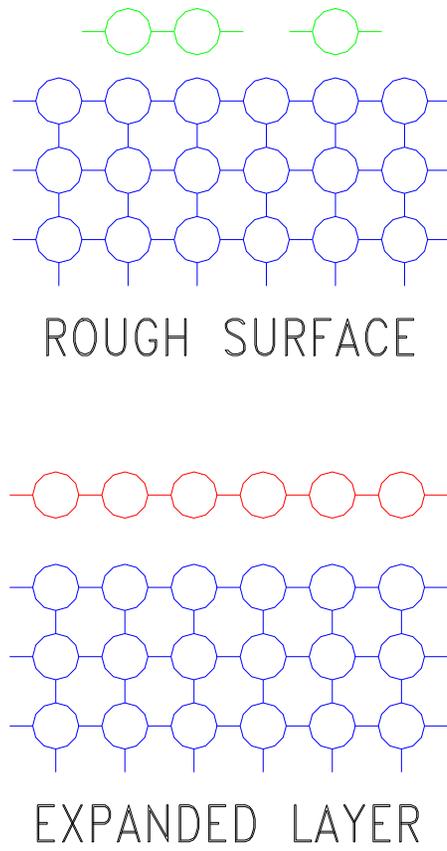


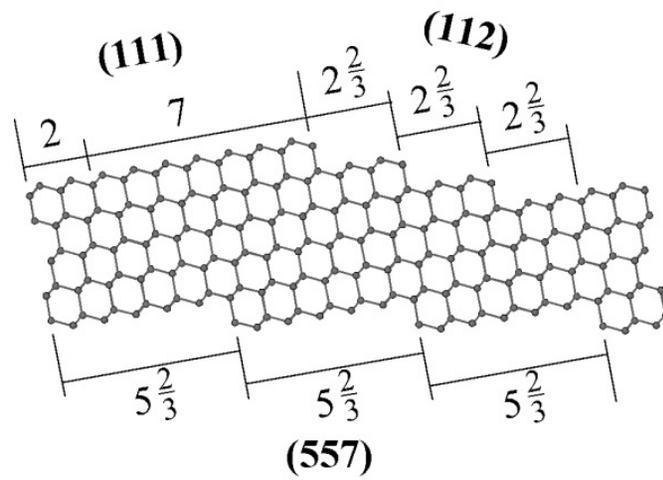
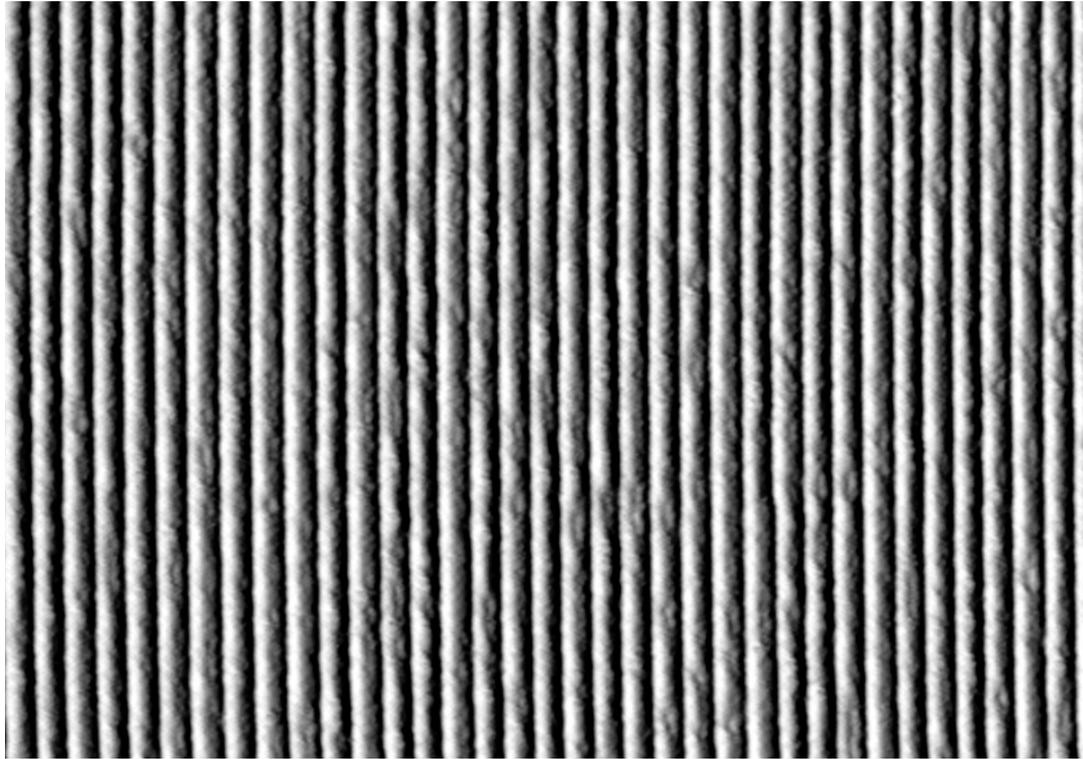
Crystal-Crystal Interface

CTR has 2D and 3D Features

Title:
C:\ikr\Publ\Pub1\RPP\RPP4C.DWG
Creator:
PSCRIPT.DRV Version 4.0
Preview:
This EPS picture was not saved
with a preview included in it.
Comment:
This EPS picture will print to a
PostScript printer, but not to
other types of printers.

