Structure of Quantum Wires in Au/Si(557)

I. K. Robinson	University of Illinois
P. A. Bennett	Arizona State University
F. J. Himpsel	University of Wisconsin

Crystal Chemistry of New Materials & Soft Matter
ESRF/ILL, Grenoble, July 2002

Outline

- Surface Crystallography
- Crystal Truncation Rods
- Crystallography of Stepped Surfaces
- Quantum Wires
- Si(557) as a Facetted Template
- Au/Si(557) Structure

Beamline X16A of the National Synchrotron Light Source

Surface X-ray Crystallography

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

Diffraction as a Surface Integral

Die äußere Form der Kristalle in ihrem Einfluß auf die Interferenzerscheinungen an Raumgittern

Von M. v. Laue

Annalen der Physik [5] 26 55 (1936)

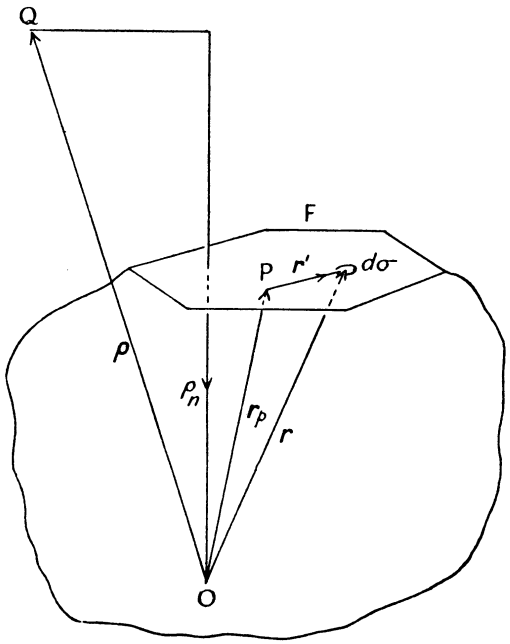
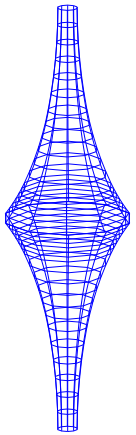
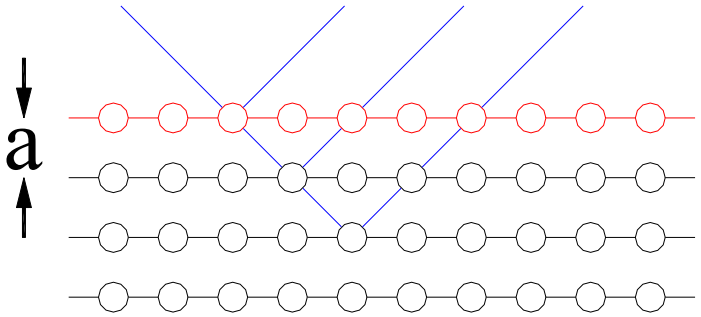


FIG. 200



"Stacheln"

