# Surface X-ray Diffraction

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

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# Outline

- Surface Diffraction

- 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 Diffraction

- 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
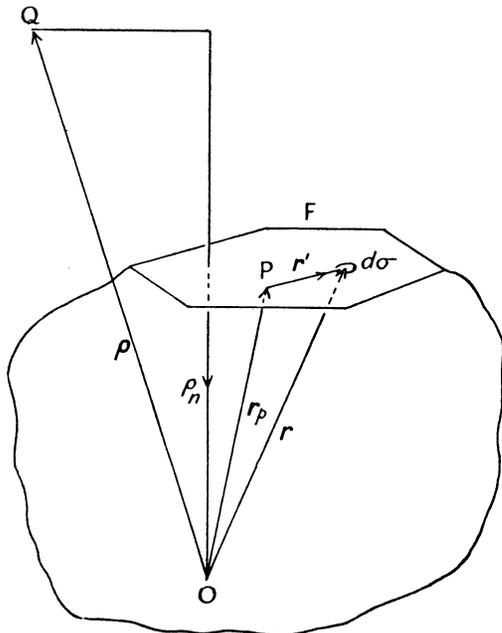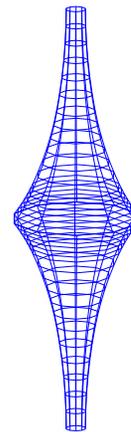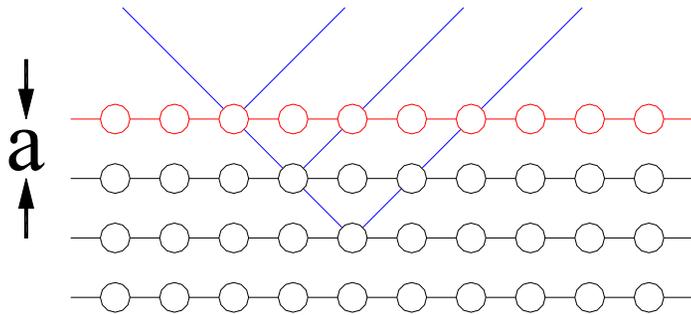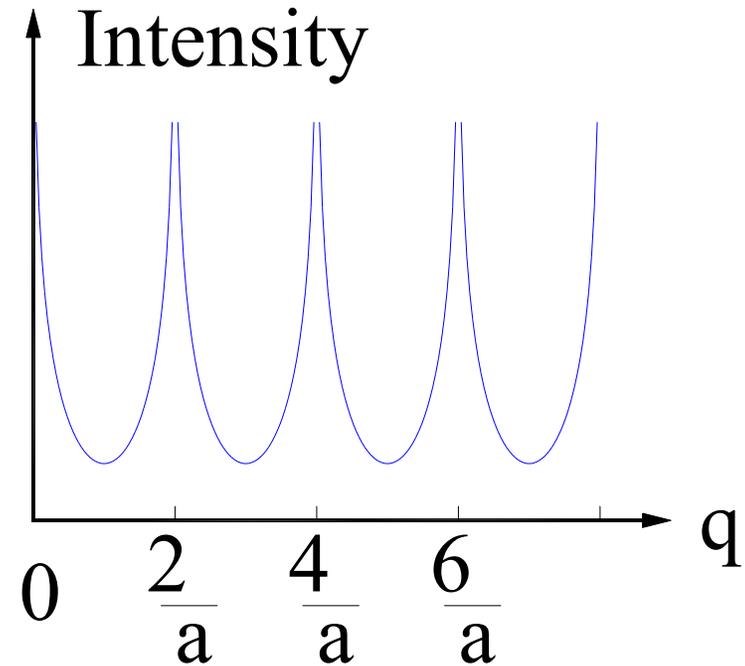
FIG. 200