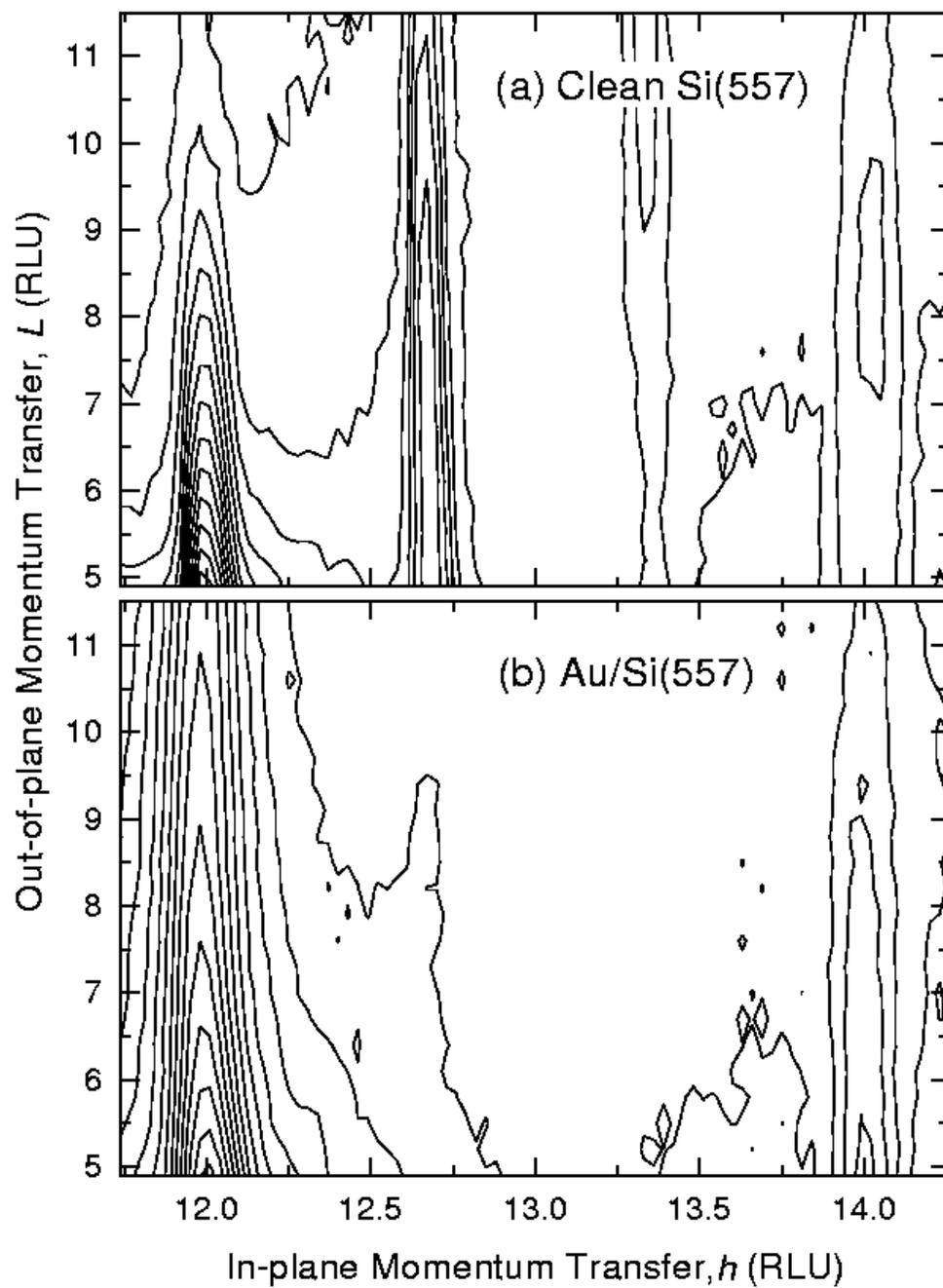
CTR is Sensitive to Surface Structure





H
5.7 nm





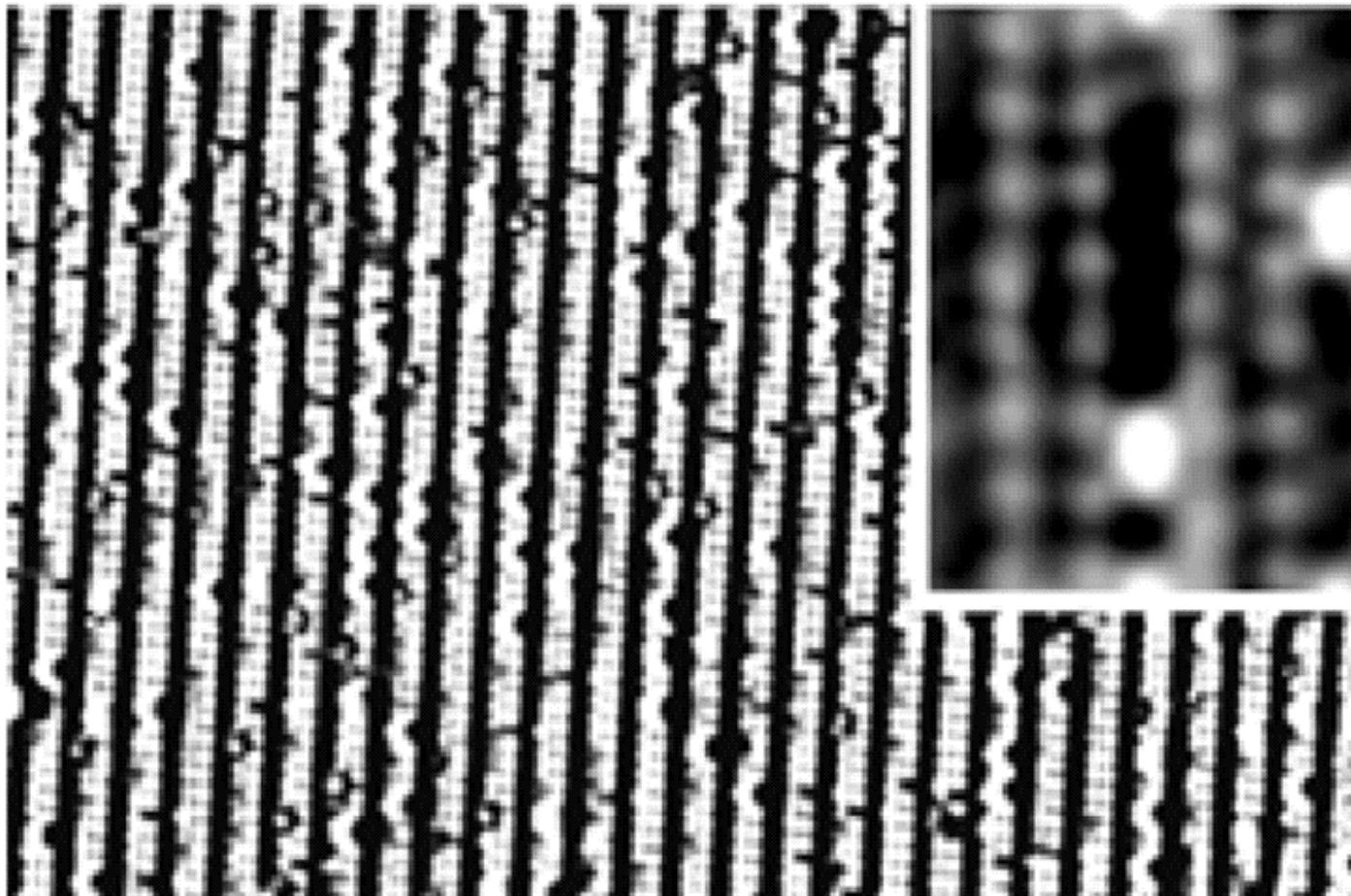
3×1 clean
surface

1×1 surface
with 0.2ML Au

