

Structure of Quantum Wires on Au/Si(557)

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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

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

Von M. v. Laue

Annalen der Physik [5] 26 55 (1936)

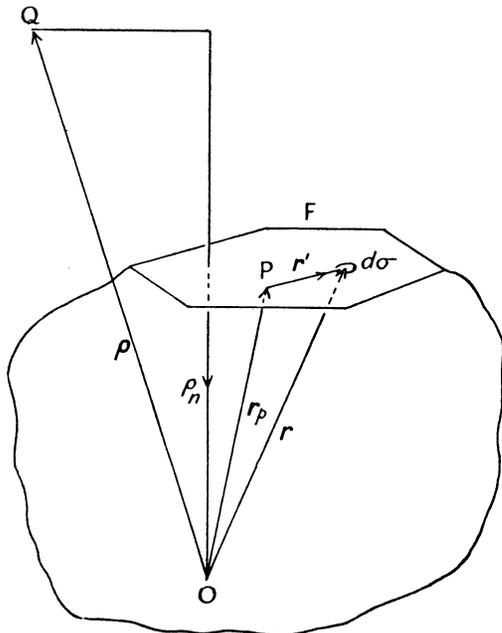
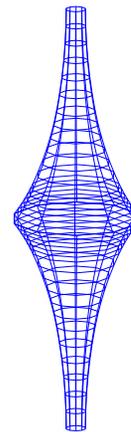
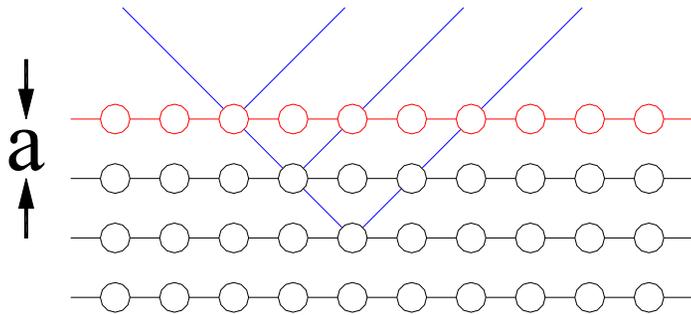


FIG. 200

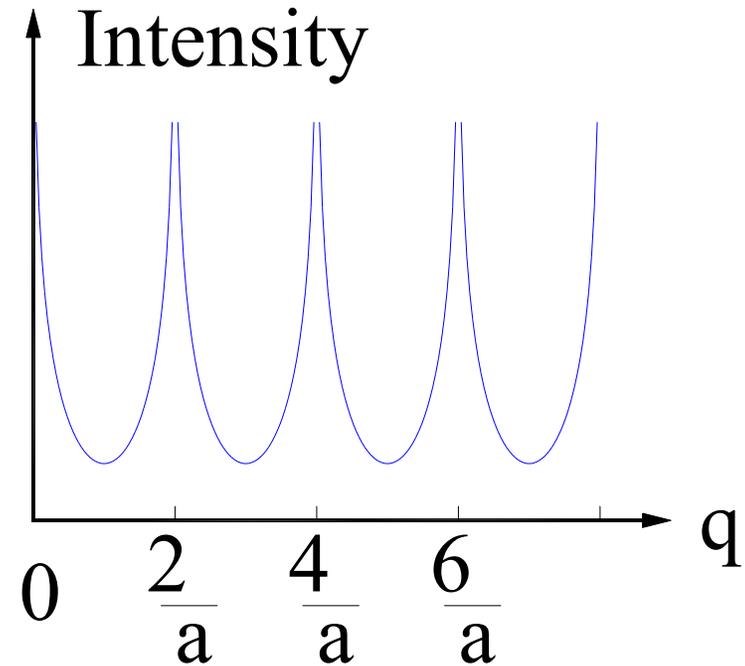


“Stacheln”