"Stacheln"
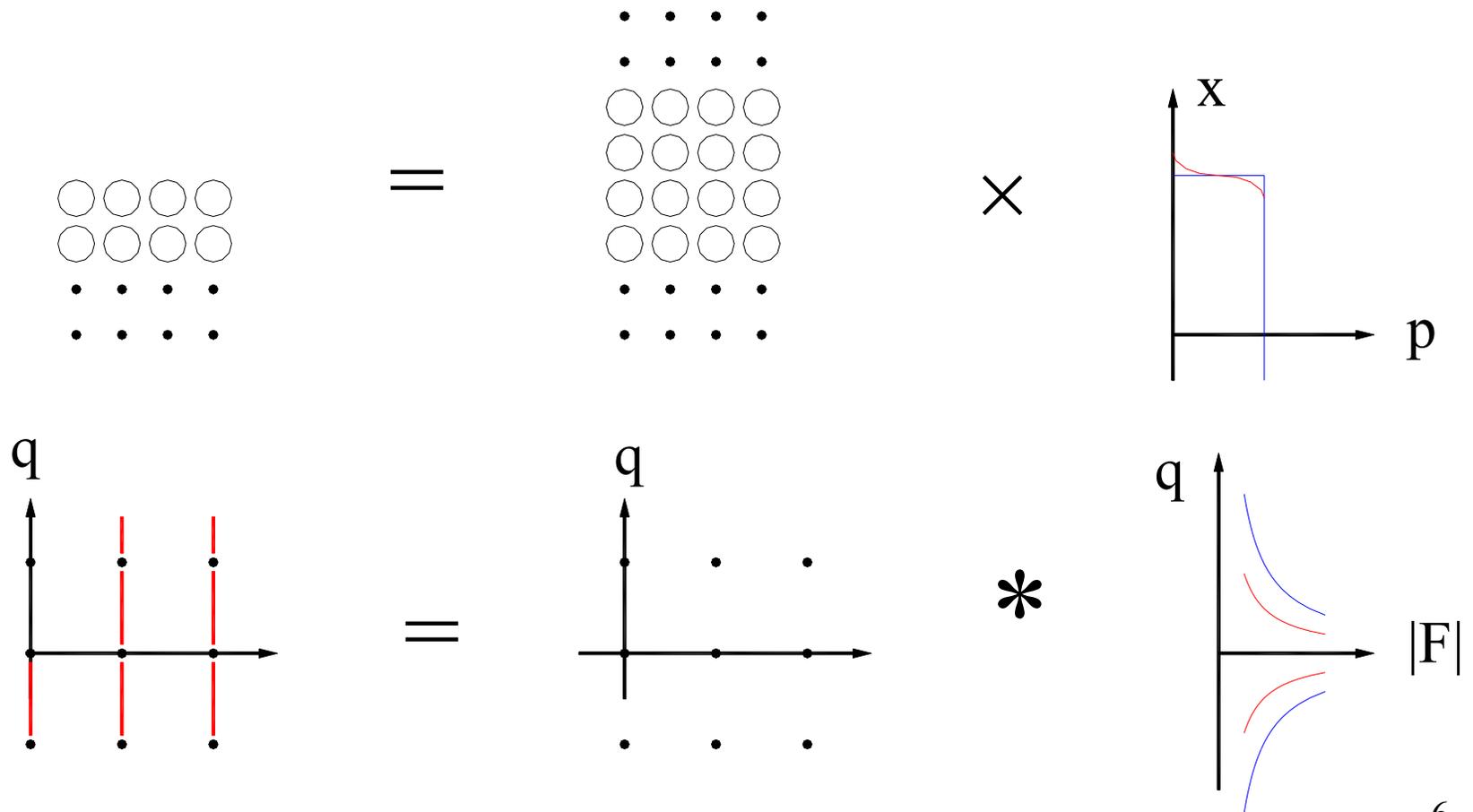
# Origin of Truncation Rods



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

$$= \sum_{n=0}^{\infty} f_L \, e^{inqa}$$
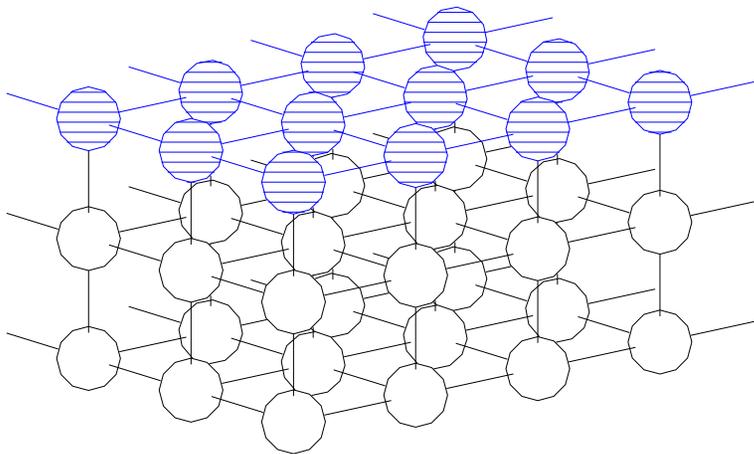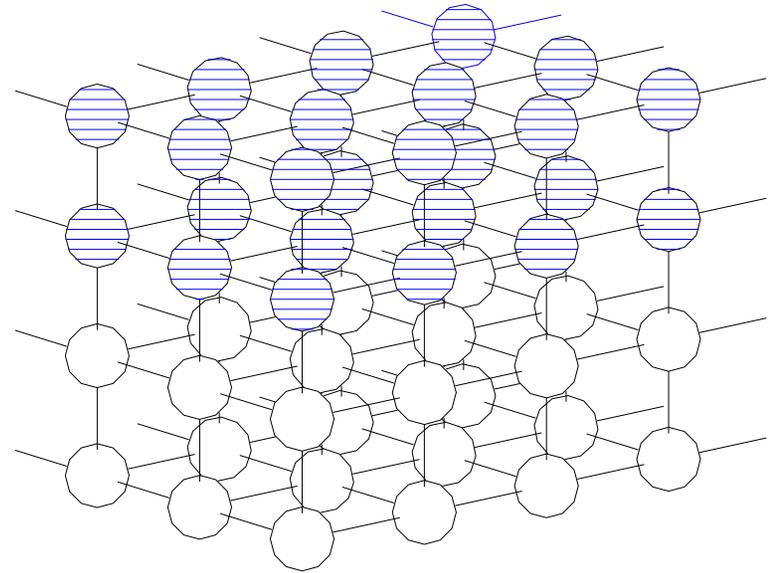
$$= \frac{f_L}{1 - e^{iqa}}$$
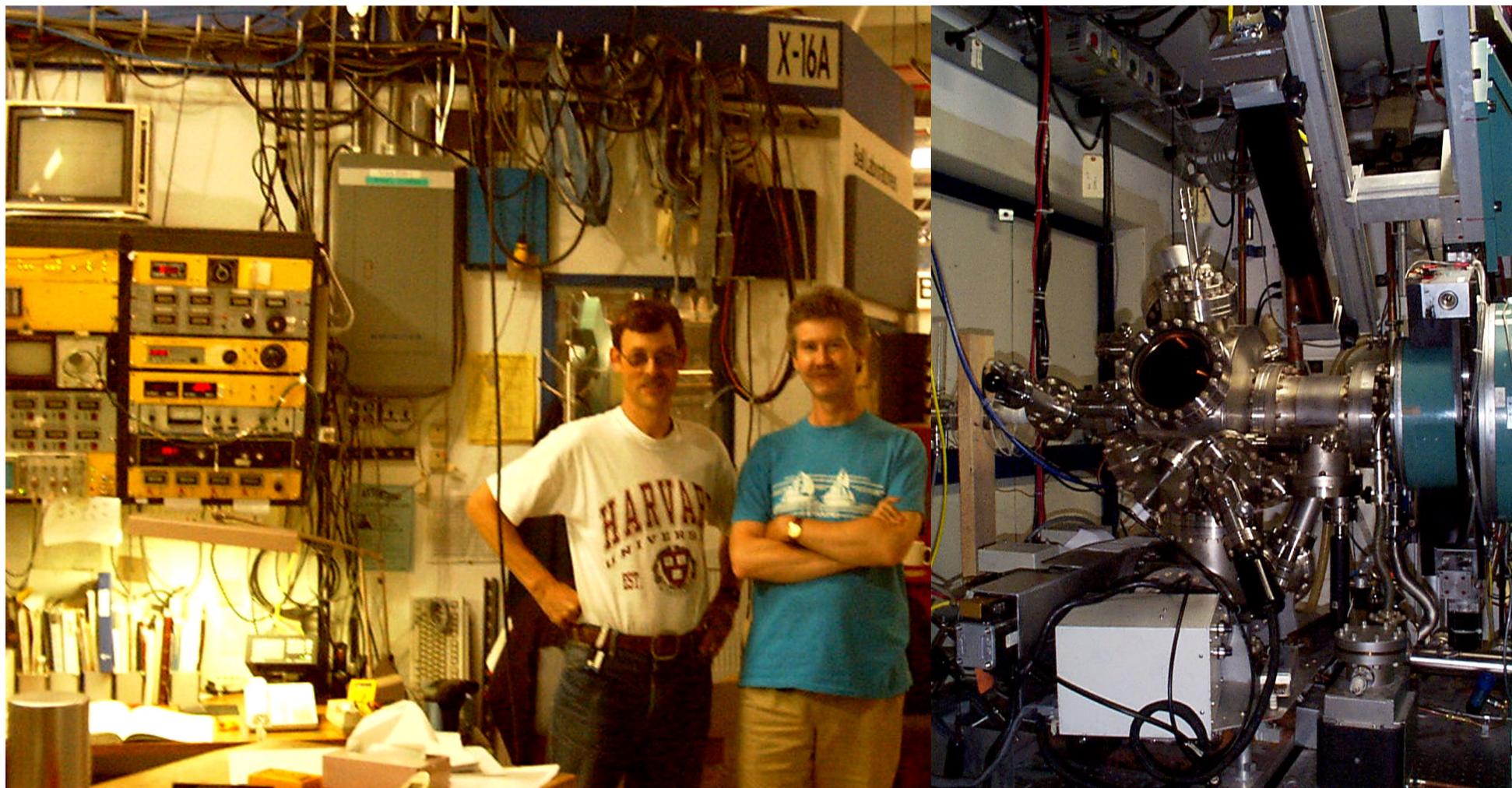
# CTR as Convolution