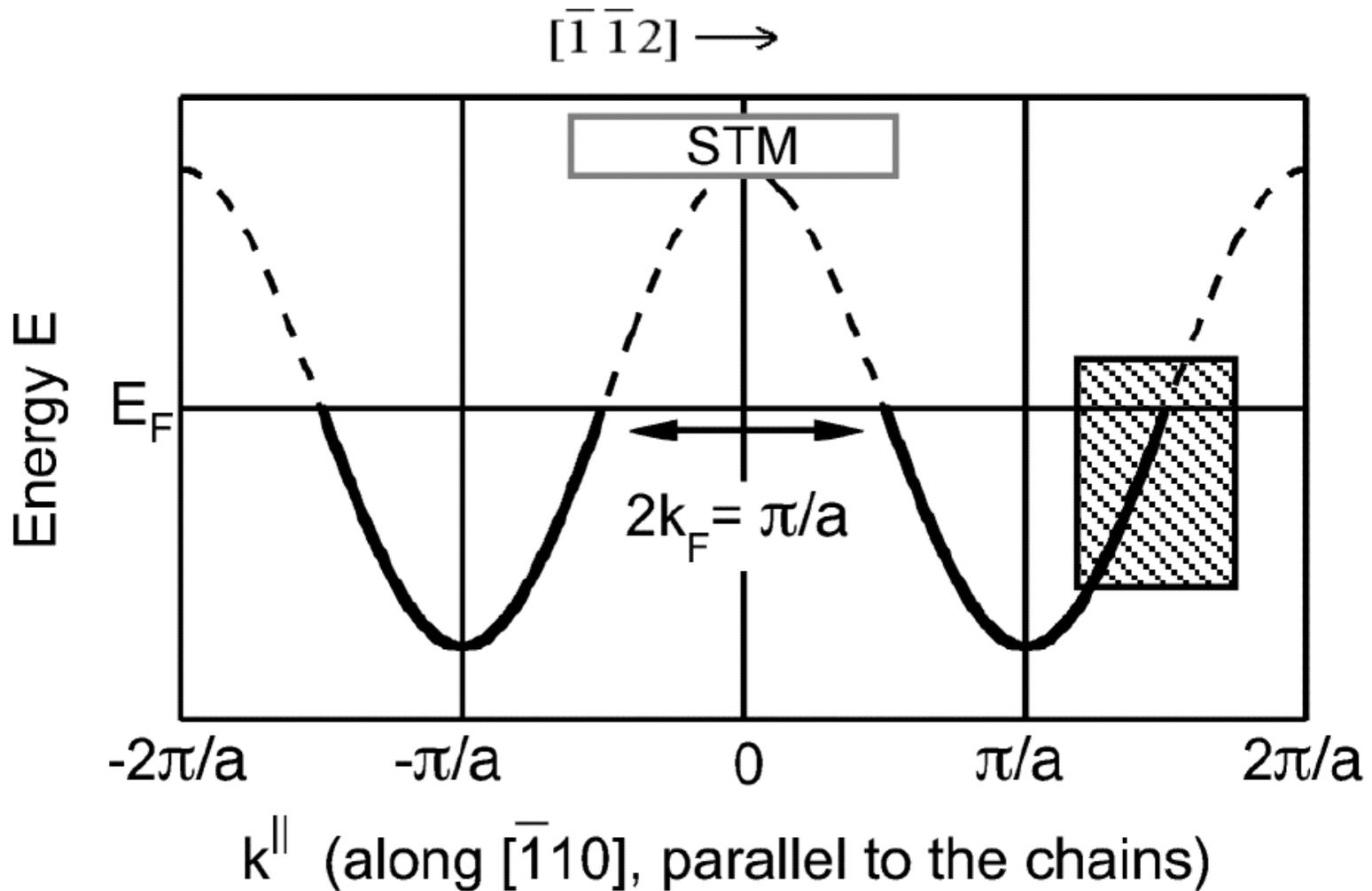
STM of Si(557)/Au

R. Losio, et. al., Phys. Rev. Lett. 86 4632 (2001)

1.9 nm



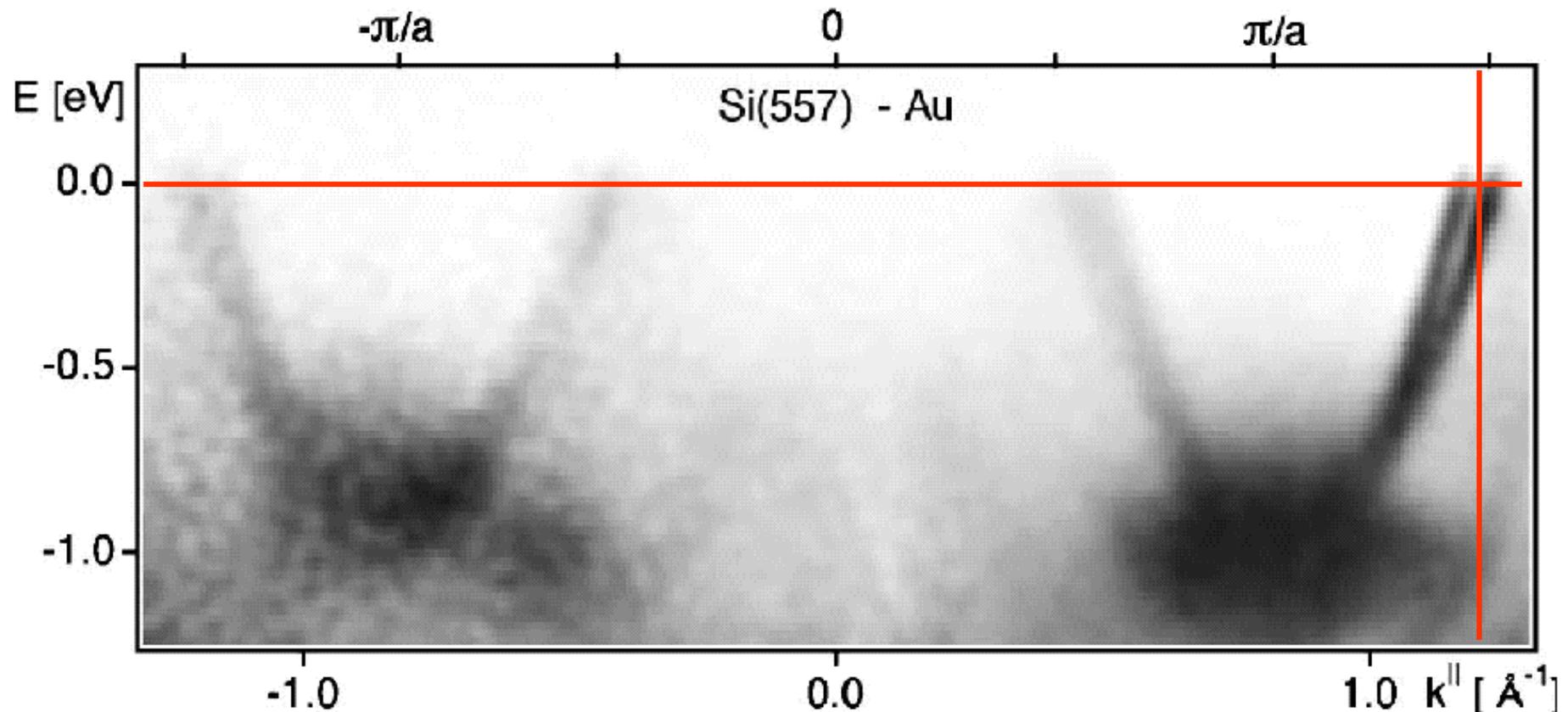
Schematic Band Topology for Au/Si(557)