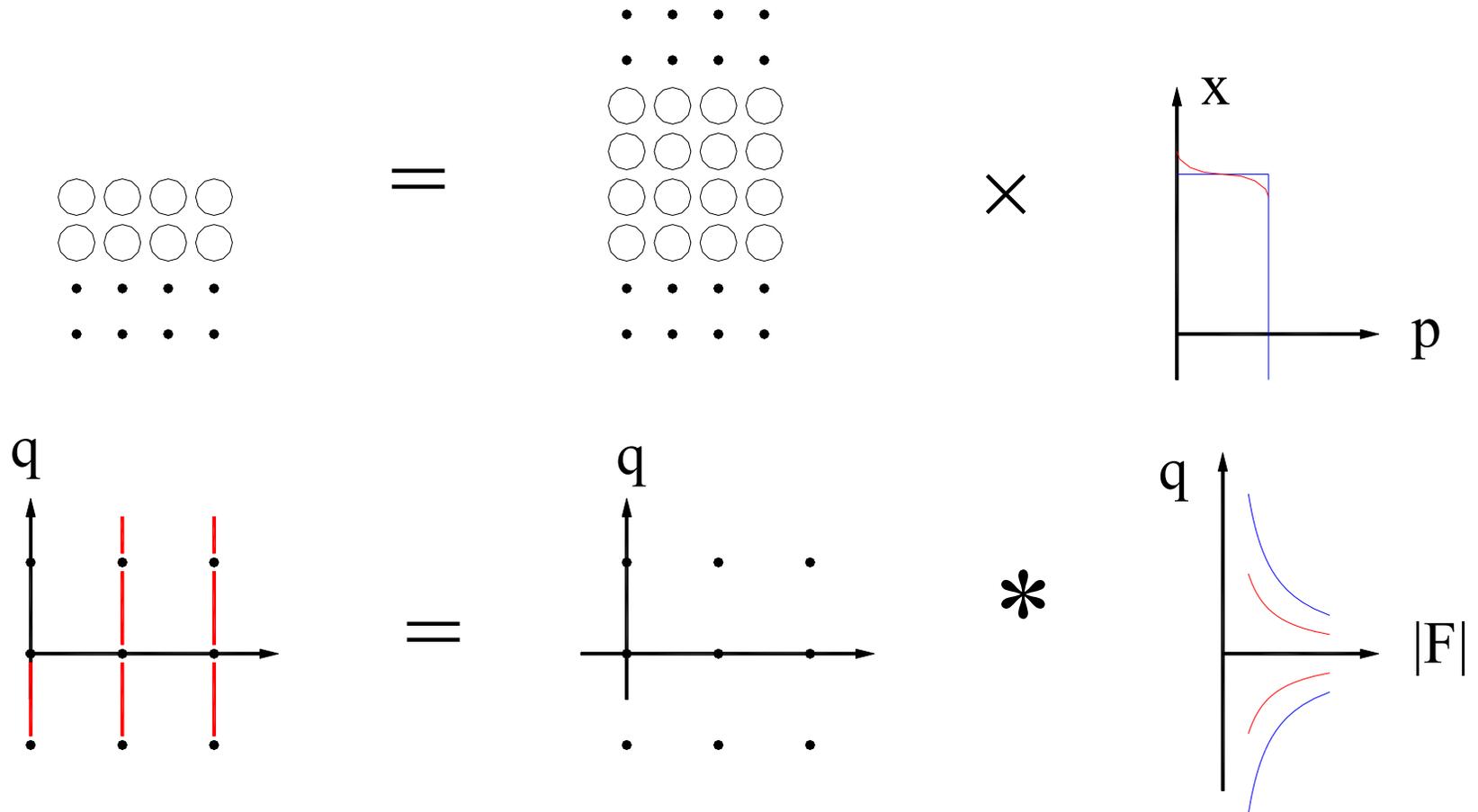
Origin of Truncation Rods



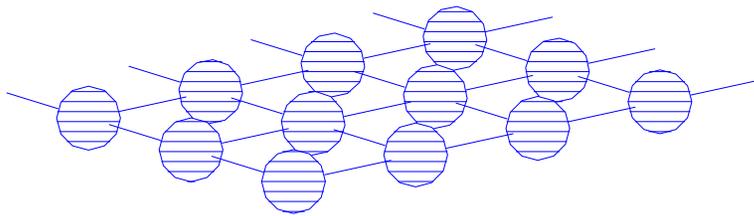
$$\begin{aligned} F_{CTR} &= \sum_{n=0}^{\infty} A_n \\ &= \sum_{n=0}^{\infty} f_L e^{inqa} \\ &= \frac{f_L}{1 - e^{iqa}} \end{aligned}$$