# Surfaces and Interfaces
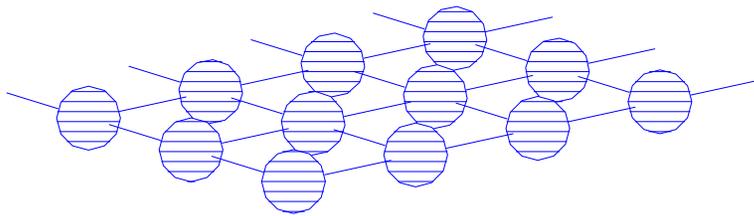
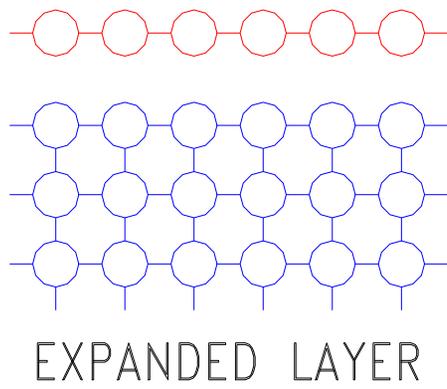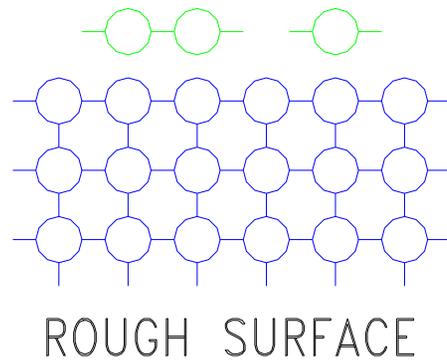Isolated monolayer
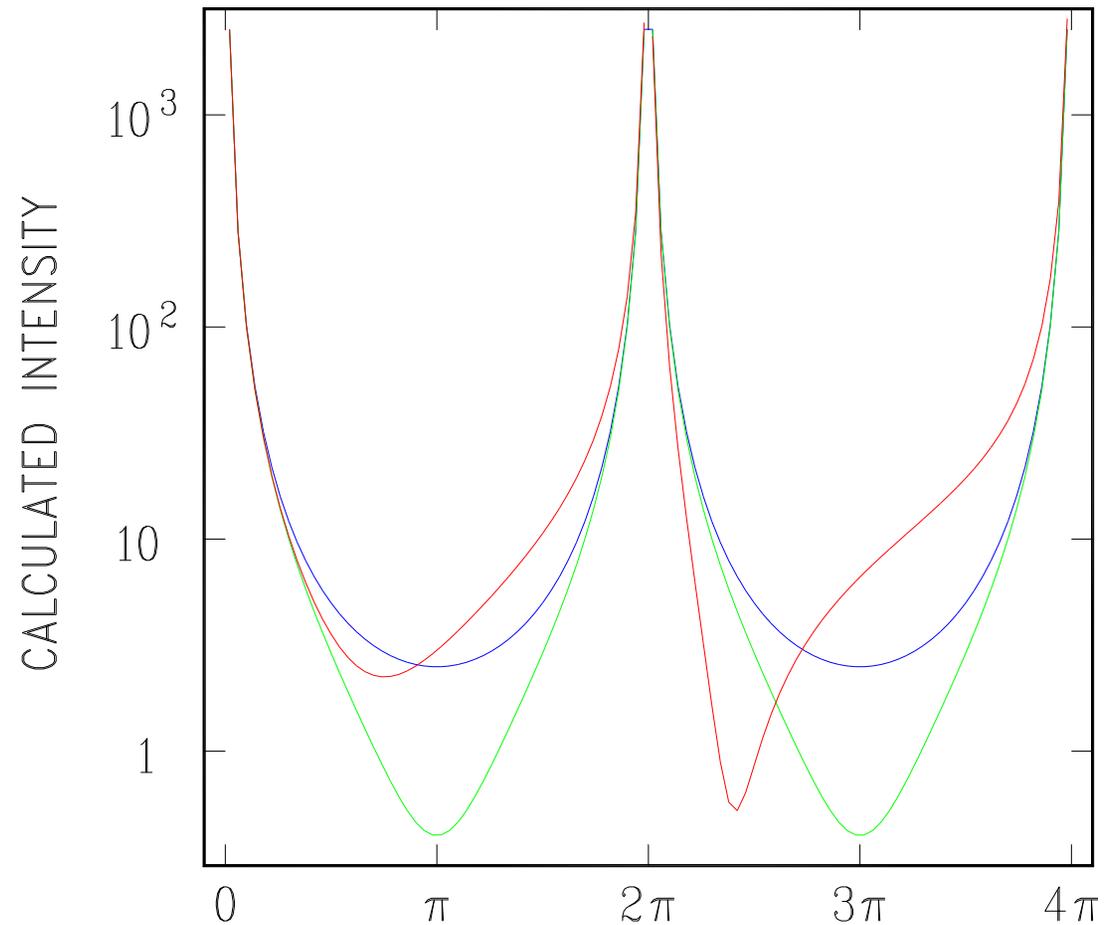
Surface of Crystal
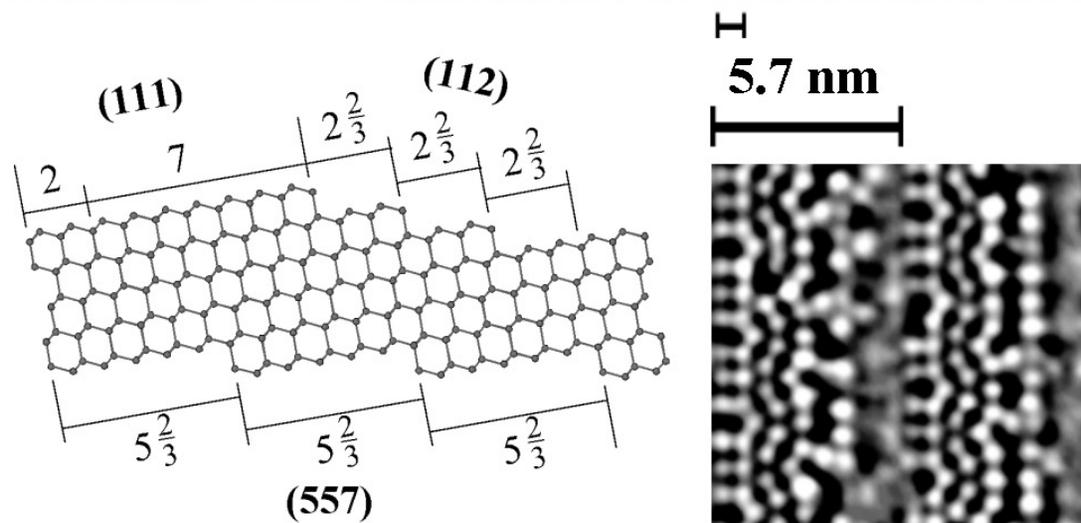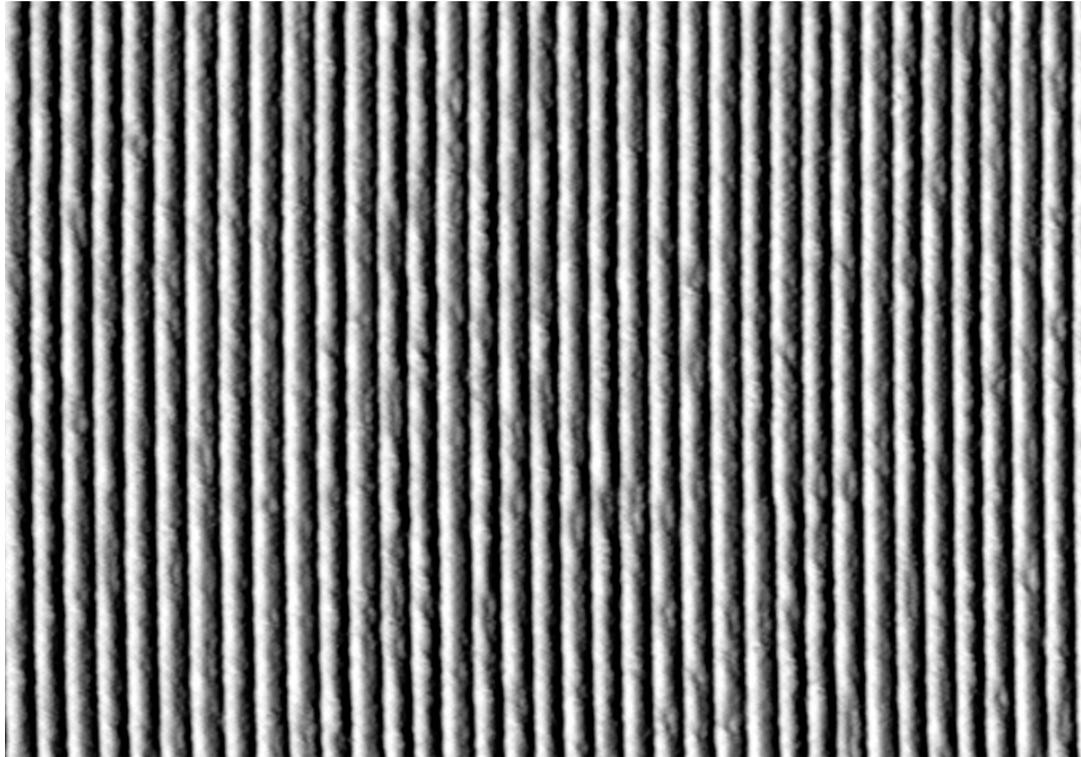
Crystal-Crystal Interface

# X16A Surface X-ray Diffraction
## operating since 1987 ...

# CTR is Sensitive to Surface Structure



ROUGH SURFACE

EXPANDED LAYER

I. K. Robins

CALCULATED INTENSITY

(111)  (112)

(557)

5.7 nm

# Crystallography of Stepped Surfaces

Silicon (111)



557

446

335

224

113        (14,0,20)

(2,0,17)220

111

002        (12,0,3)

11-1
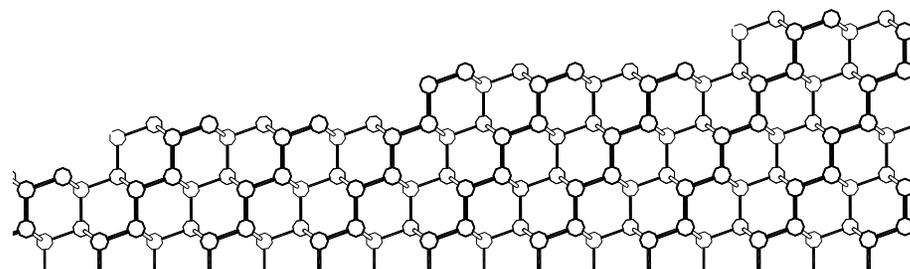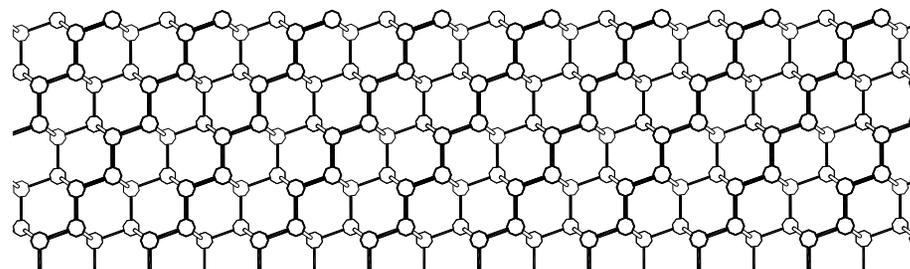
Si(557) surface