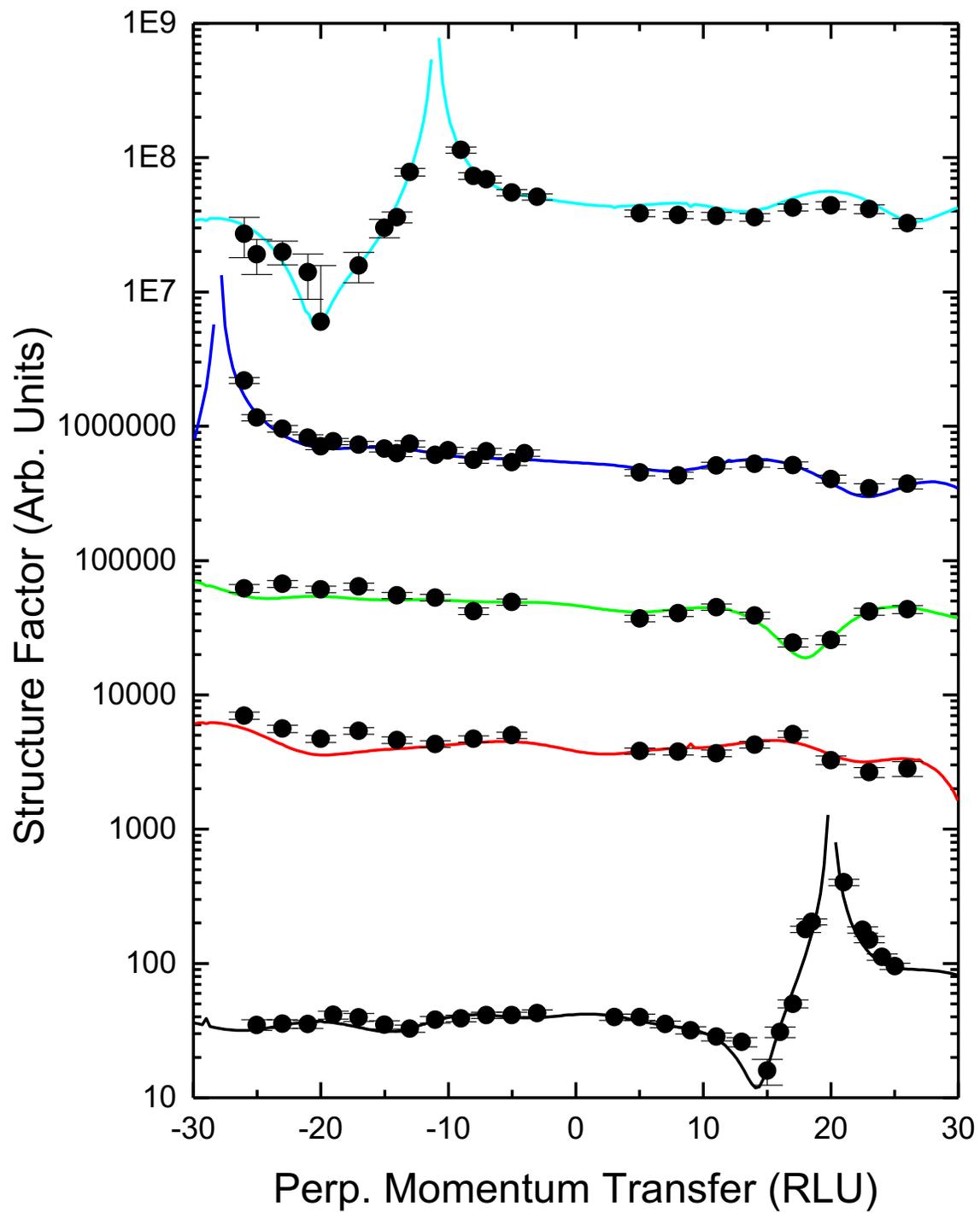


Photoemission from Surface States

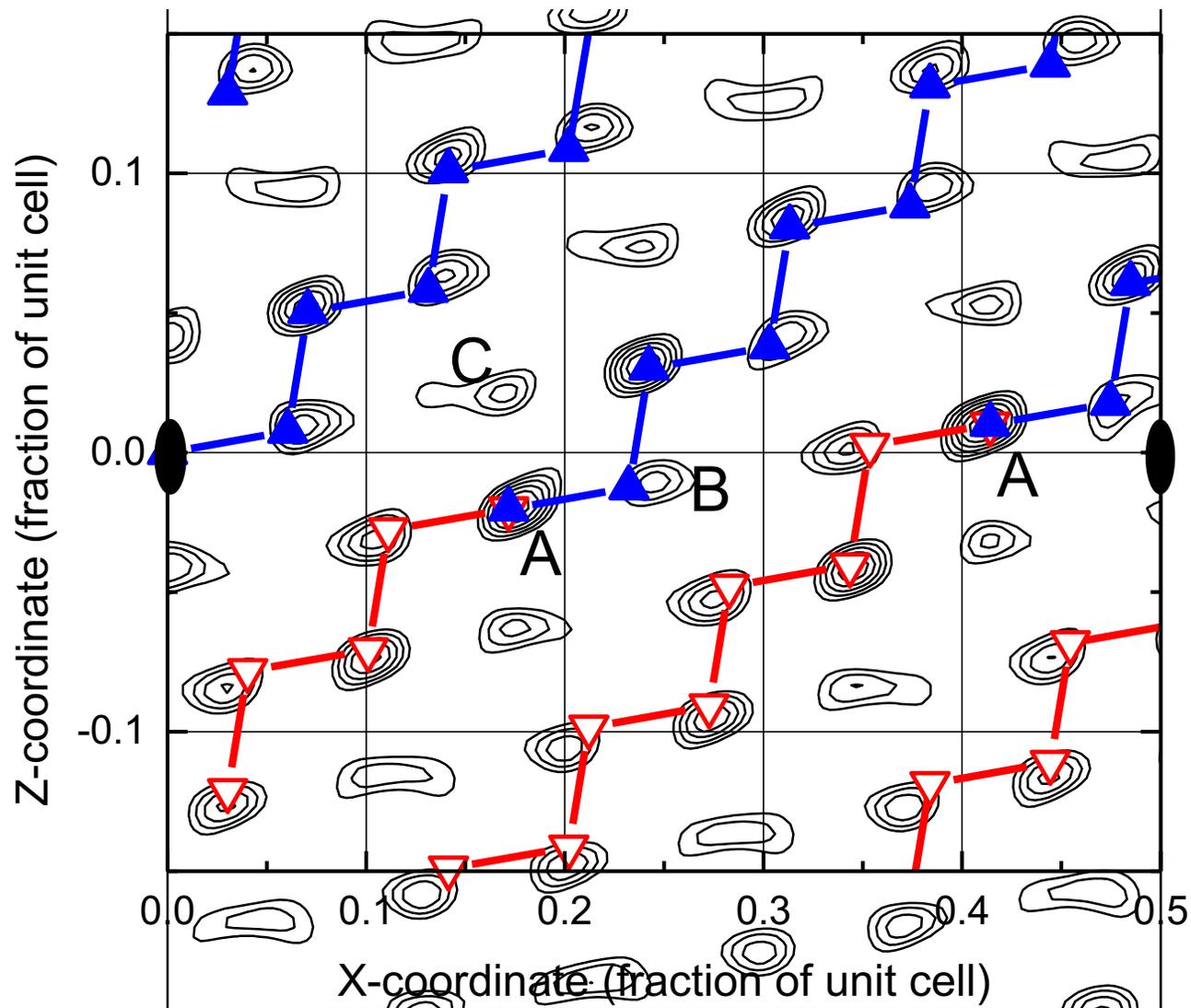
Parallel to the Au Chains in Au/Si(557)