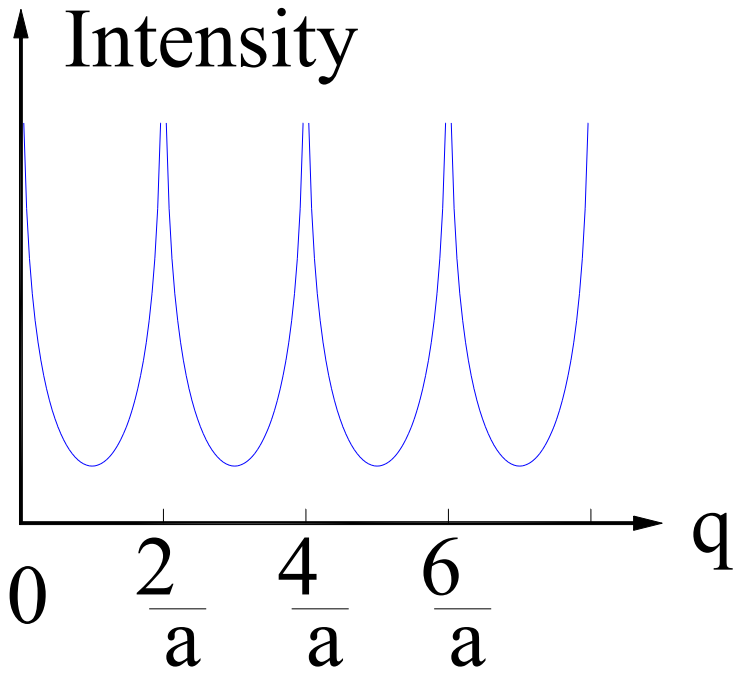
Origin of Truncation Rods



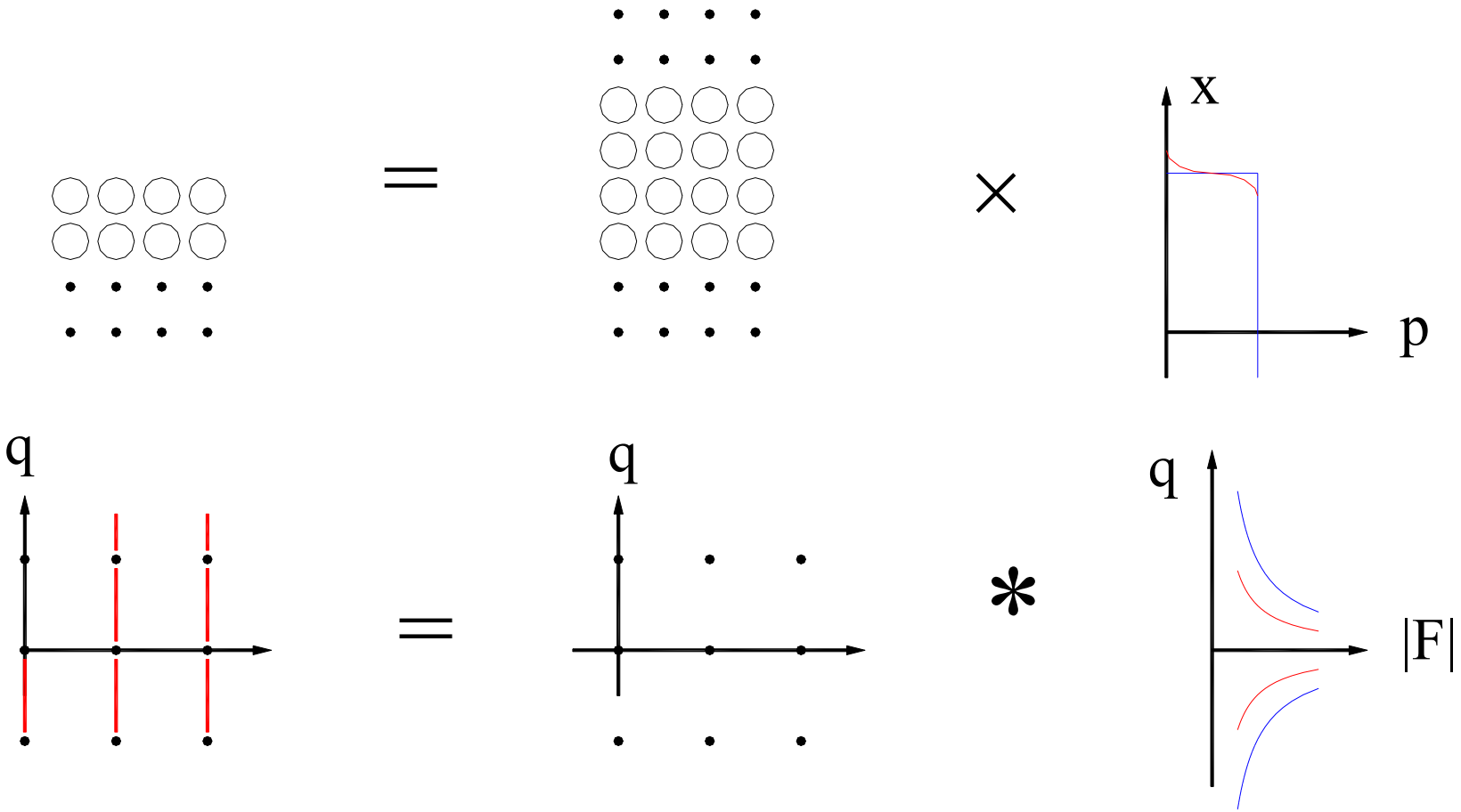
$$F_{CTR} = \sum_{n=0}^{\infty} A_n$$

$$= \sum_{n=0}^{\infty} f_L \; e^{inqa}$$

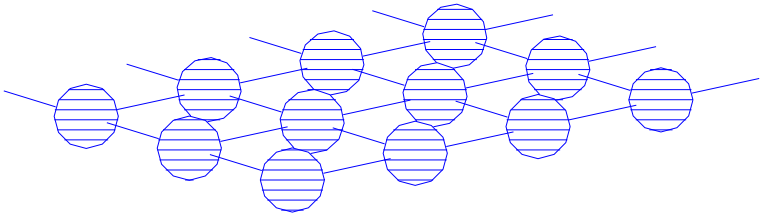
$$= \frac{f_L}{1 - e^{iqa}}$$



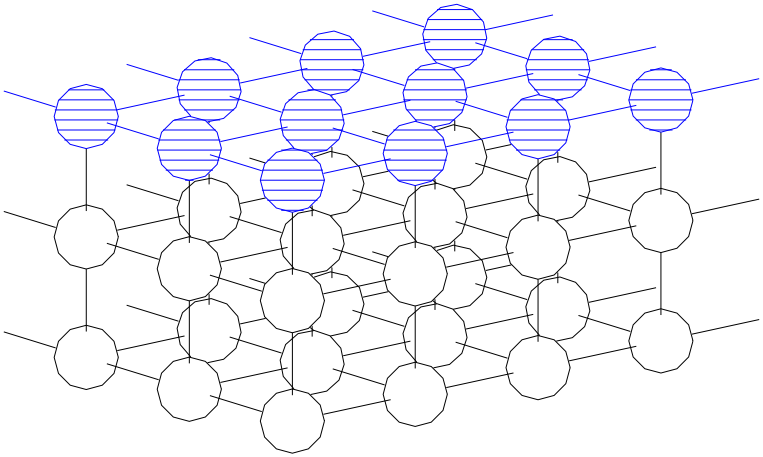
CTR as Convolution



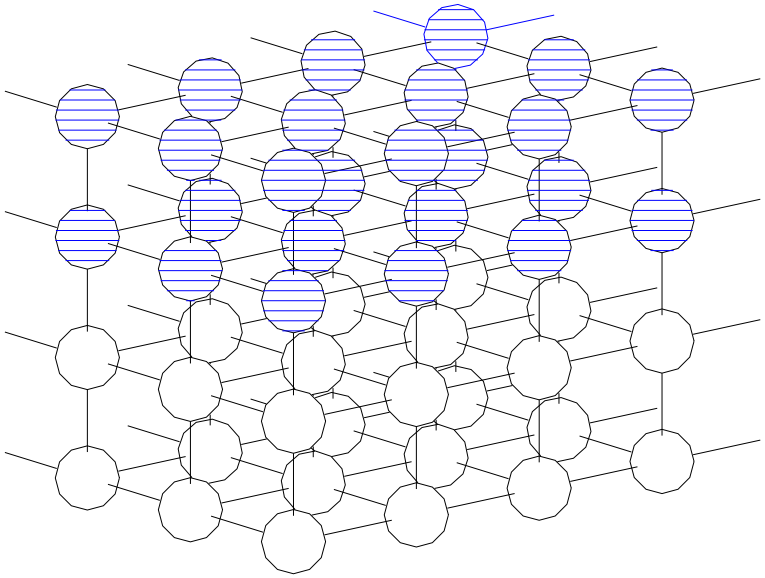
Surfaces and Interfaces



Isolated monolayer



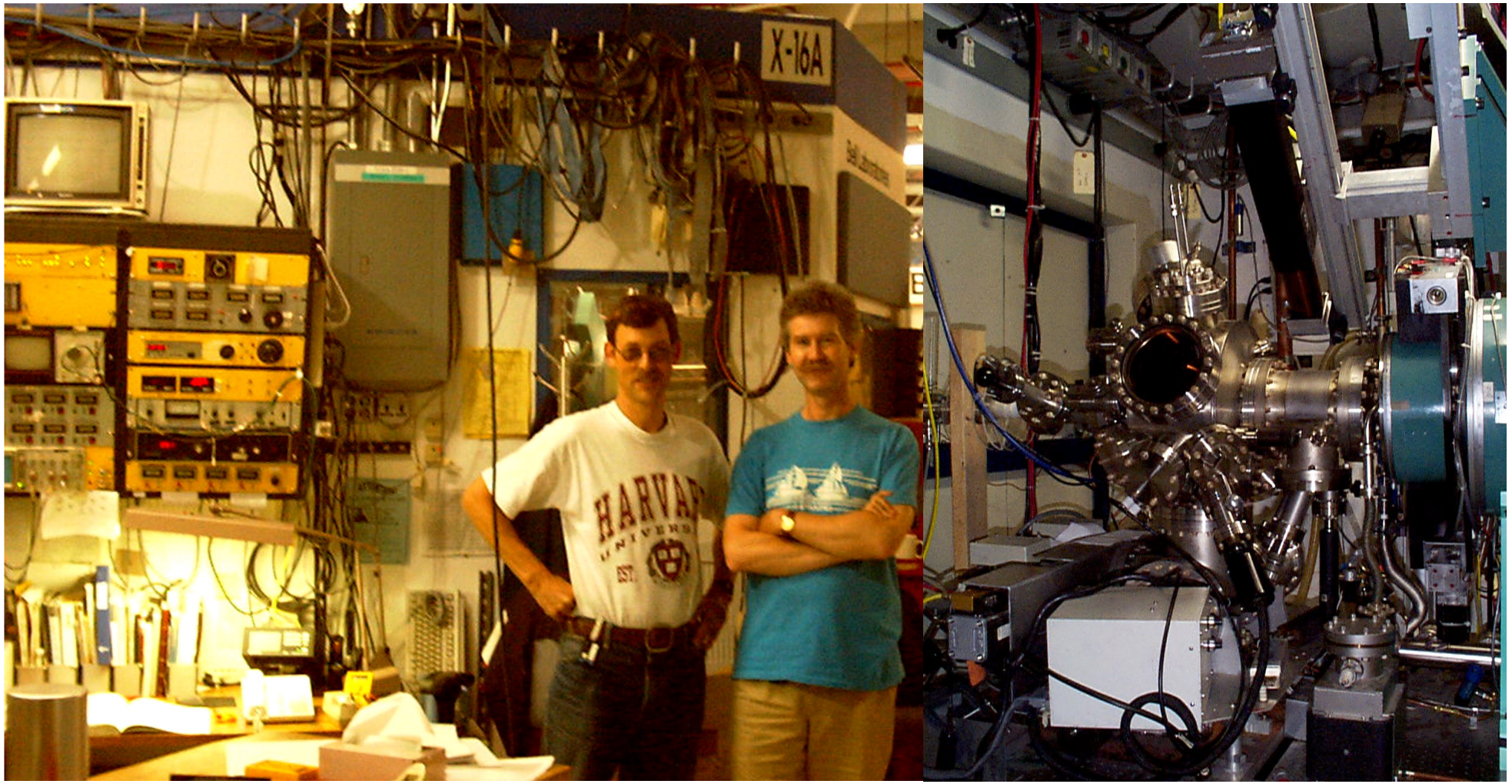
Surface of Crystal



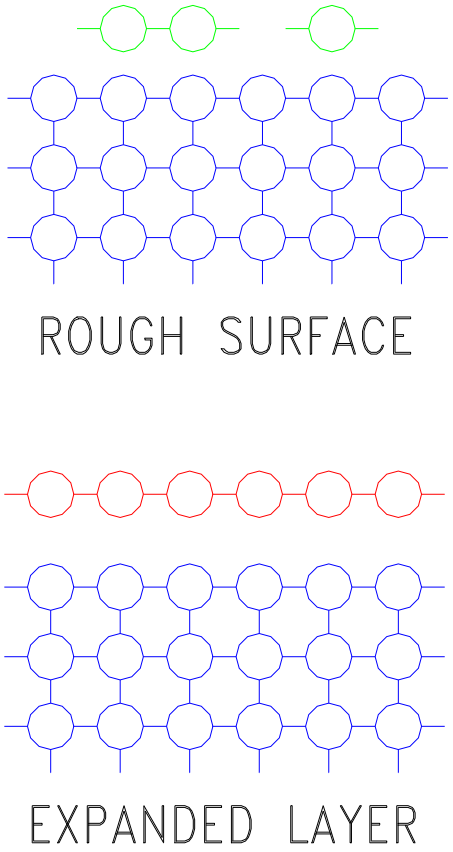