# Alignment can be 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:
```
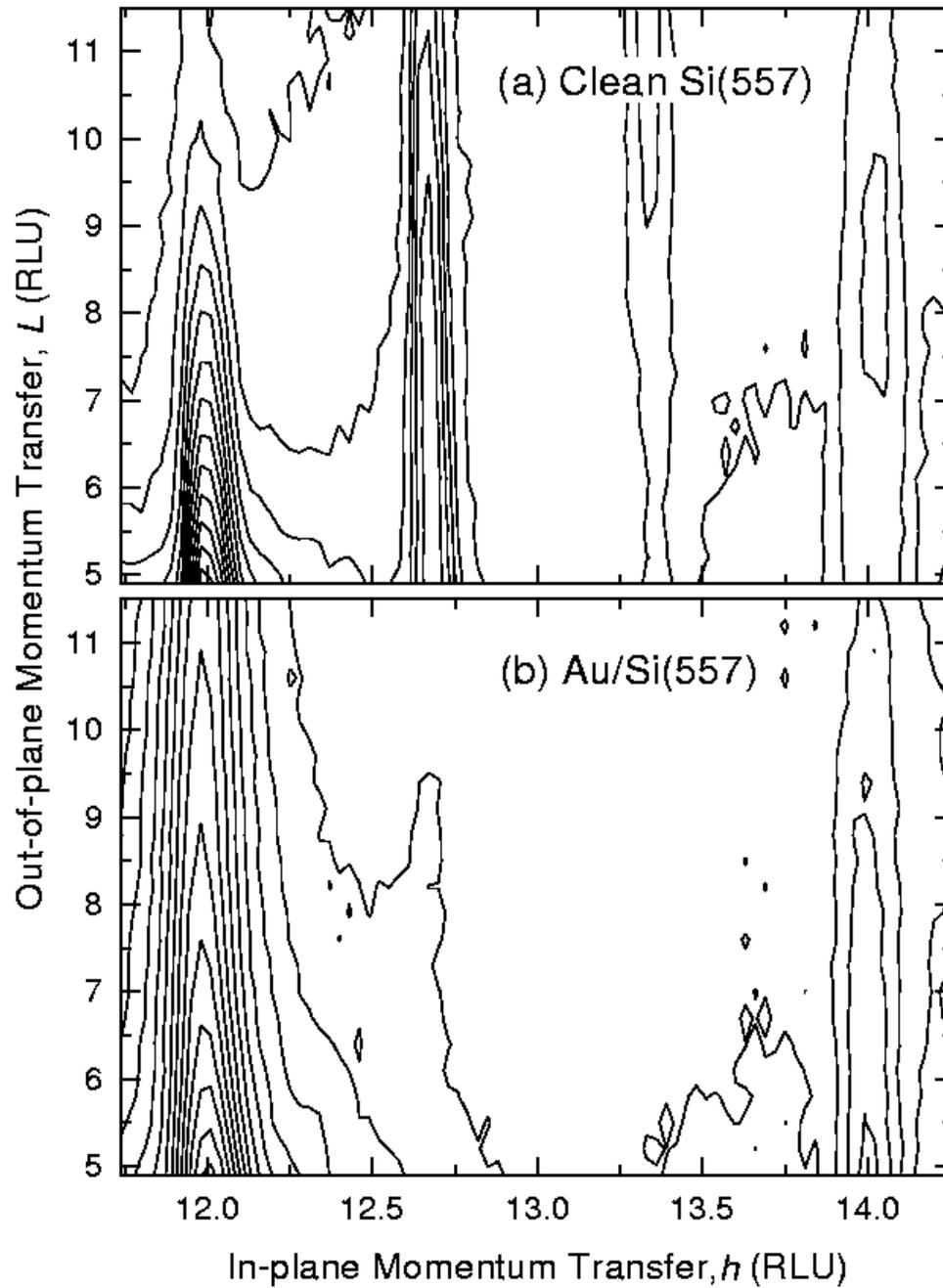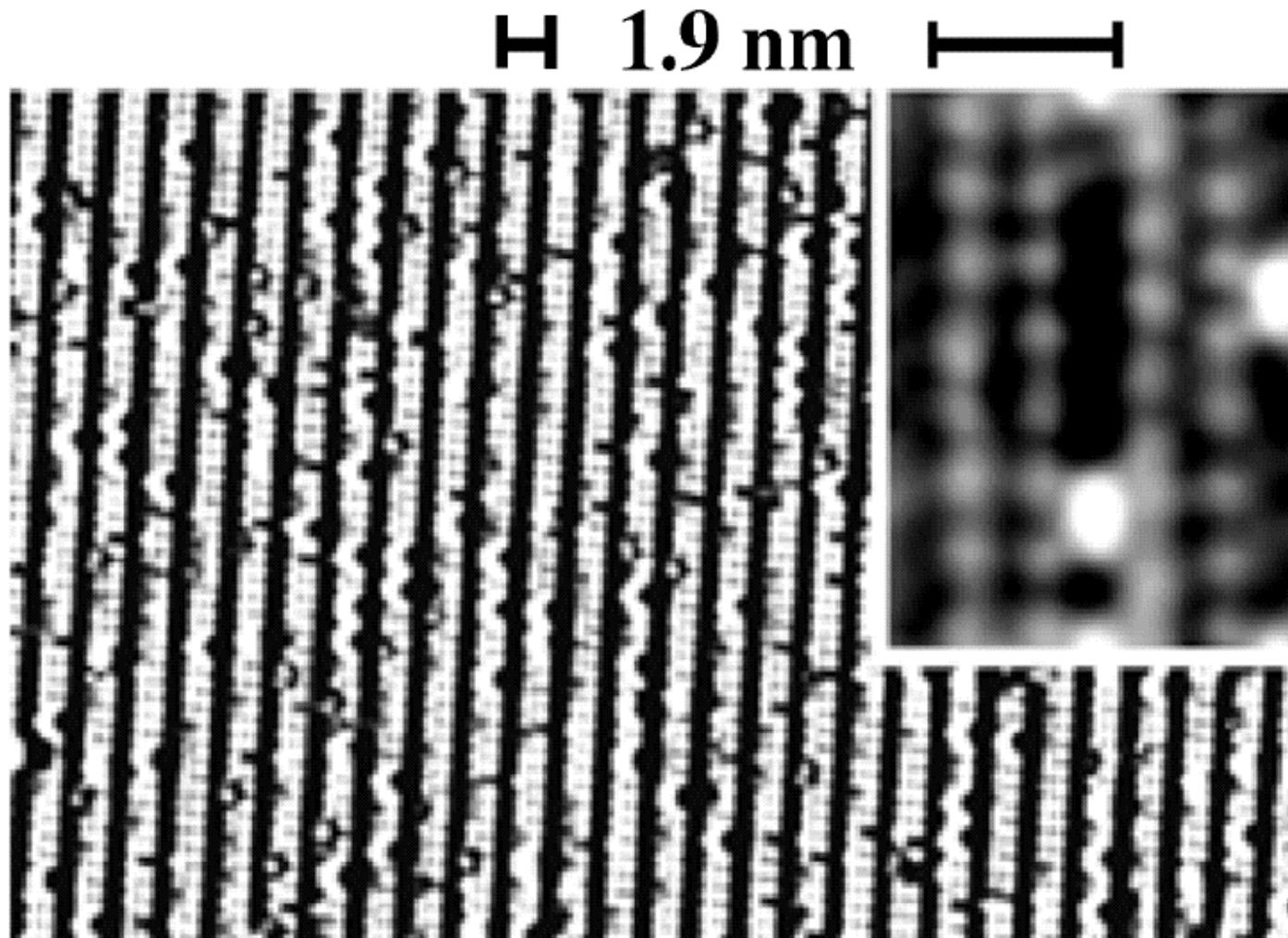
Centered Orthorhombic unit cell contains two steps.
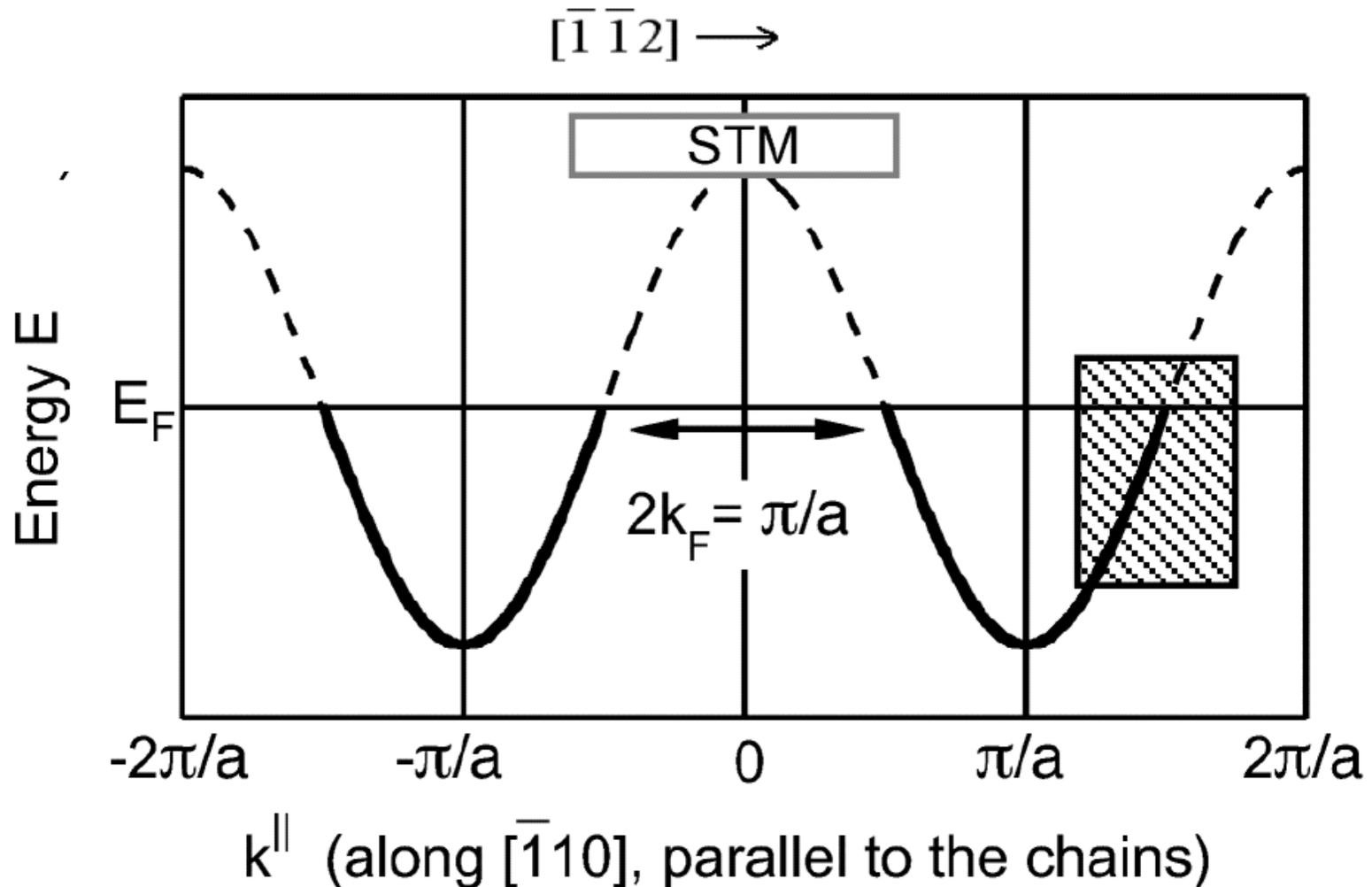
3×1 clean surface

1×1 surface with 0.2ML Au at 600C

# STM of Si(557)/Au
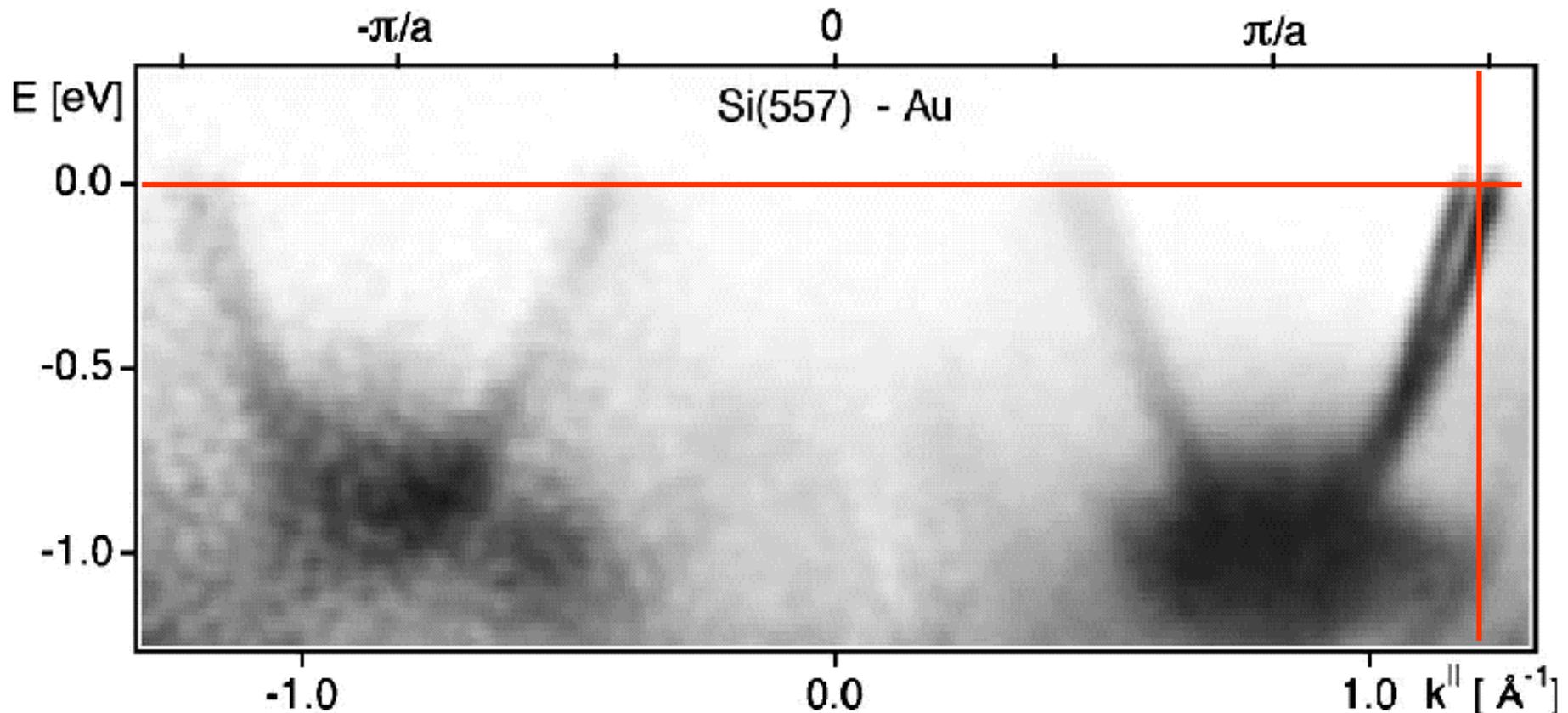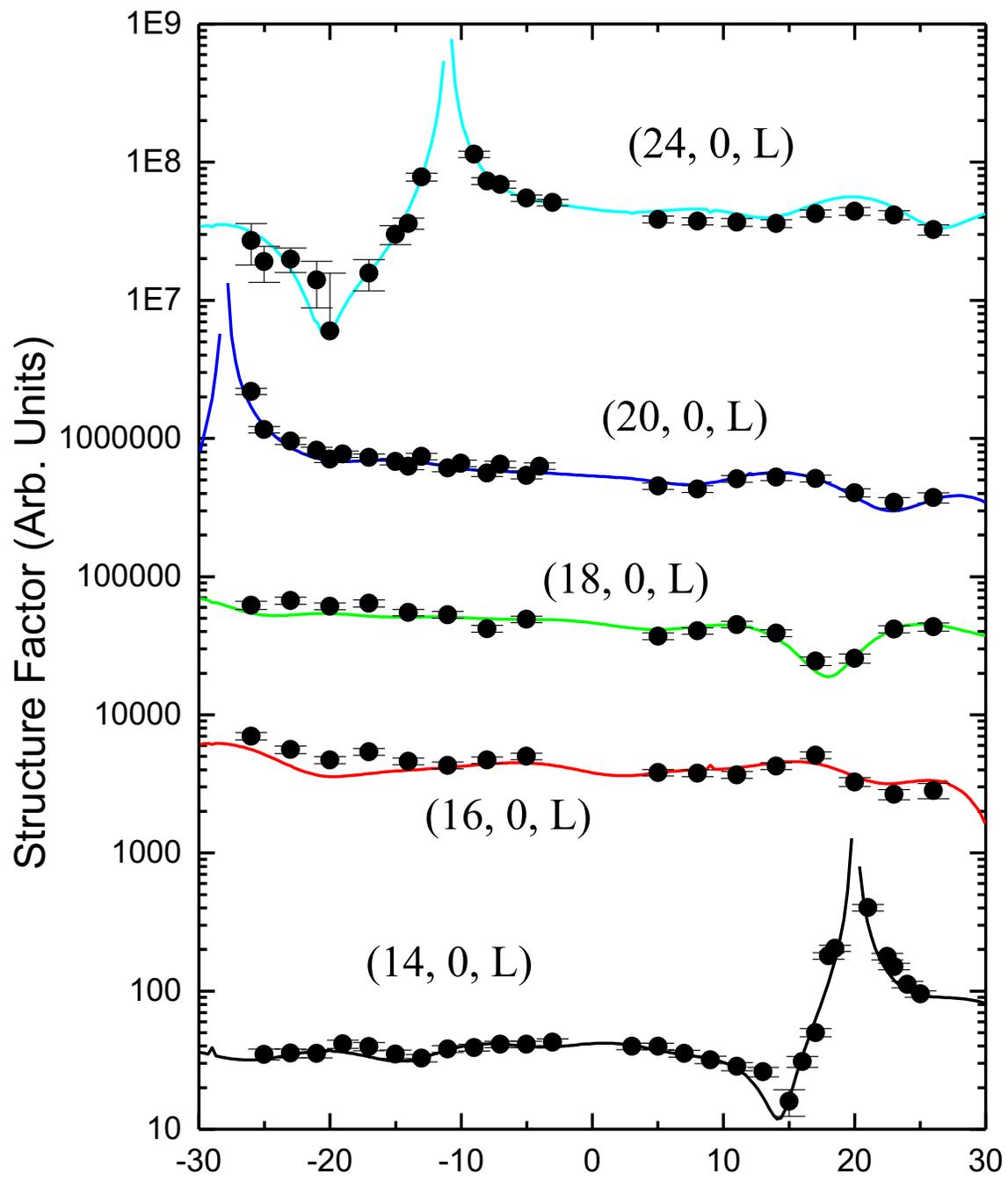