K. N. Altmann et. al. Phys Rev B 64 035406 (2001)



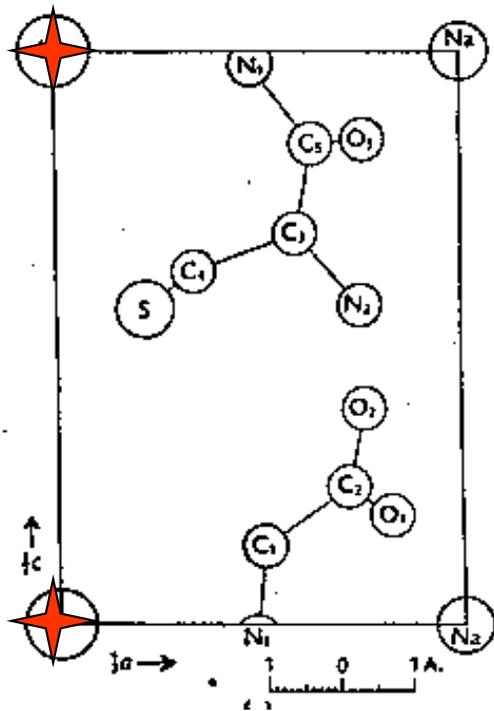


X-Z Patterson of Au/Si(557)

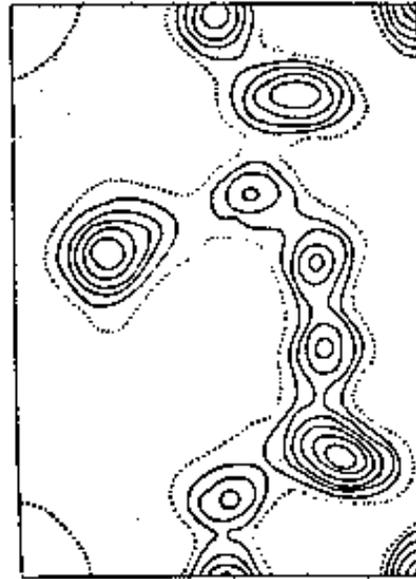


Phasing by a Single Heavy Atom

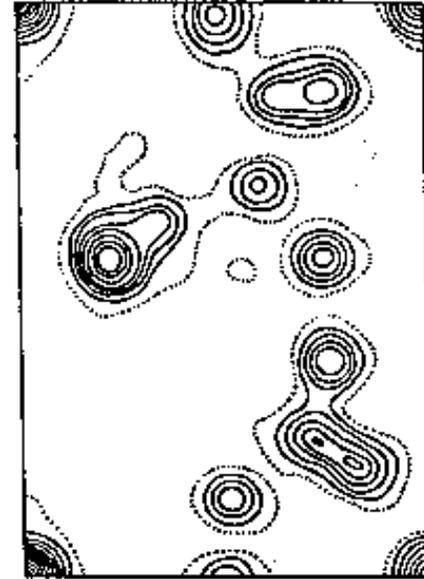
H. B. Dyer, Acta Cryst. 4 42 (1951)