Crystal-Crystal Interface

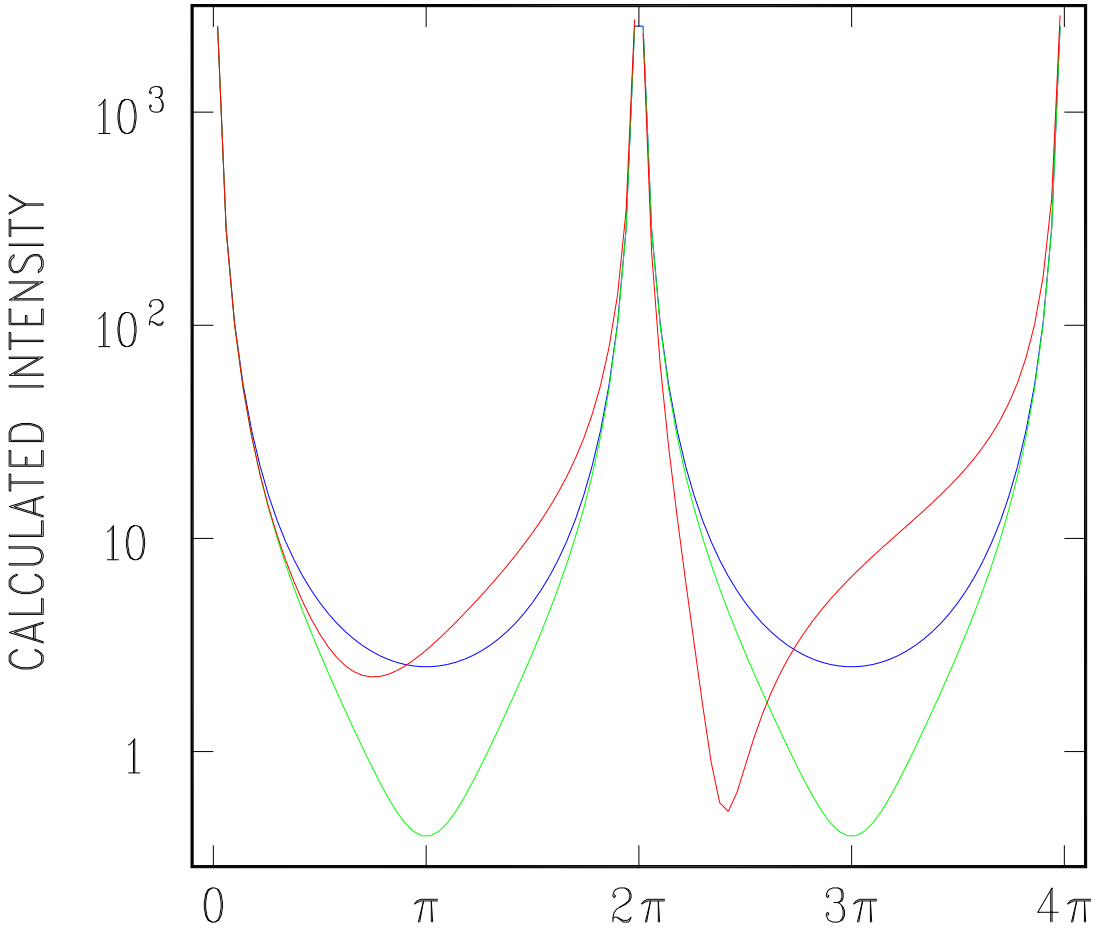
X16A Surface X-ray Diffraction

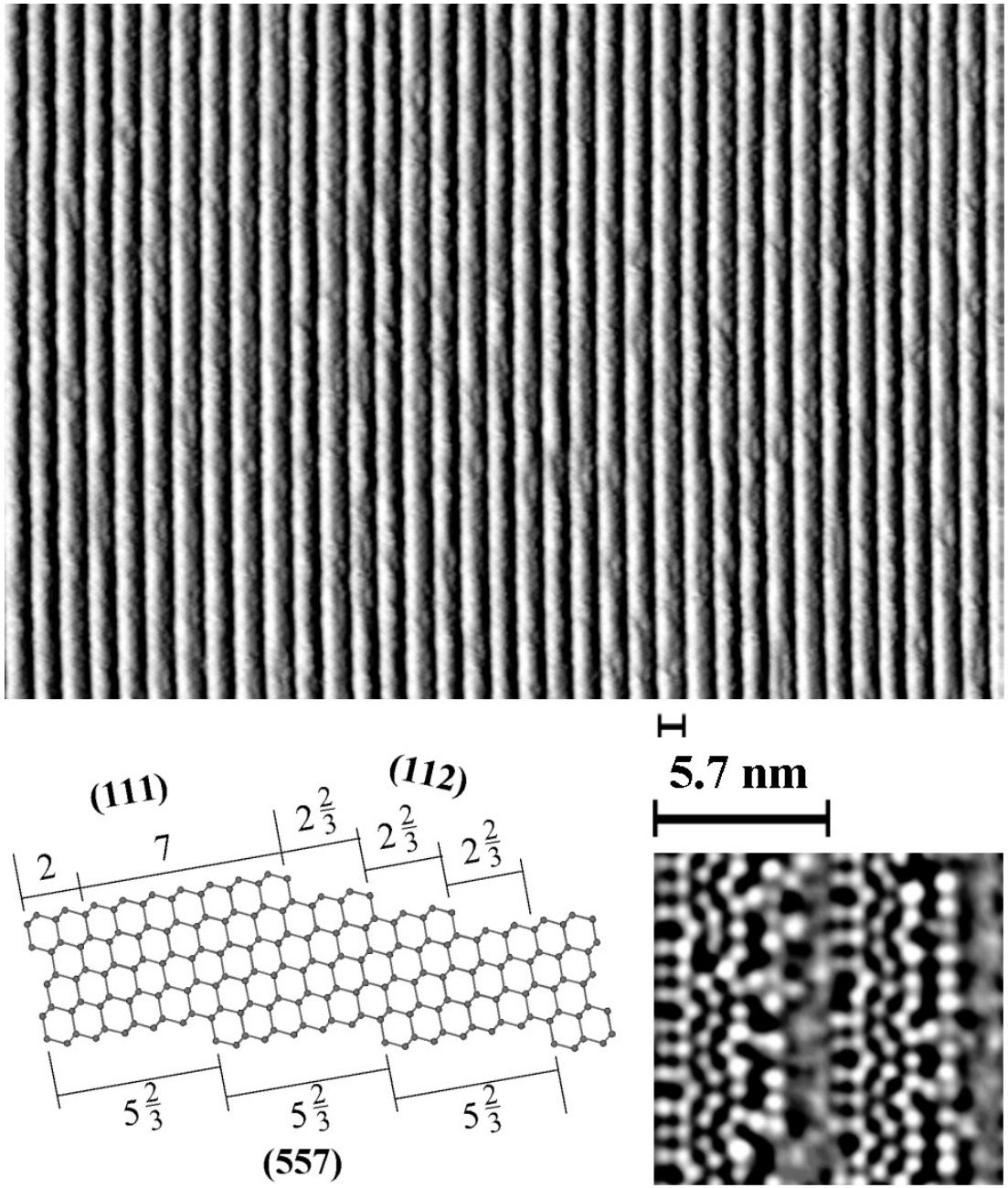
operating since 1987 ...



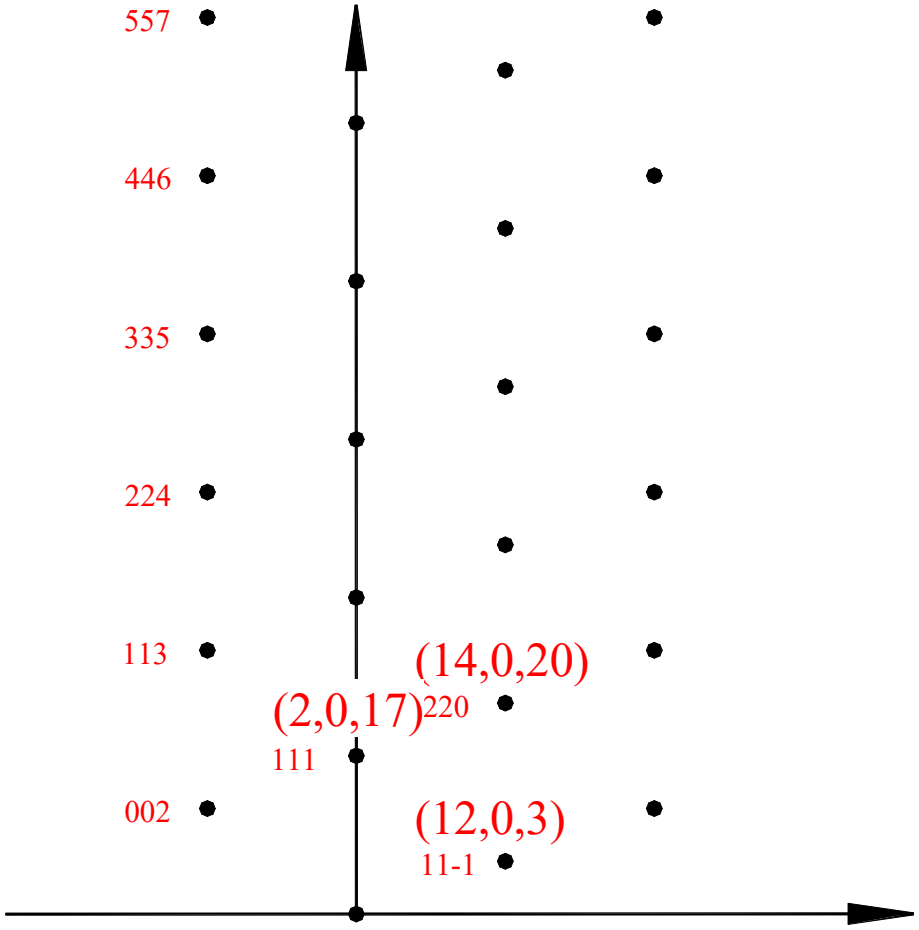
CTR is Sensitive to Surface Structure



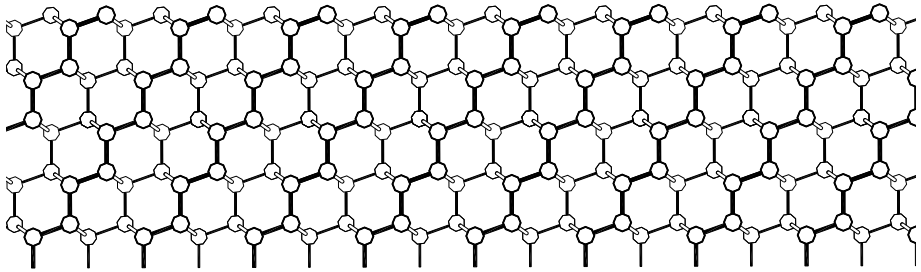


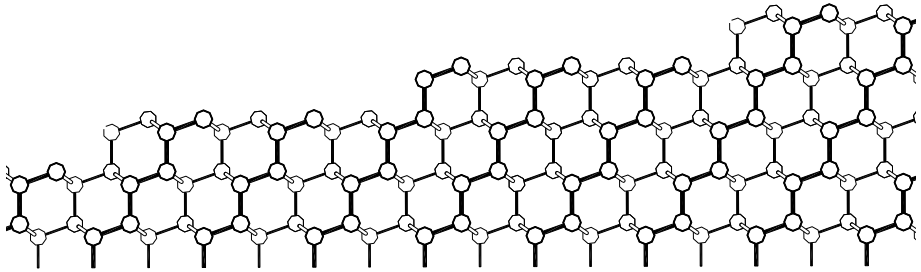

5.7 nm
(111)
(112)
2
7
$2\frac{2}{3}$
$2\frac{2}{3}$
$2\frac{2}{3}$
$5\frac{2}{3}$
$5\frac{2}{3}$
$5\frac{2}{3}$
(557)

Crystallography of Stepped Surfaces



Silicon (111)