## R. Losio, et. al., Phys. Rev. Lett. 86 4632 (2001)

# 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)
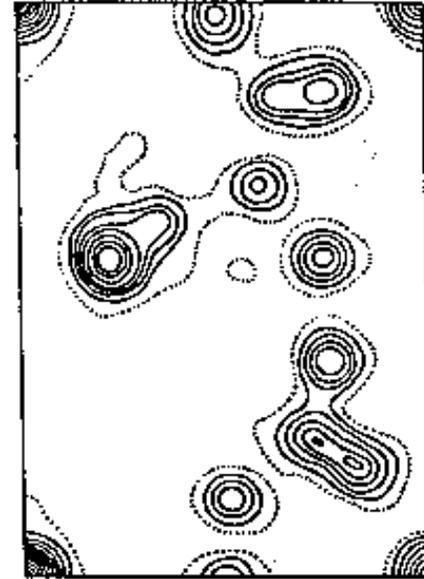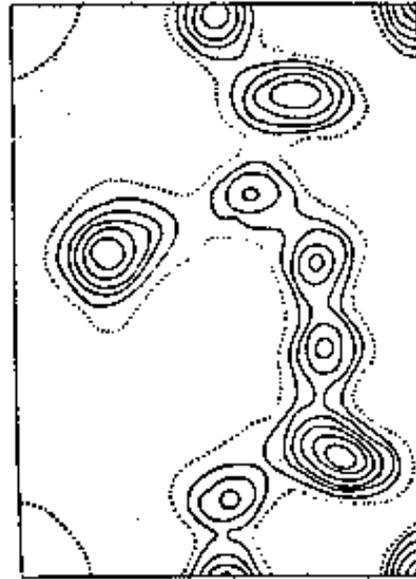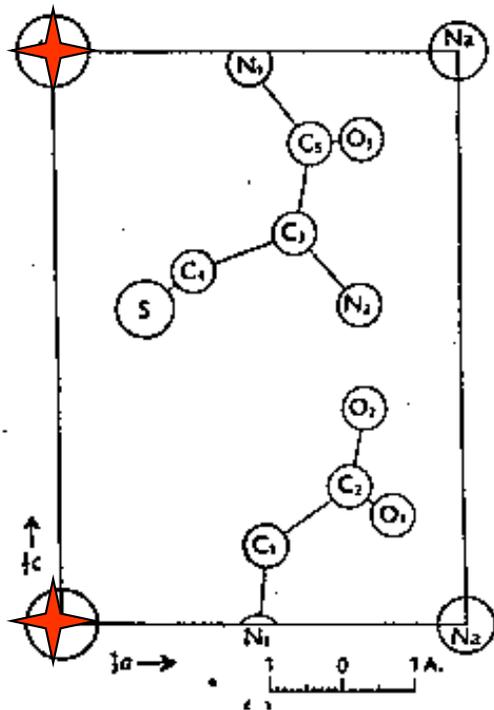
(24, 0, L)

(20, 0, L)

(18, 0, L)

(16, 0, L)

(14, 0, L)

Structure Factor (Arb. Units)

# Phasing by a Single Heavy Atom
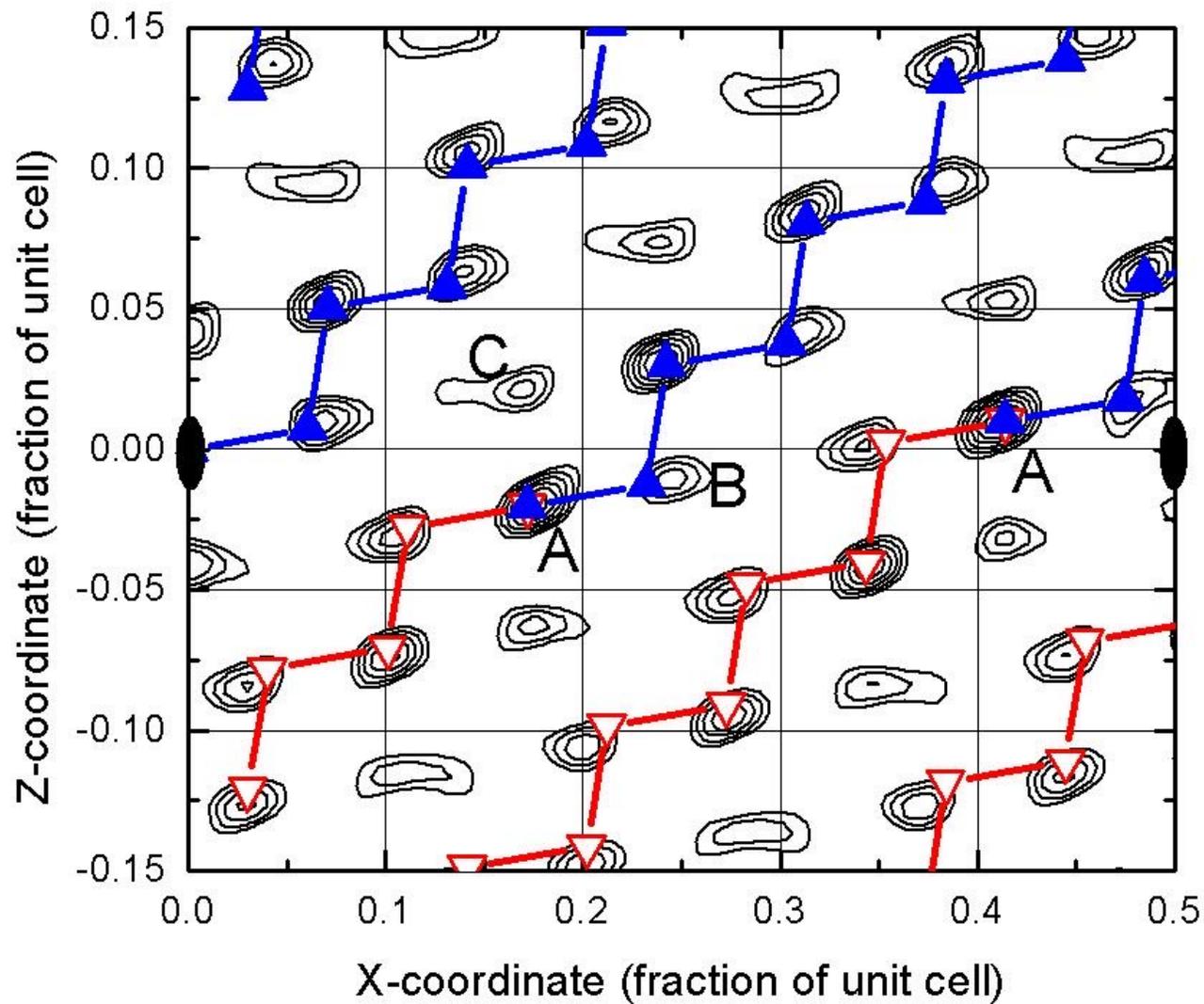## H. B. Dyer, Acta Cryst. $\underline{4}$ 42 (1951)



Cysteinylglycine