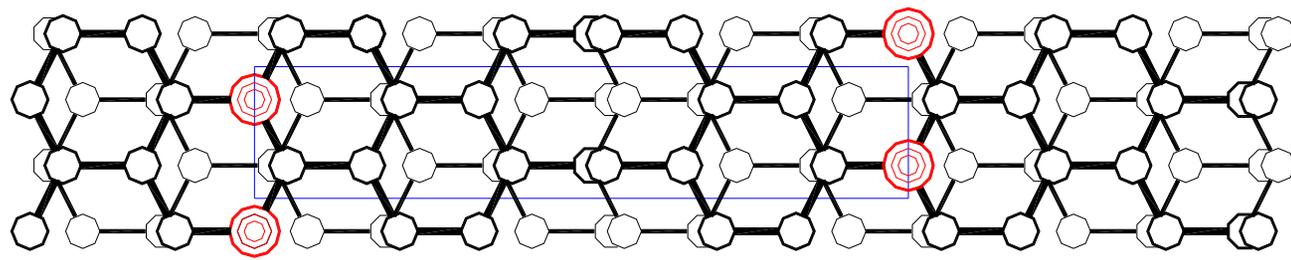
Cysteinylglycine
sodium iodide



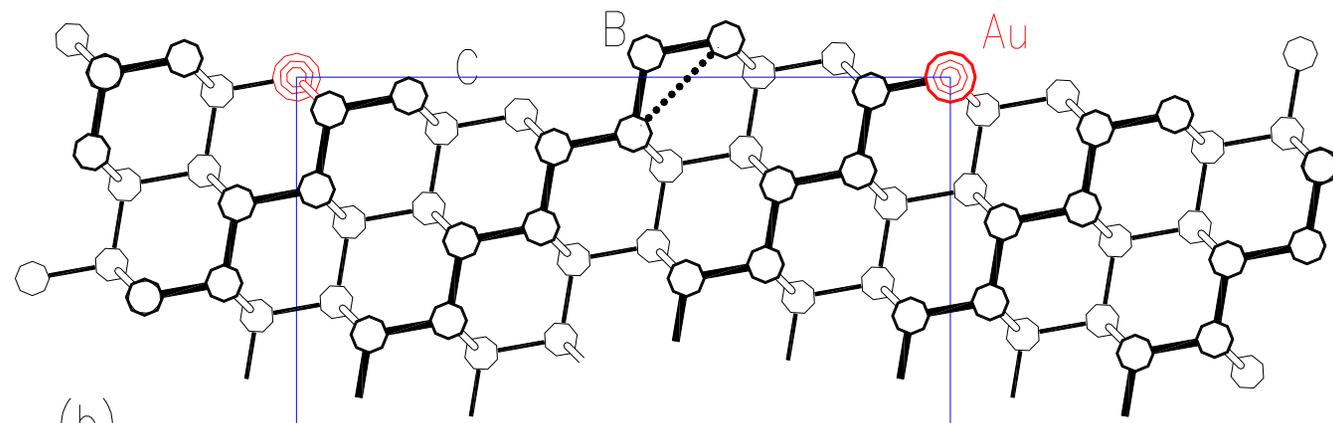
Patterson



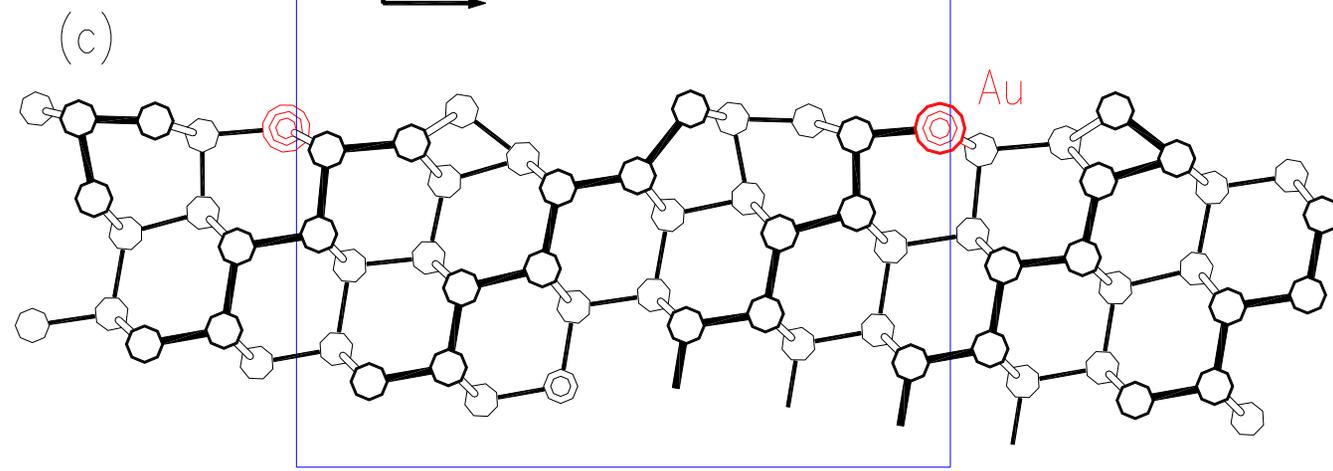
Electron density



(a) A coordinate system with a vertical y-axis and a horizontal x-axis.

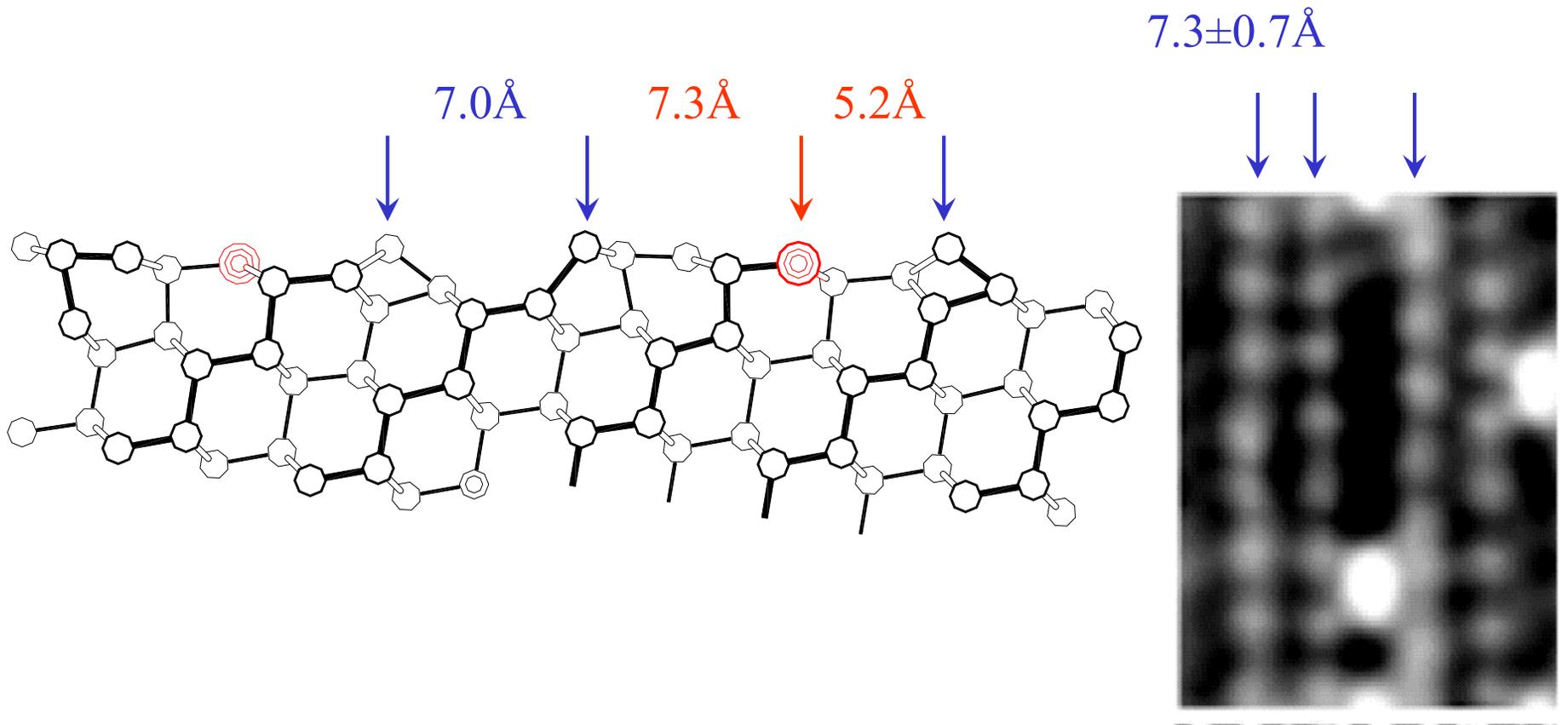


(b) A coordinate system with a horizontal x-axis and a vertical z-axis.