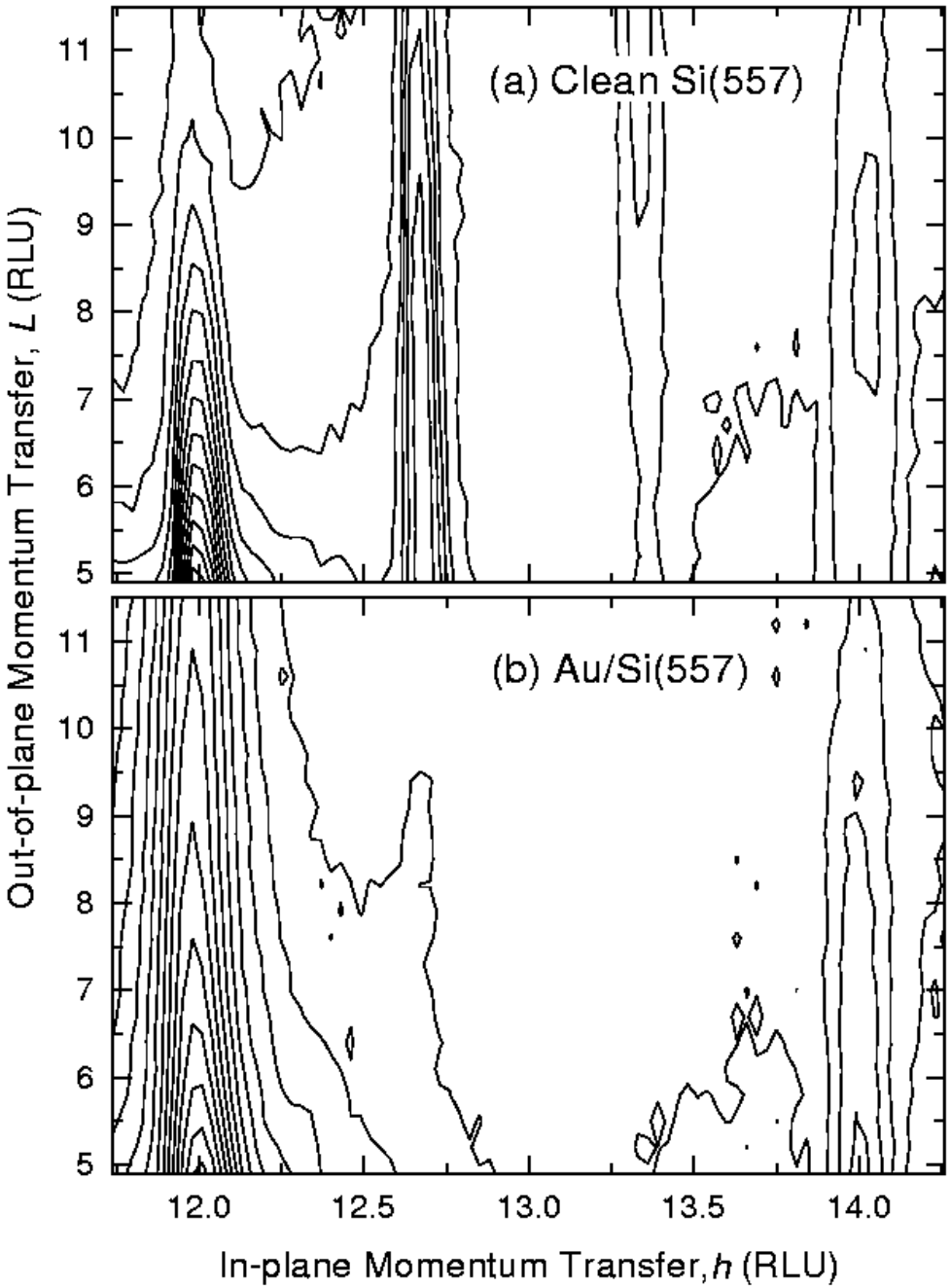


Si(557) surface

Alignment is Straightforward

```
CALCULATED PARAMETERS:
          A           B           C       ALFA    BETA    GAMMA
REC:  0.164431    1.63392    0.116412   90.06   90.03   89.93
DIR:   38.2118    3.84548     53.9736   89.94   89.97   90.07
          H    K     L     TTH      TH      PHI      CHI      ALP      CTS    ERROR
OR 1 = 12.0  0.0   3.0  21.938 112.920   50.308   -1.137    3.841    22456  0.0027
OR 2 = -5.0  1.0   7.0  20.284  97.018  307.482   -2.259    9.179    20719  0.0018
OR 3 = 14.0  0.0  20.0  26.411 113.142   40.844   -1.290   26.483    13639  0.0009
OR 4 = 12.0  2.0   3.0  43.135 110.470    4.520   -2.092    4.313    12772  0.0009
Lambda = 1.20913 A, wv = 5.19647, Energy = 10.2542 keV (FIXED)
Five-Circle Mode using alm = 2 and bem = 2:
```

Centered Orthorhombic unit cell contains two steps.