sodium iodide

Patterson

Electron density

# X-Z Patterson of Au/Si(557)
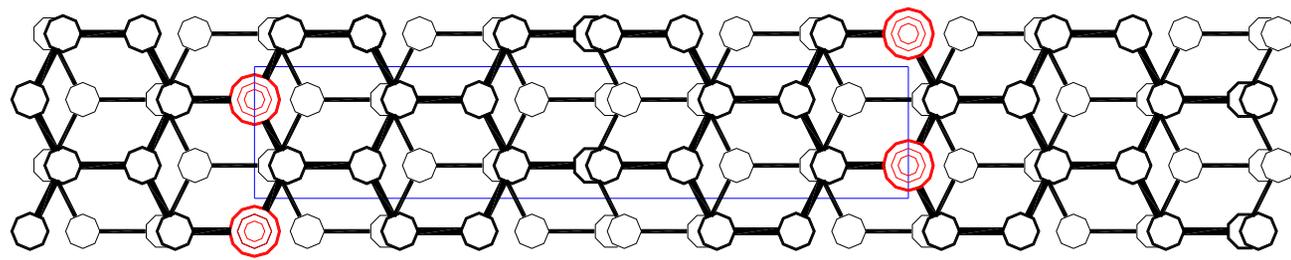
(a)

y
x

(b)

B
C
Au

(c)

z
x

Au

20
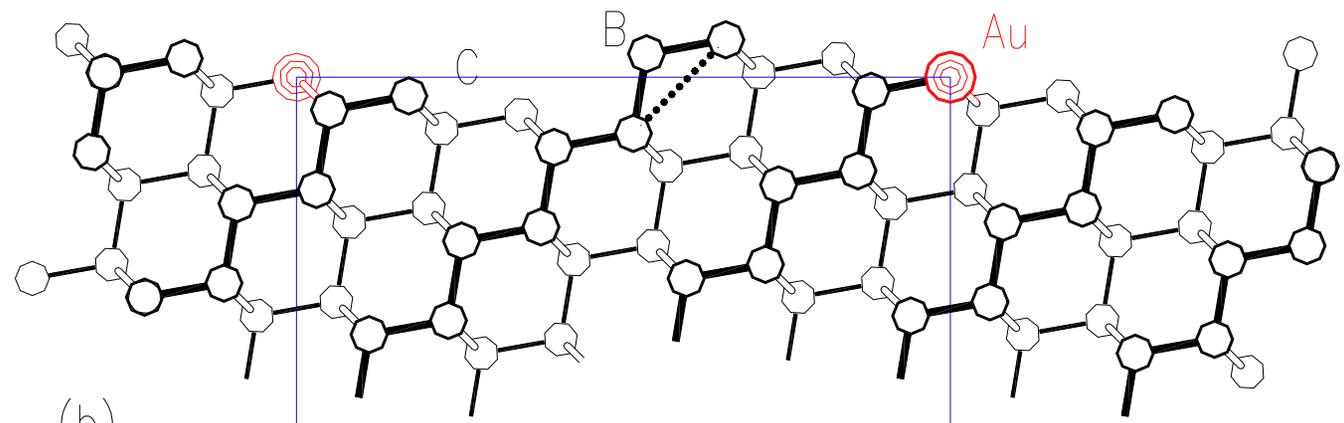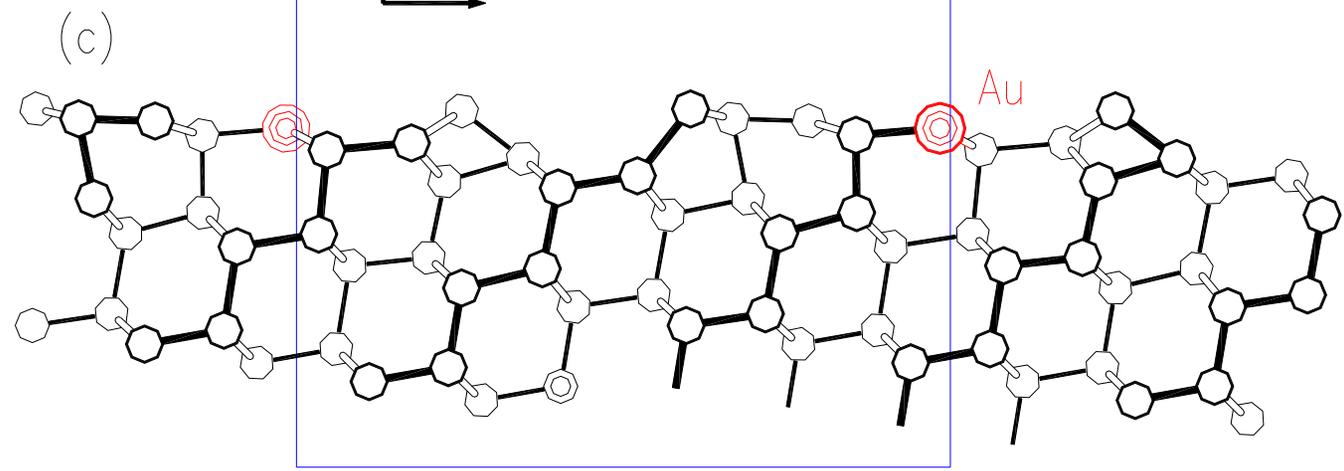
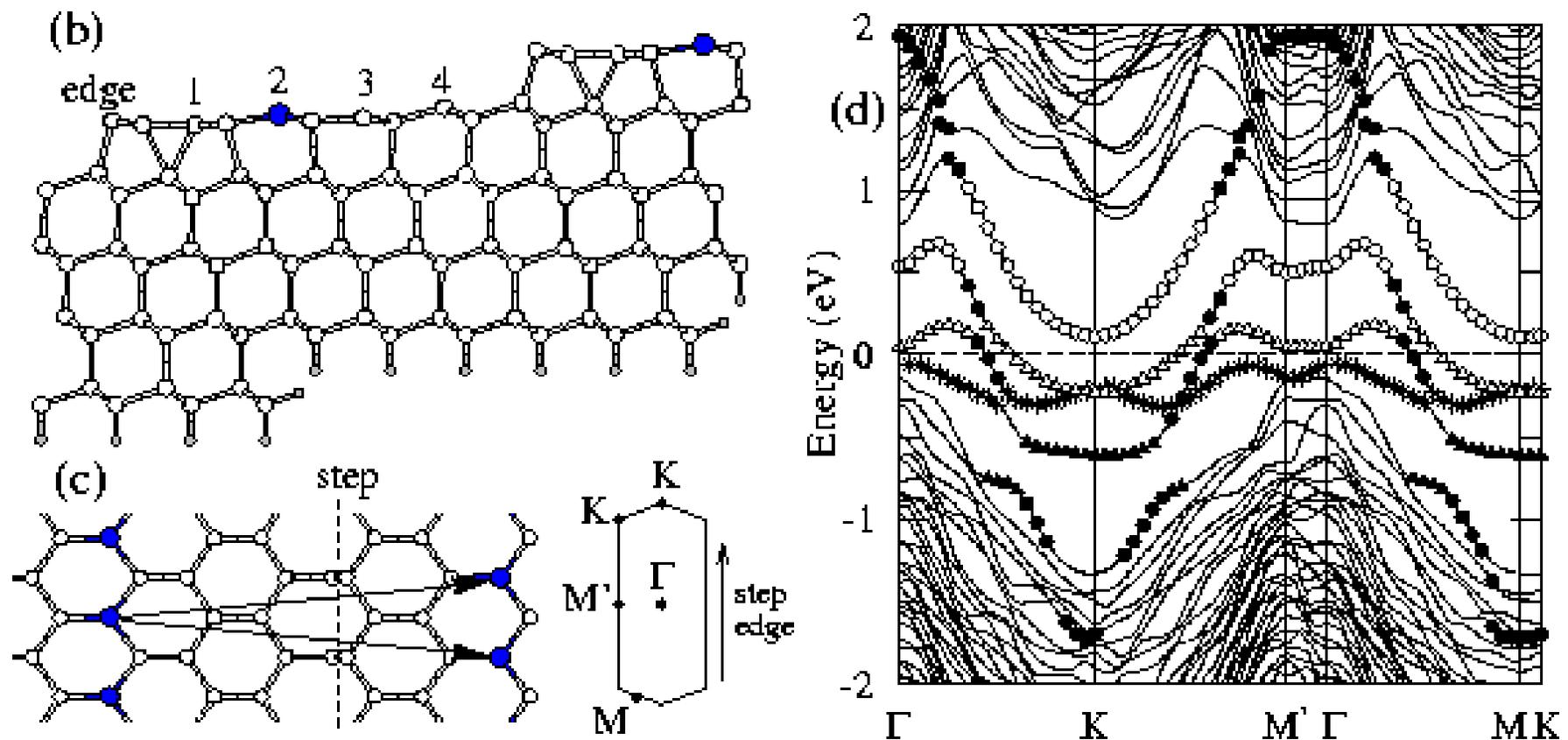# Comparison with STM



7.0Å    7.3Å    5.2Å    7.3±0.7Å
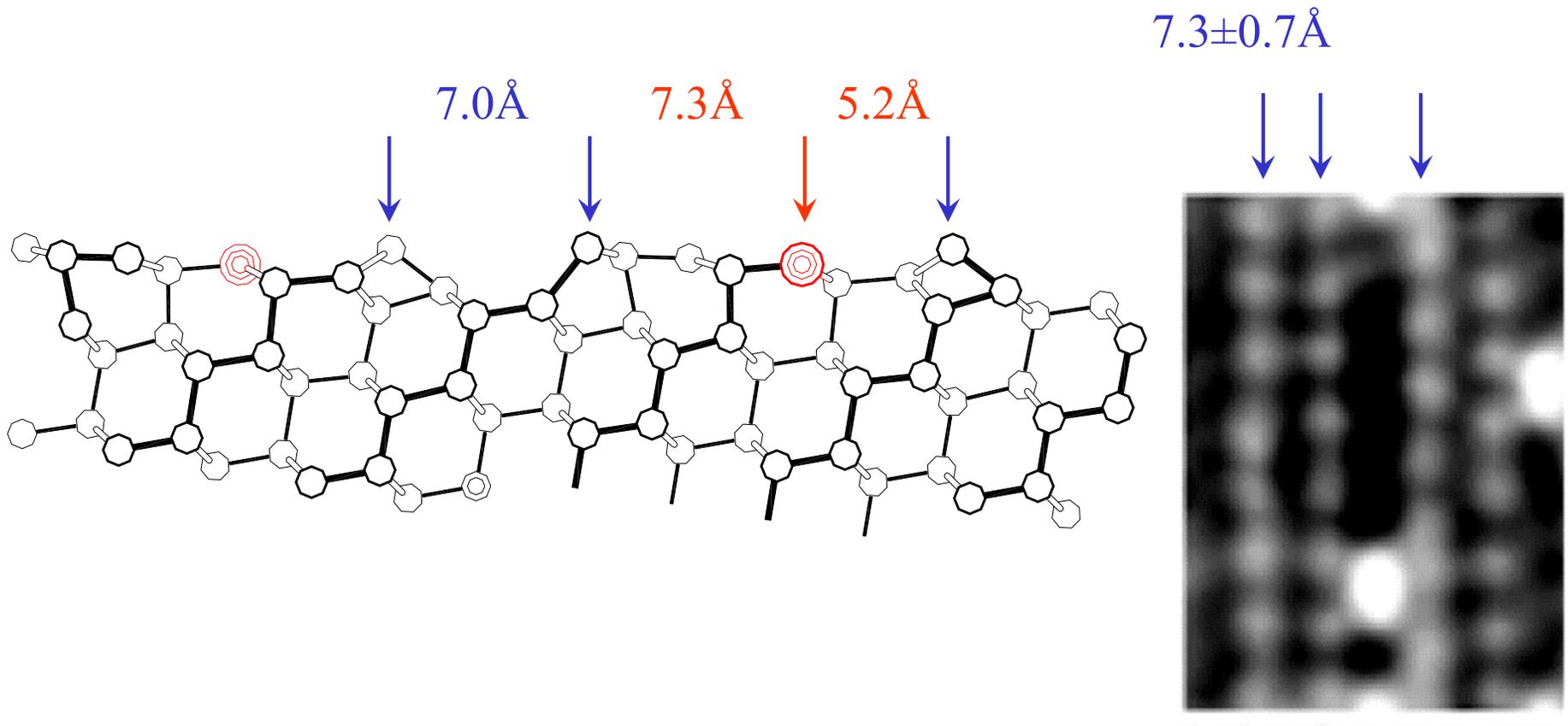