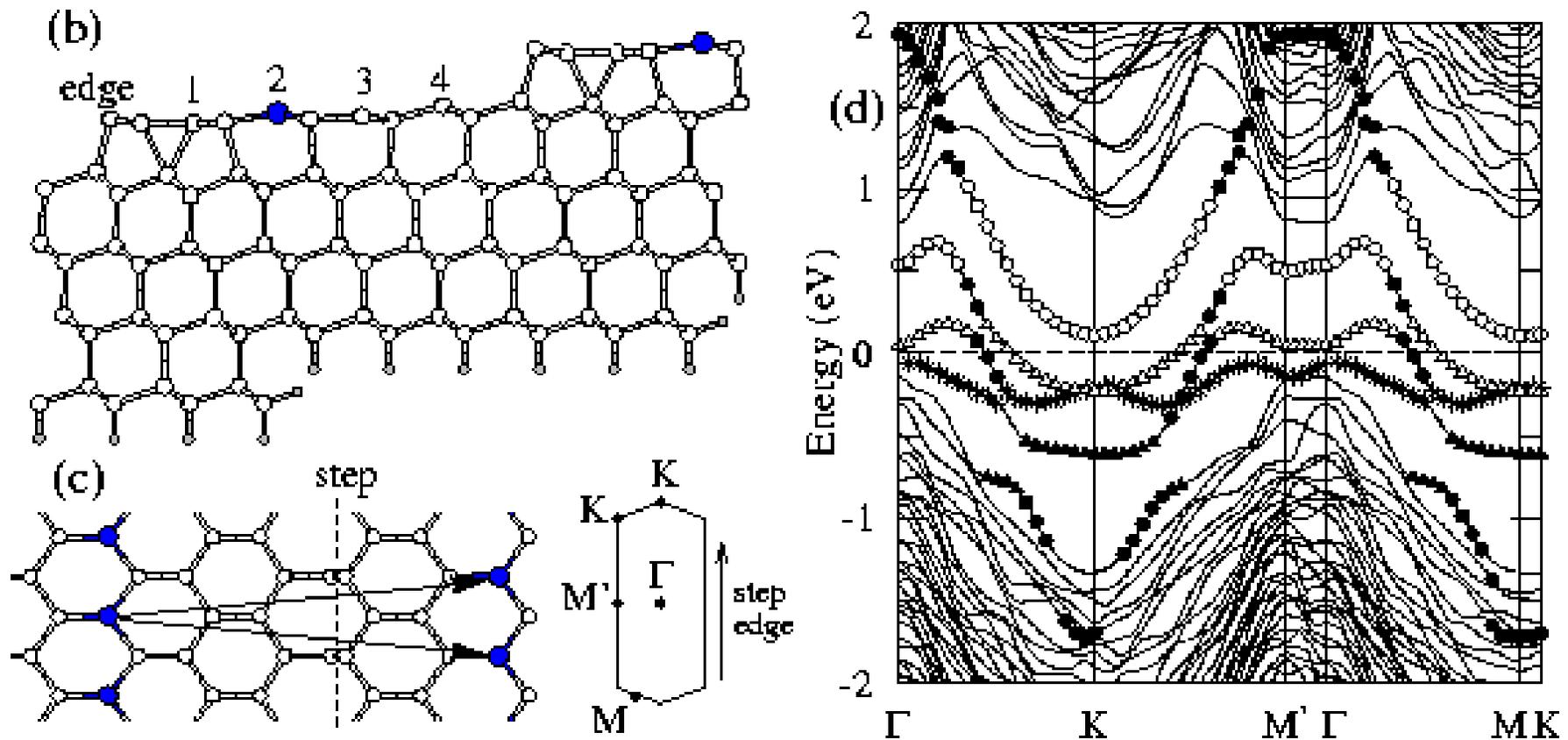
(c)

Comparison with STM



Calculated Electronic Band Structure of Au/Si(557) using SIESTA code

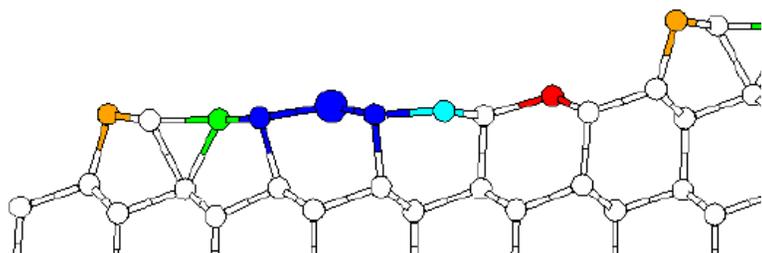
D. Sanchez-Portal et. al. (to be published)



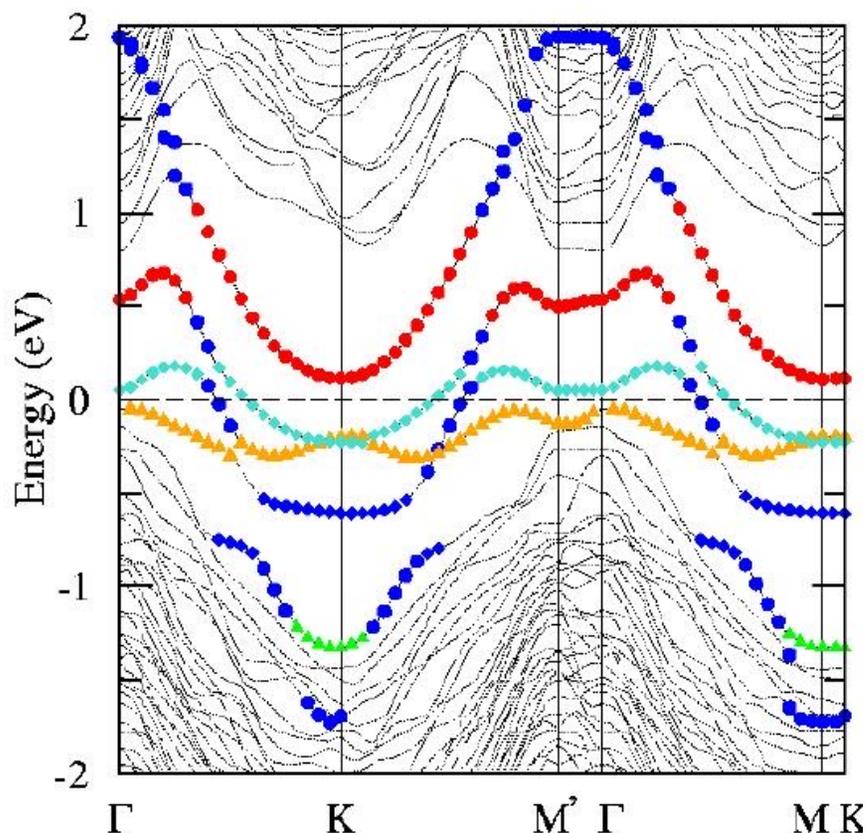
Si(557)-Au: calculated band structure

D. Sanchez-Portal et. al. (to be published)

Mulliken populations allow to identify the origin of each band



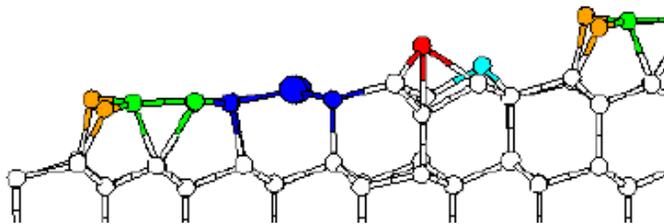
- Directions Γ - K - M' and Γ - M are parallel to the gold chains
- “Gold bands” (blue) are strongly hybridized with the Si neighboring atoms
- Orange band corresponds to the step edge
- Red and cyan bands are due to dangling bonds in the terraces
- The inclusion of adatoms saturating some of the Si dangling-bonds do not modify the main features of this band structure.