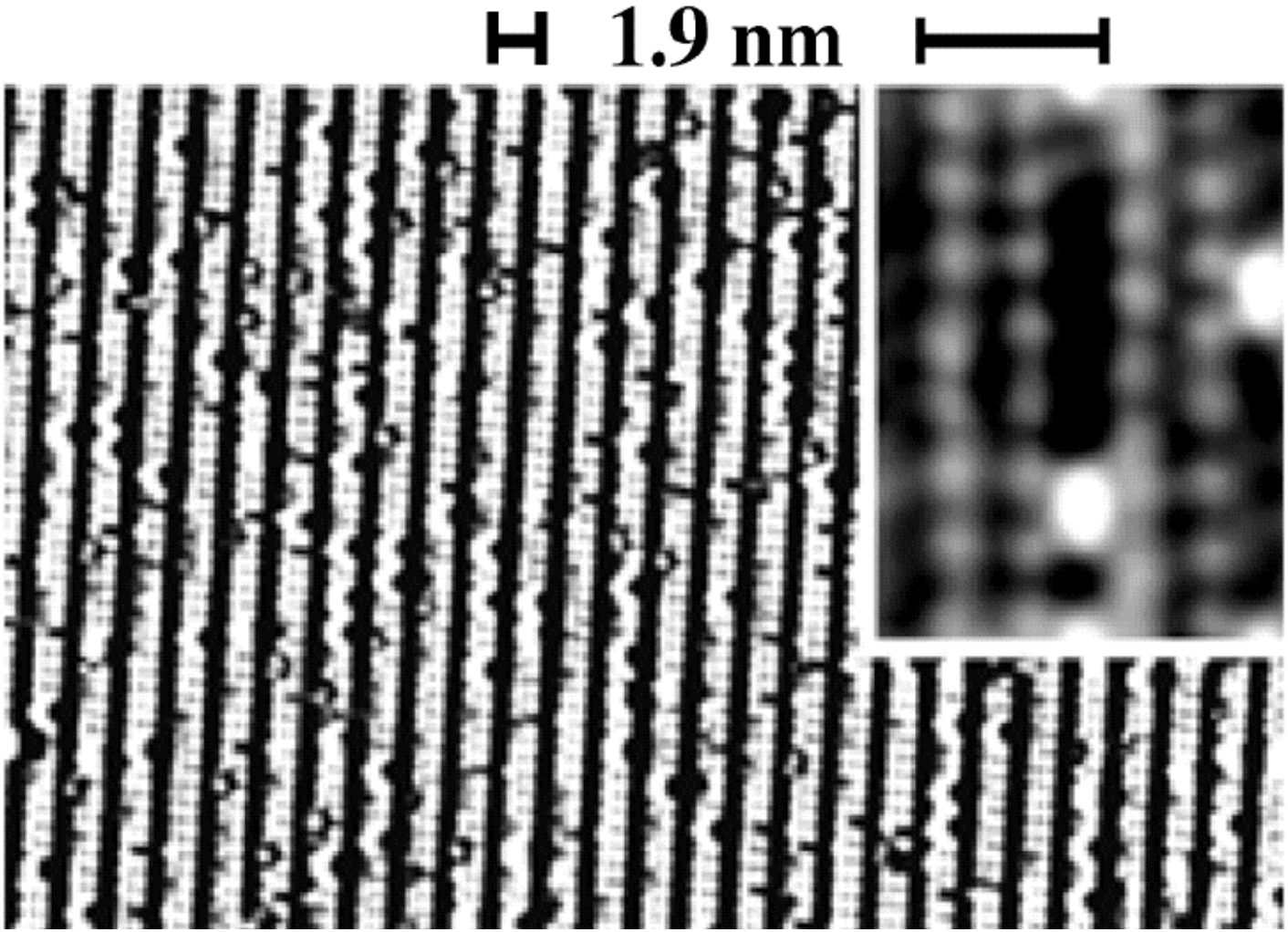


3×1 clean surface

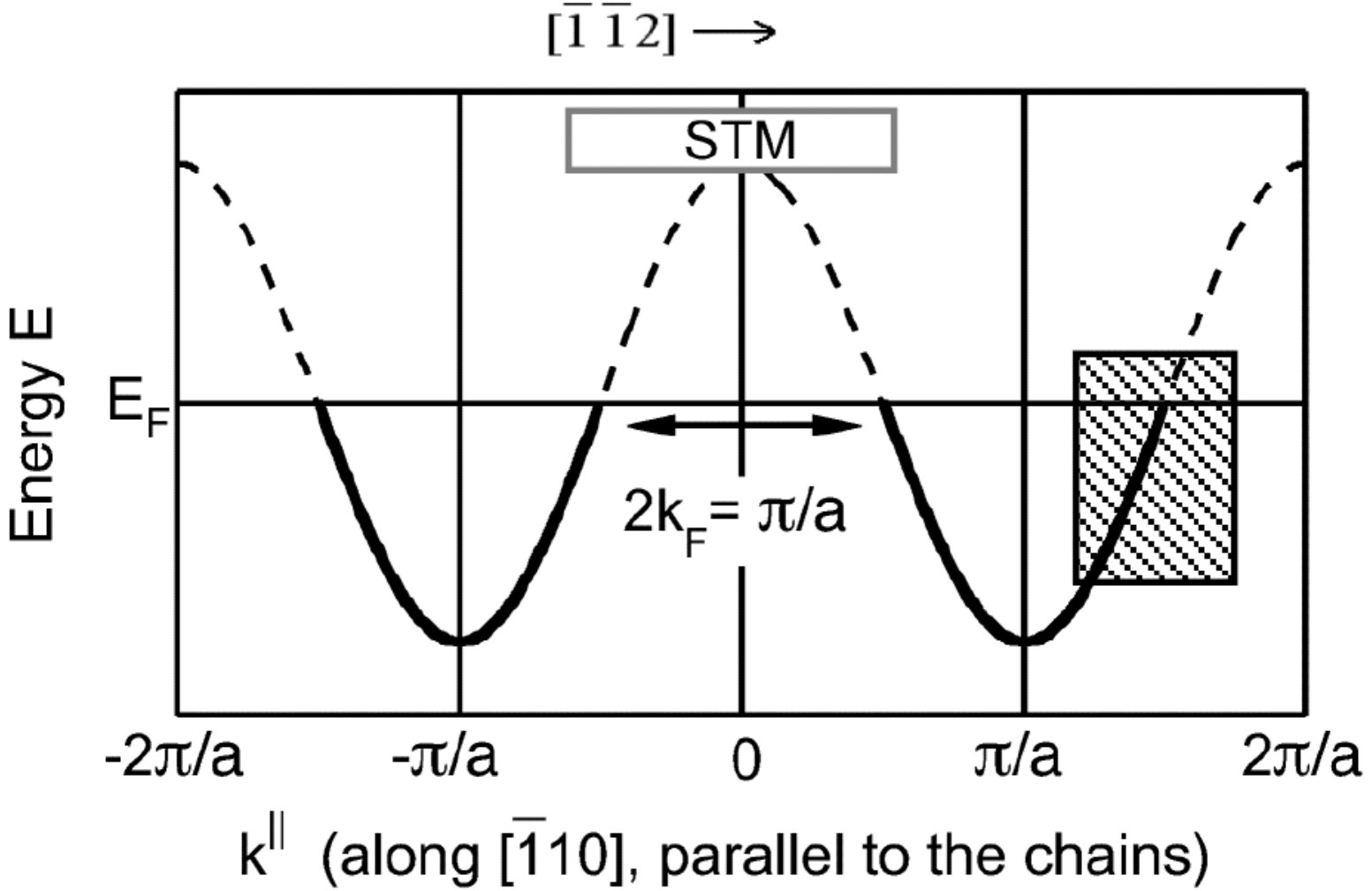
1×1 surface with 0.2ML Au at 600C

STM of Si(557)/Au

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

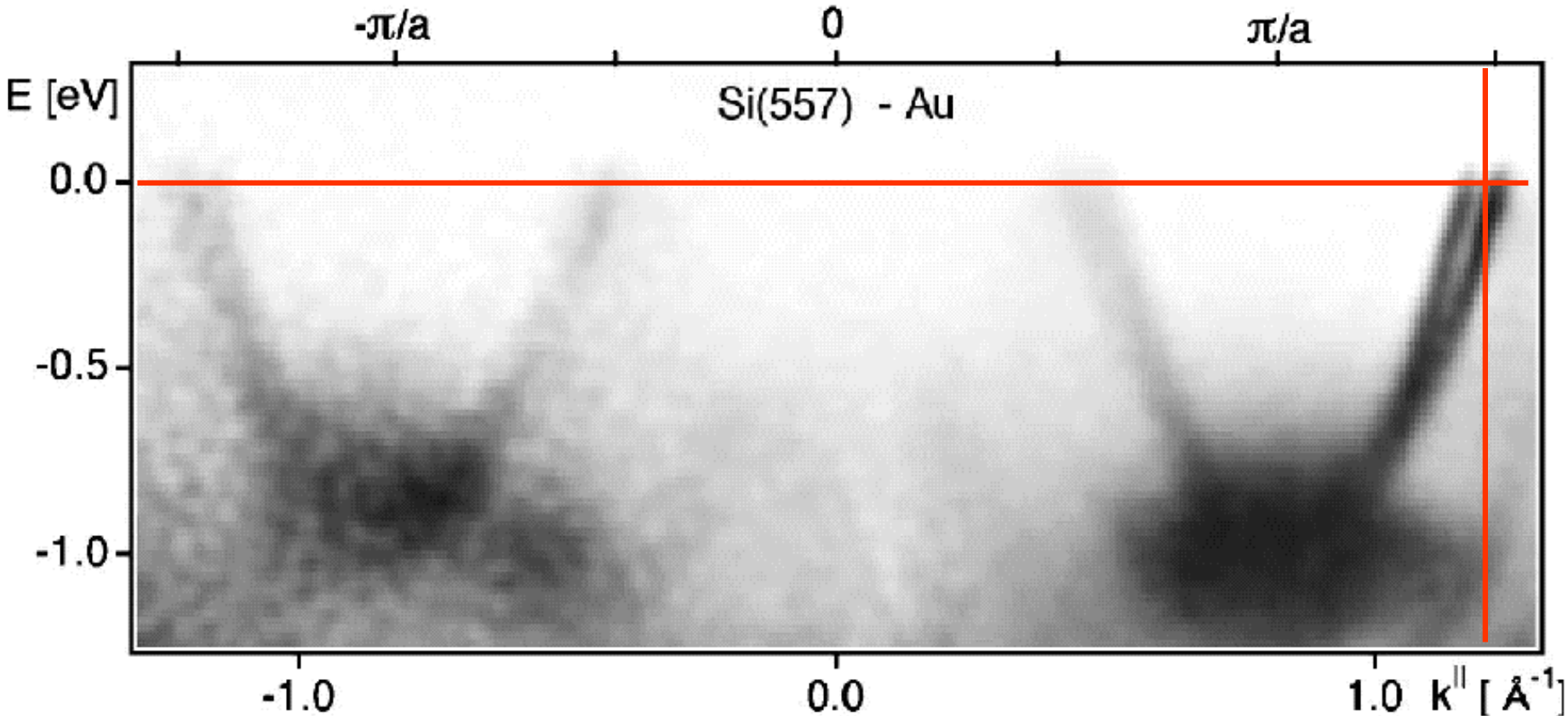


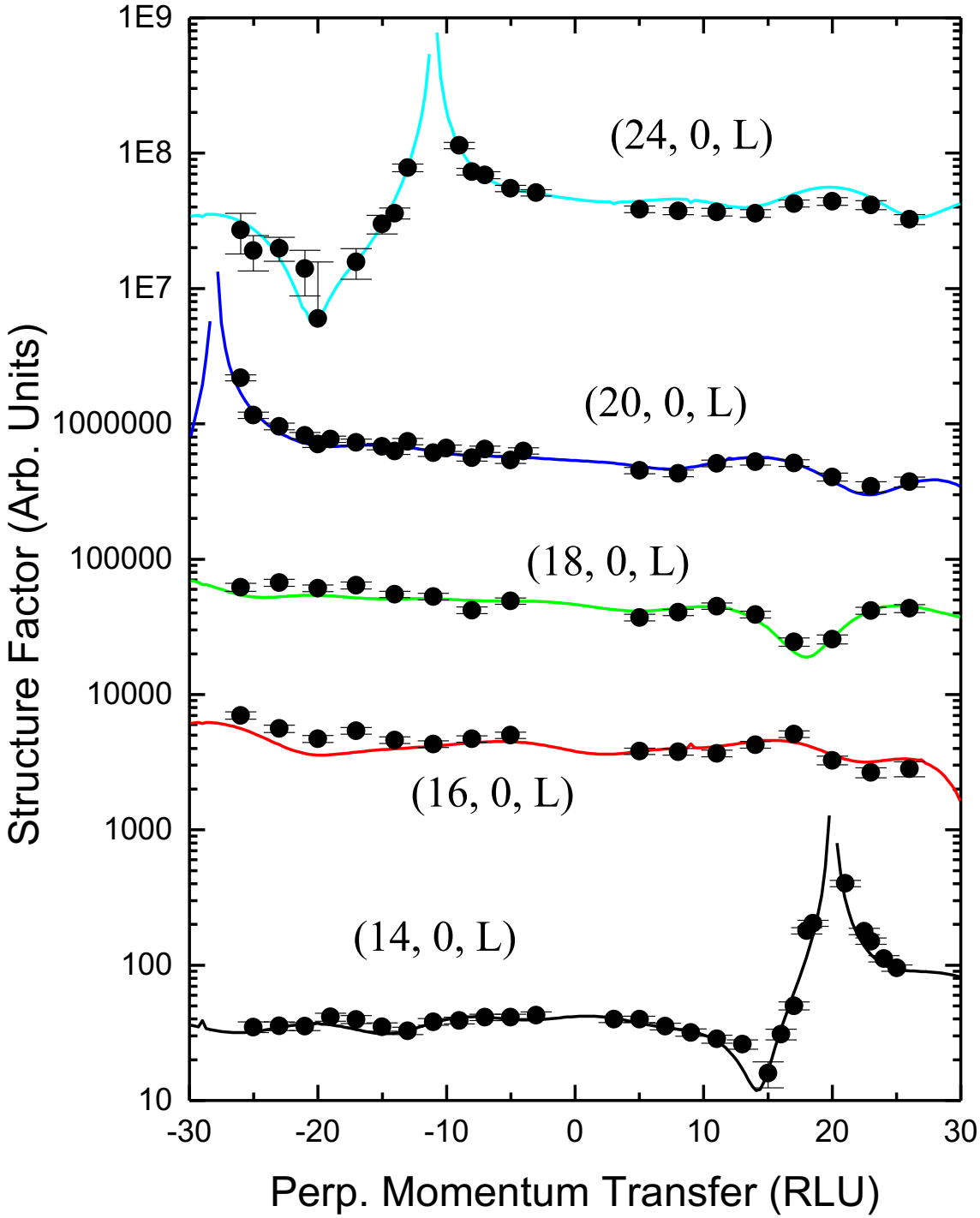
Schematic Band Topology for Au/Si(557)