# Calculated Electronic Band Structure of Au/Si(557) using SIESTA code

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

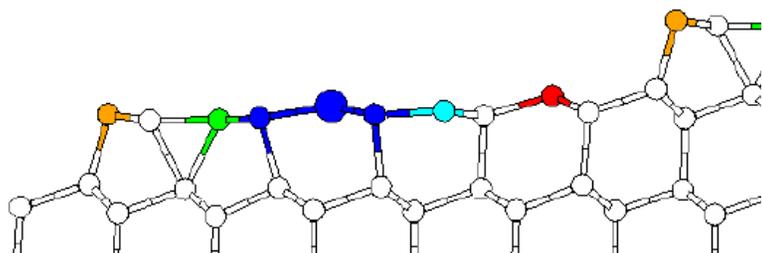# Si(557)-Au: calculated band structure
## D. Sanchez-Portal et. al. Phys. Rev. B **65**, 081401 (2002)

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.
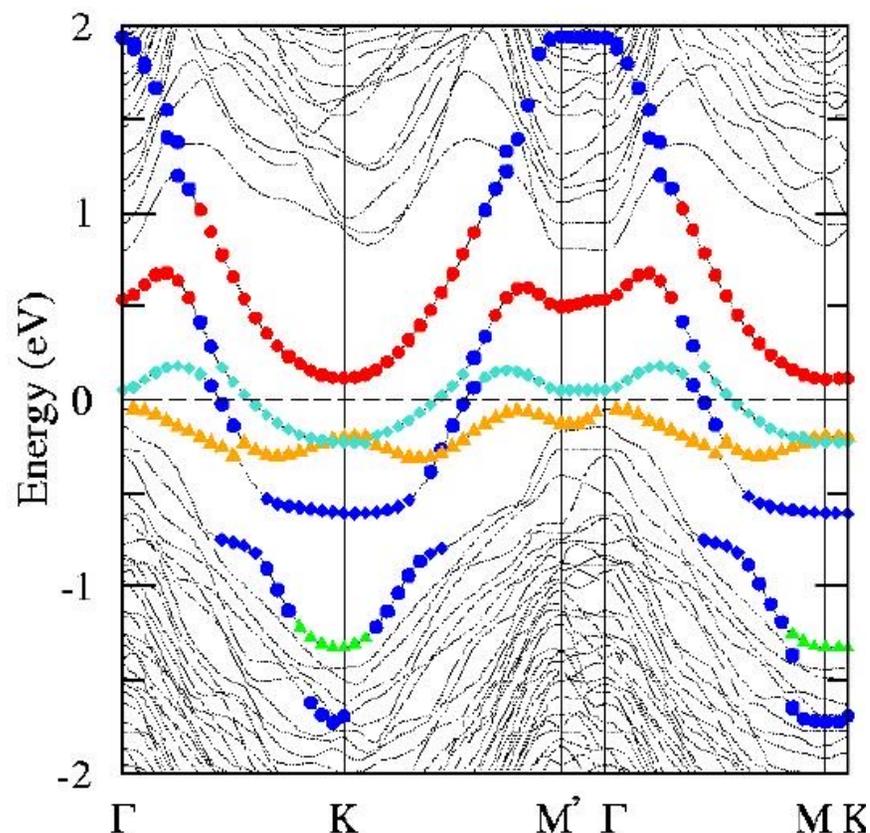
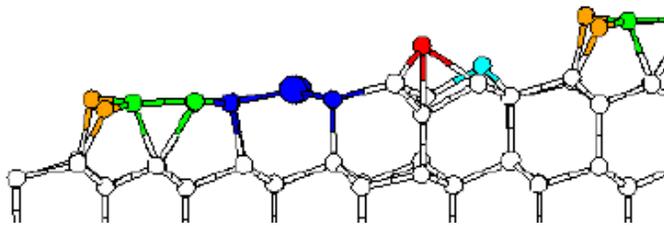# Si(557)-Au: role of adatoms

## 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

Adatom