Si(557)-Au: role of adatoms

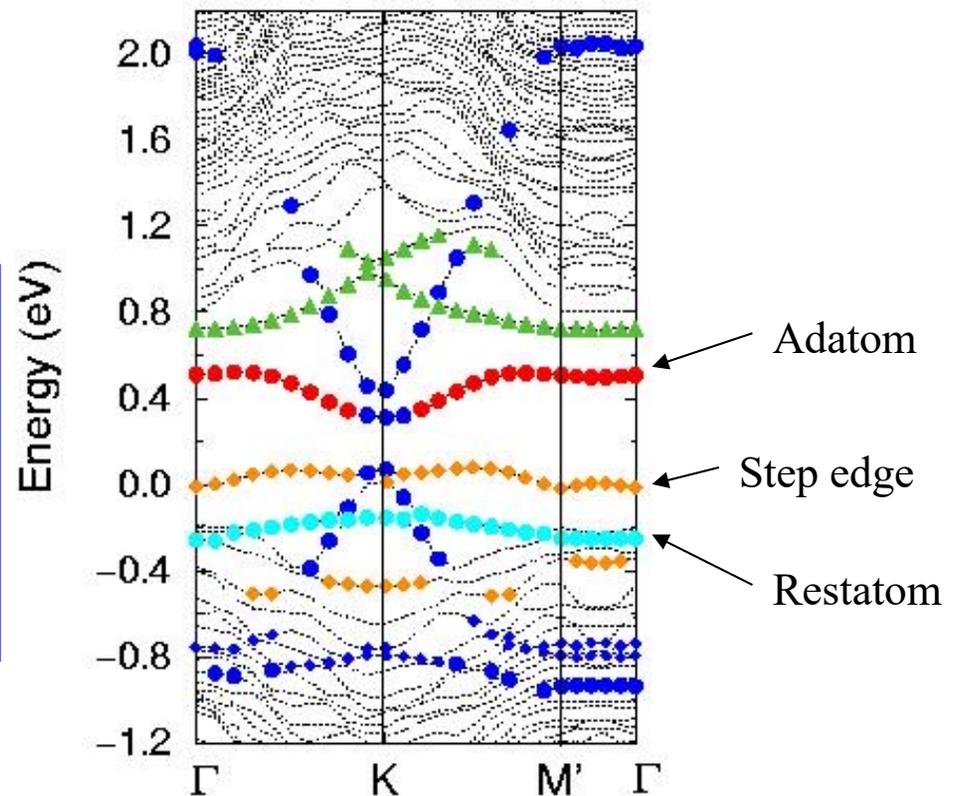
D. Sanchez-Portal et. al. (to be published)

The presence of **one row of adatoms** partially saturating some of the dangling bonds **do not modify** our main conclusions
However it is slightly **favorable energetically**, with a gain of ~ 0.14 eV/Au



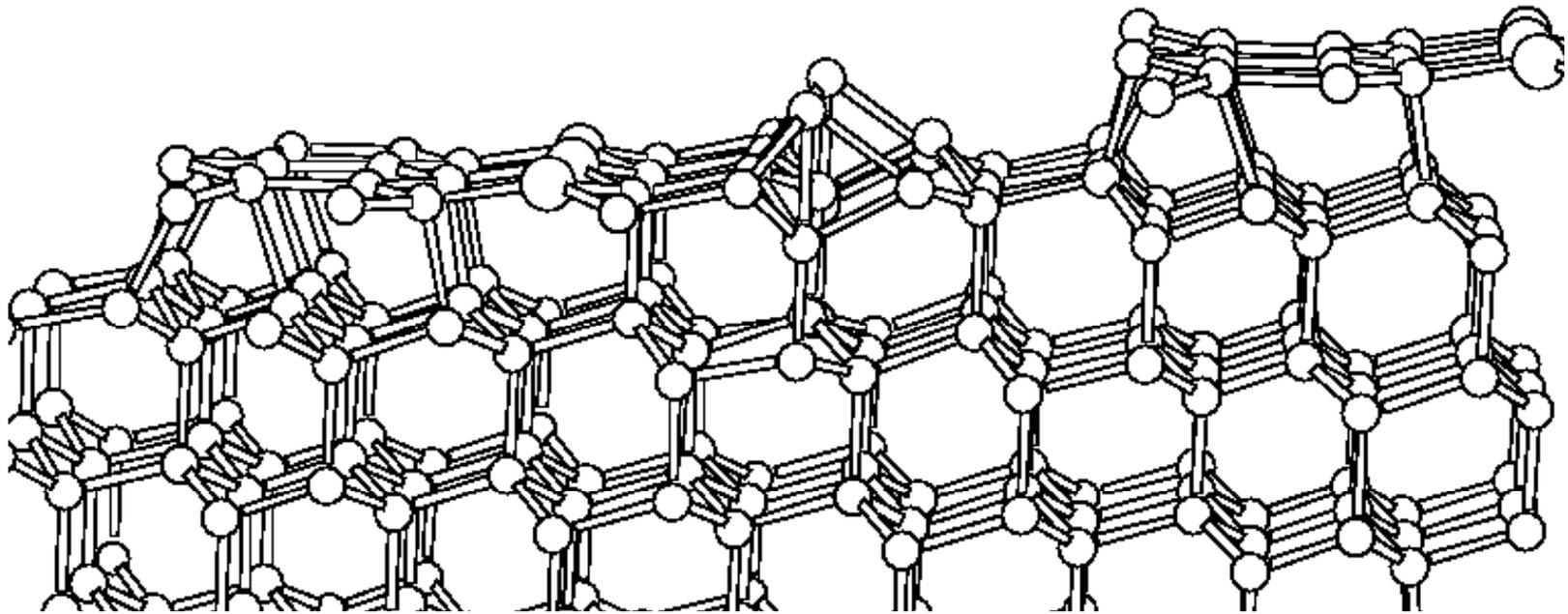
- The **step-edge band** (orange) is located precisely at the Fermi energy
- Still **two bands*** (blue symbols) associated to the gold chain.

*They appear as four bands due to the folding associated to the doubling of the unit cell



Energy-minimized Model of Au/Si(557) 1x2 with Adatom

D. Sanchez-Portal et. al. (to be published)



Conclusions

- Direct imaging of structure containing heavy atom
- Au stabilizes terraced Si(557) substrate
- Au substitutes for Si in **middle** of terrace
- 1D quantum wires seen in photoemission
- Superstructure yet to be resolved