Photoemission from Surface States Parallel to the Au Chains in Au/Si(557)

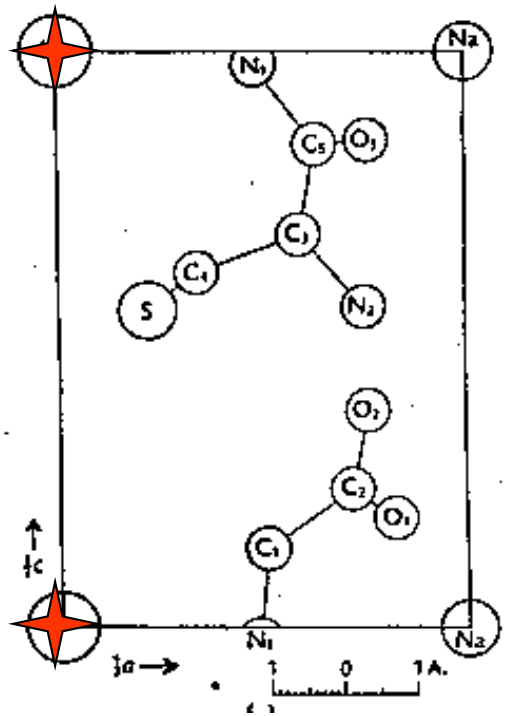
K. N. Altmann et. al. Phys Rev B 64 035406 (2001)



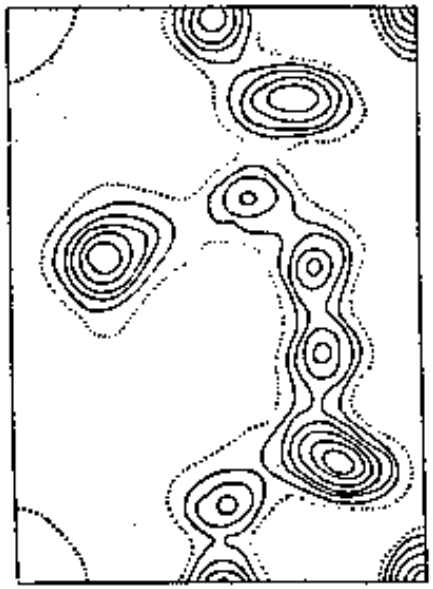

1E9
1E8
1E7
1000000
100000
10000
1000
100
10
Structure Factor (Arb. Units)
(24, 0, L)
(20, 0, L)
(18, 0, L)
(16, 0, L)
(14, 0, L)
-30
-20
-10
0
10
20
30
Perp. Momentum Transfer (RLU)

Phasing by a Single Heavy Atom

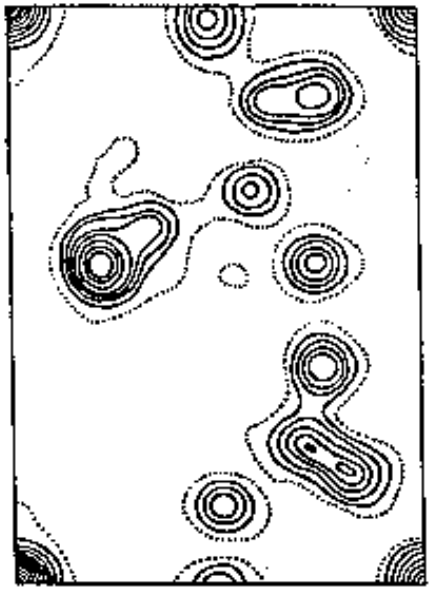
H. B. Dyer, Acta Cryst. 4 42 (1951)