Step edge

Restatom

24
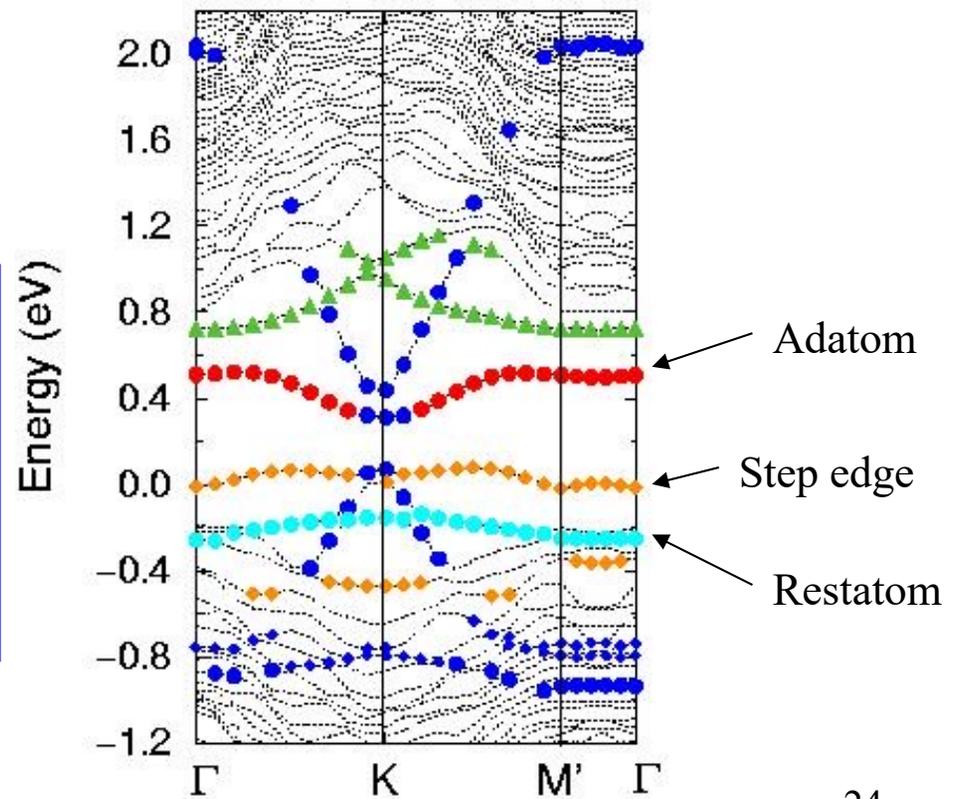
# Energy-minimized Model of Au/Si(557) 1x2 with Adatom
## D. Sanchez-Portal et. al. (to be published)
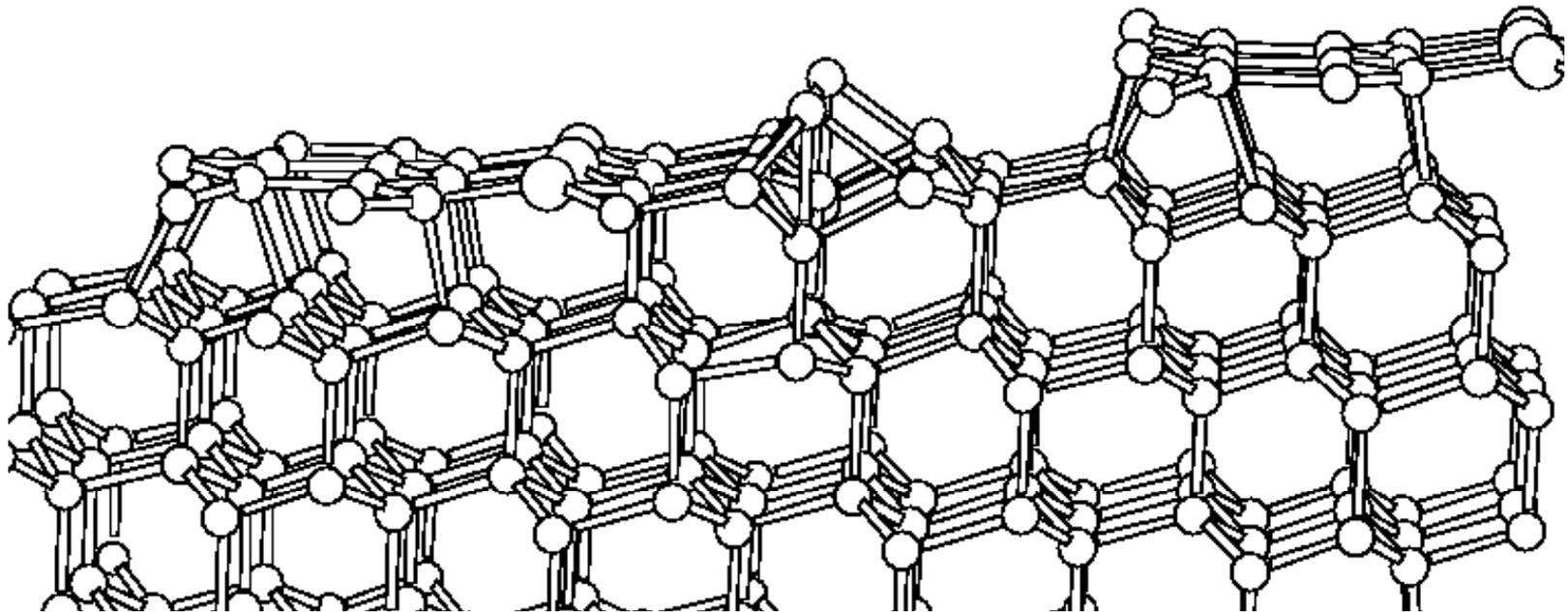
# Conclusions

- Surface sensitivity from symmetry of CTR

- Direct imaging is possible for structure containing a single heavy atom

- Au stabilizes terraced Si(557) substrate

- Au substitutes for Si in middle of terrace