Cysteinylglycine
sodium iodide

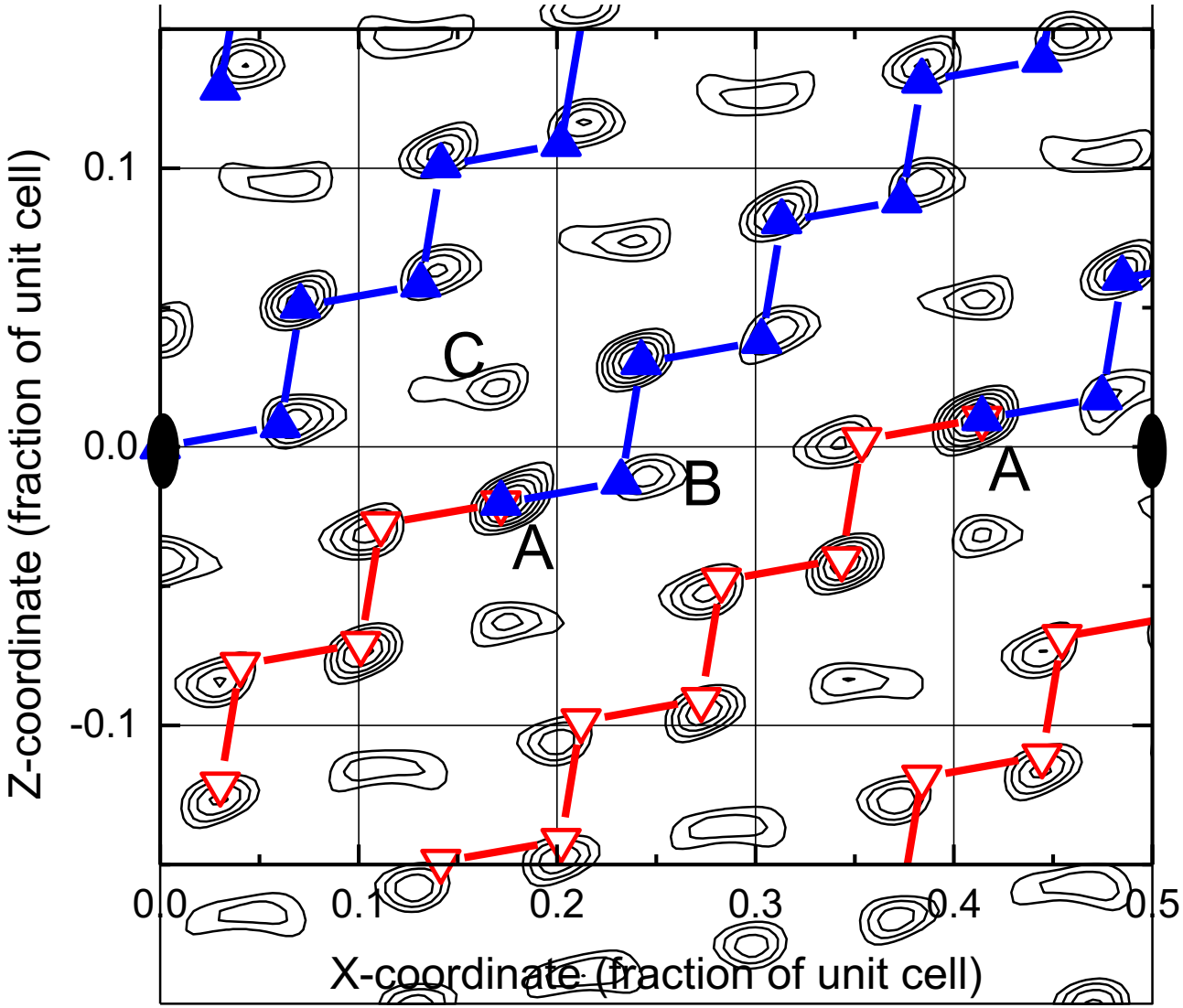


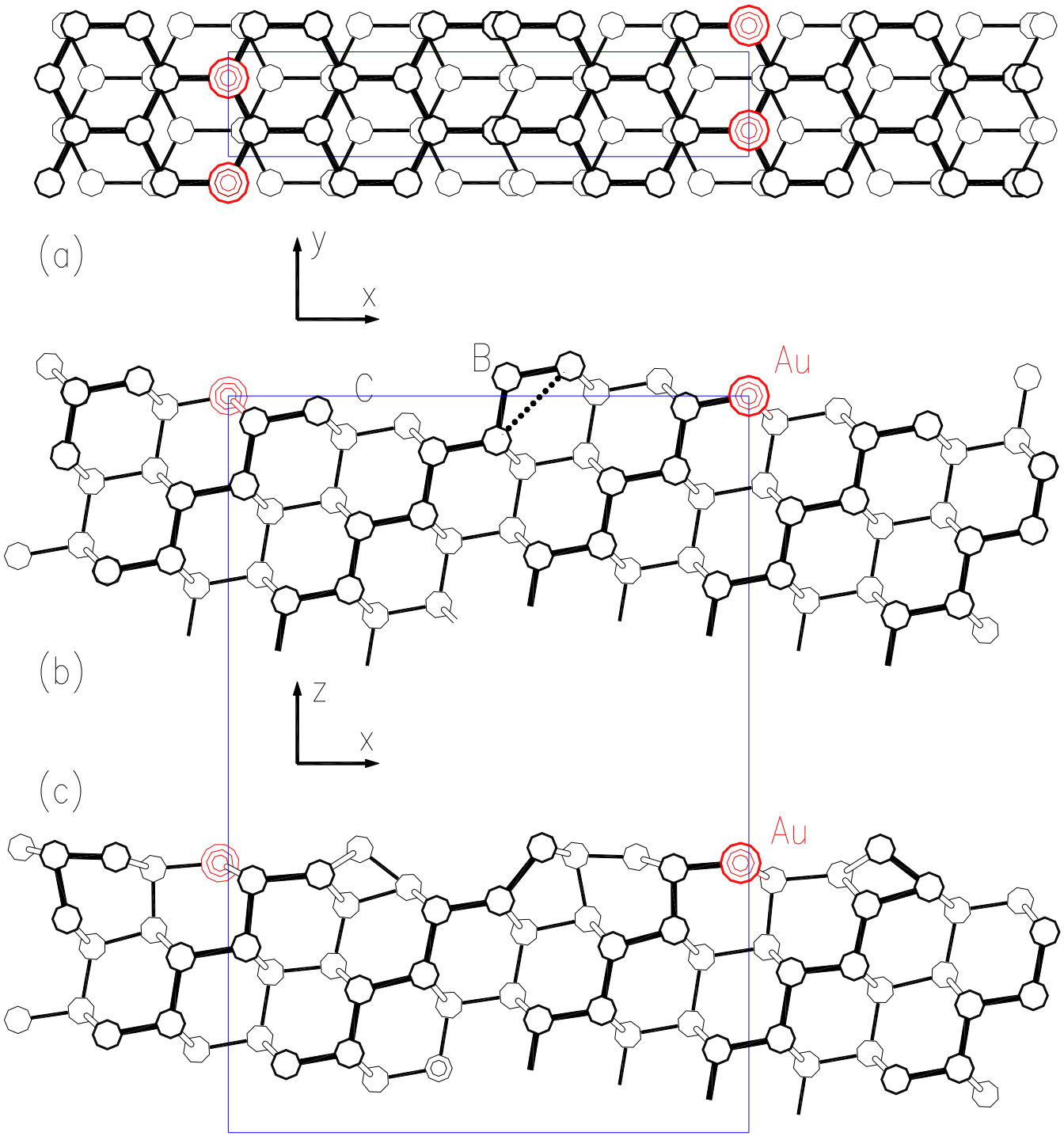
Patterson



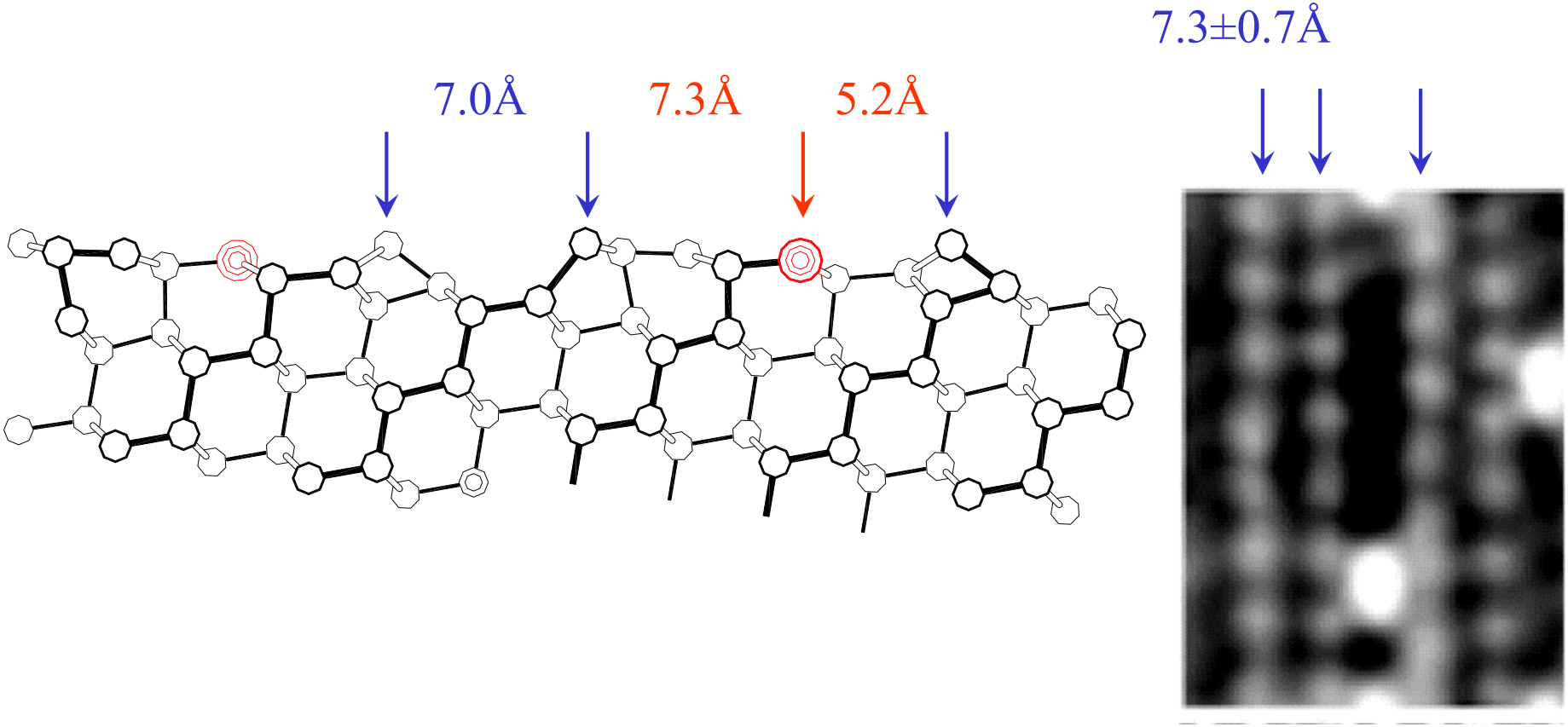
Electron density

X-Z Patterson of Au/Si(557)



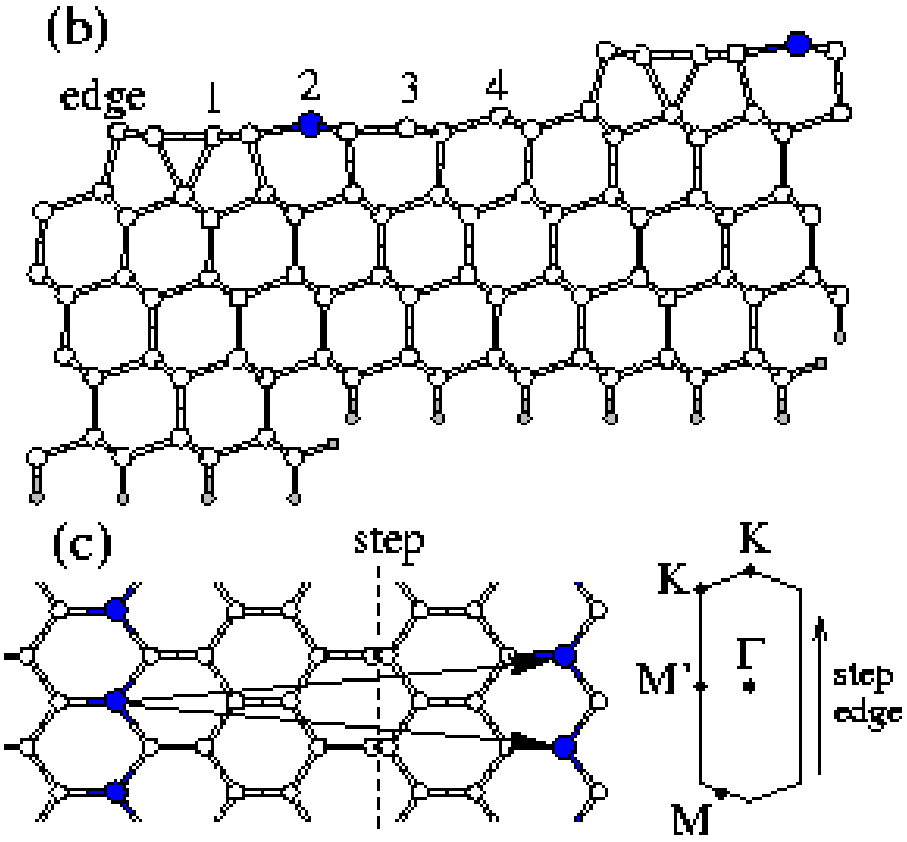

(a)
y
x
B
C
Au
(b)
z
x
(c)
Au

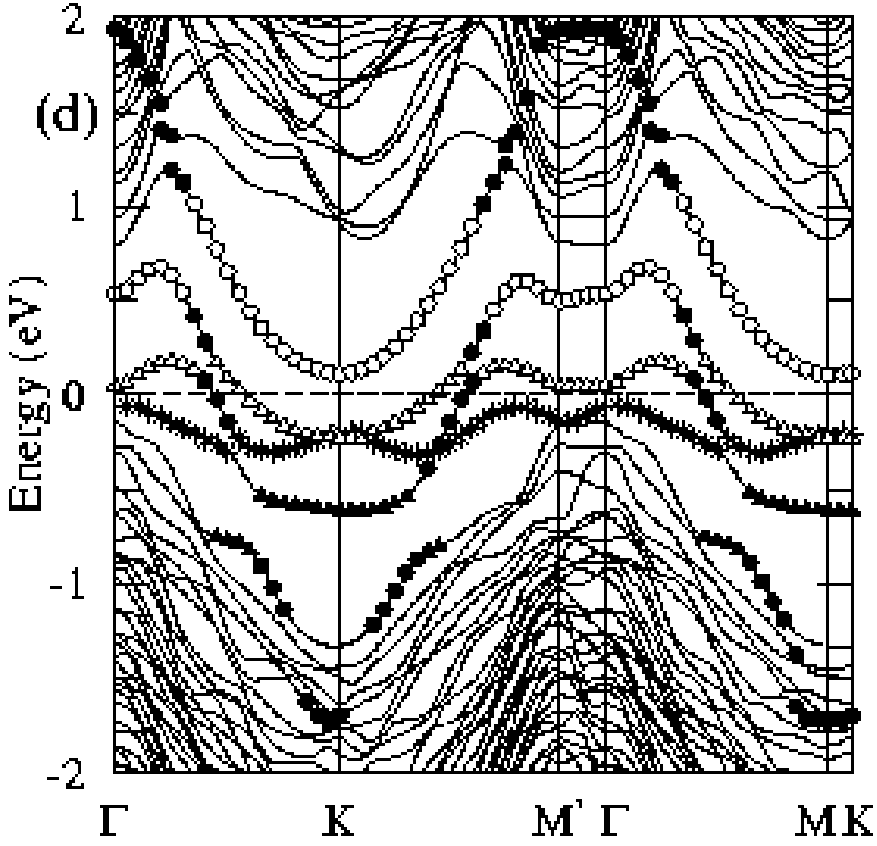
Comparison with STM



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

D. Sanchez-Portal et. al. Phys. Rev. B **65**, 081401 (2002)

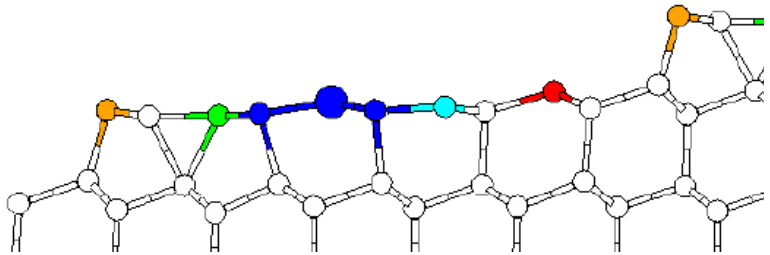




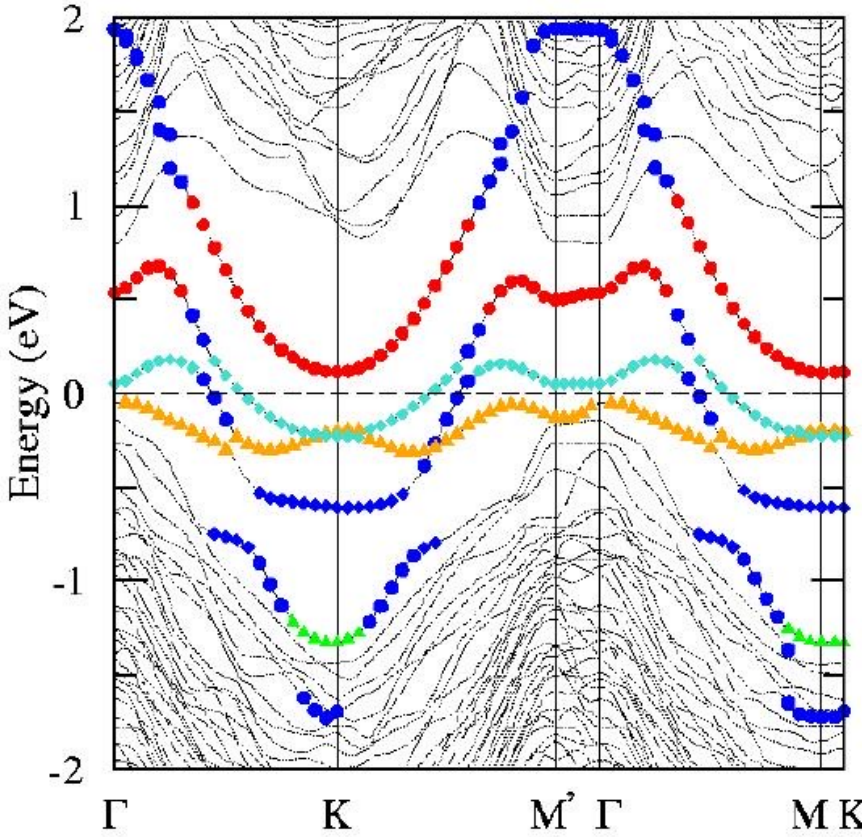
Si(557)-Au: calculated band structure

D. Sanchez-Portal et. al. Phys. Rev. B **65**, 081401 (2002)

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.

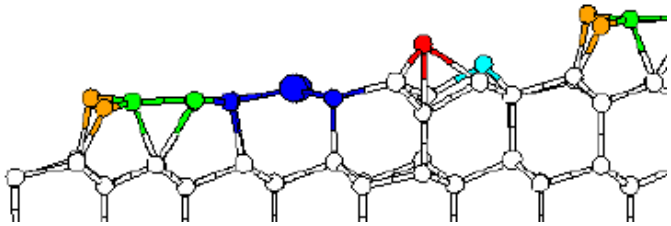


Si(557)-Au: role of adatoms

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

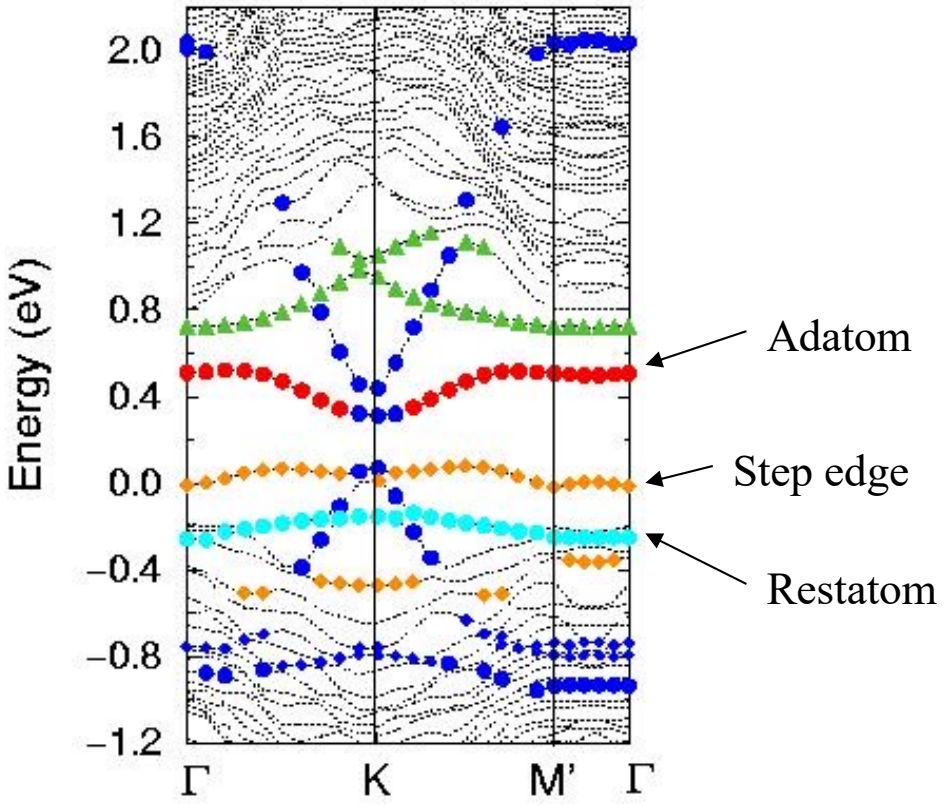
The presence of one row of adatoms partially saturating some of the dangling bonds do not modify our main conclusions

However it is slightly favorable energetically, with a gain of ~ **0.14 eV/Au**



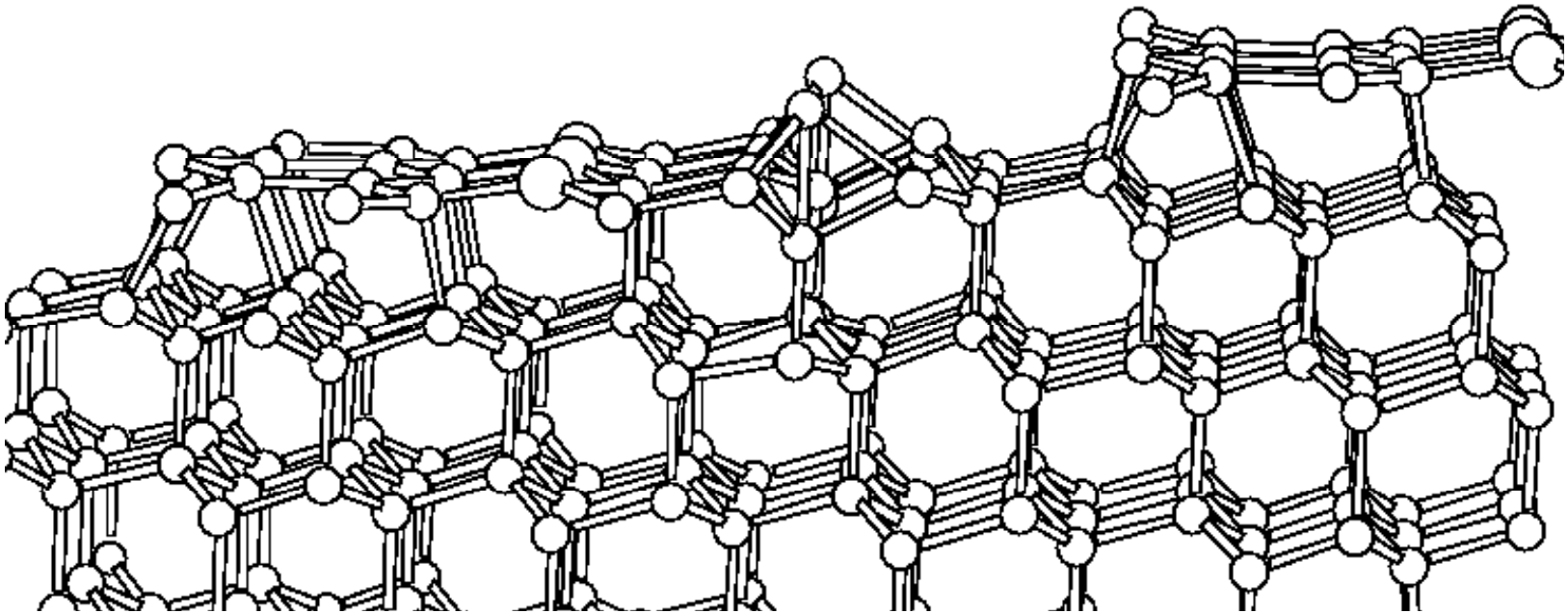
- The step-edge band (orange) is located precisely at the Fermi energy
- Still two bands* (blue symbols) associated to the gold chain.

*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