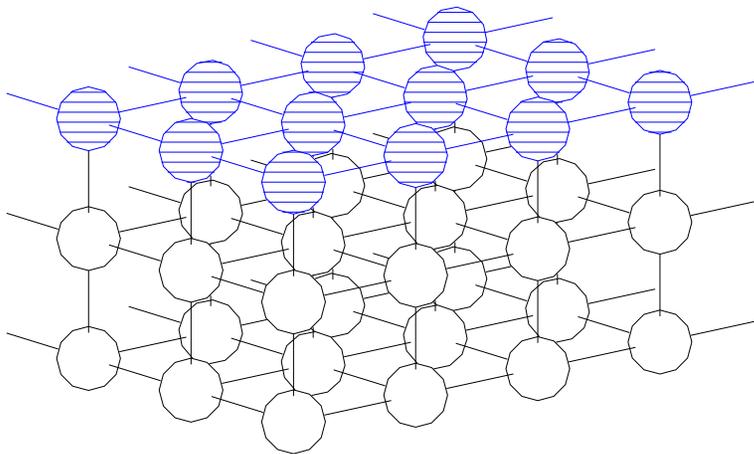
CTR as Convolution



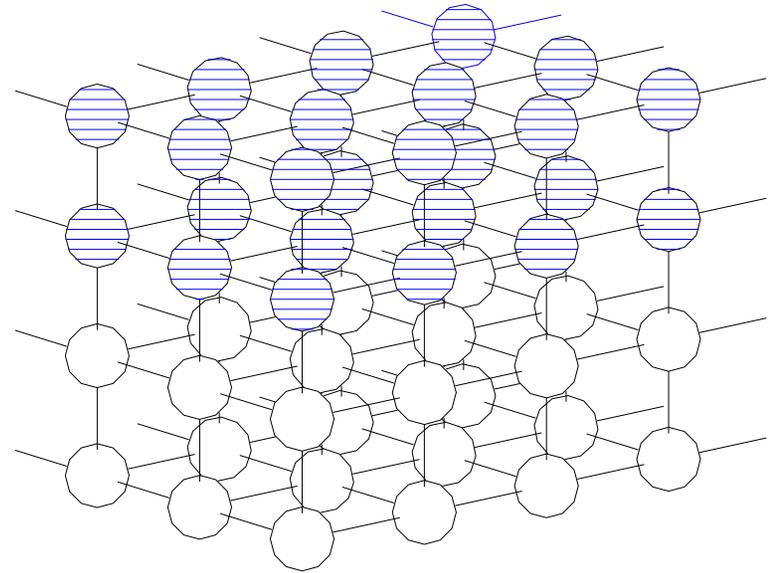
Surfaces and Interfaces



Isolated monolayer

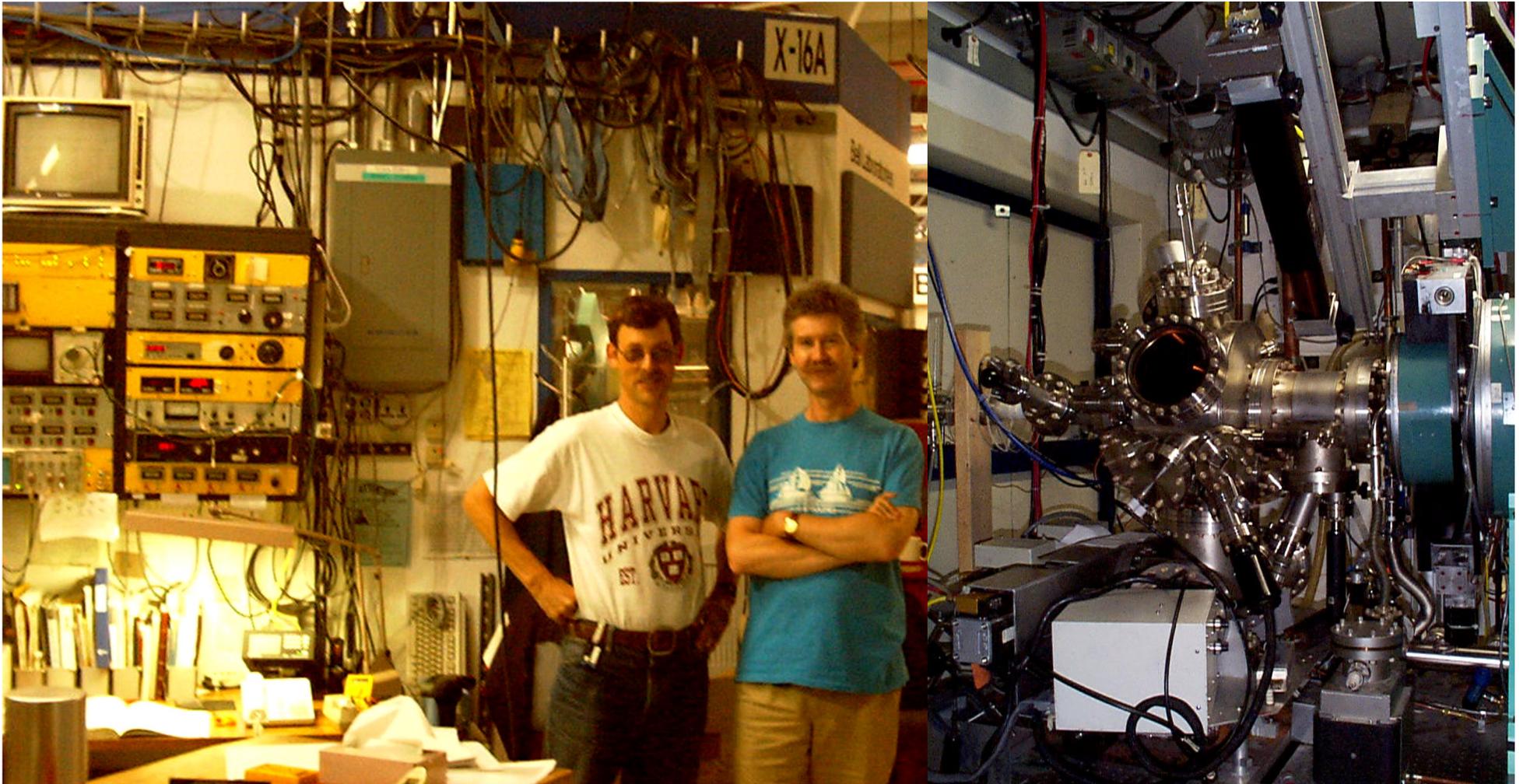


Surface of Crystal



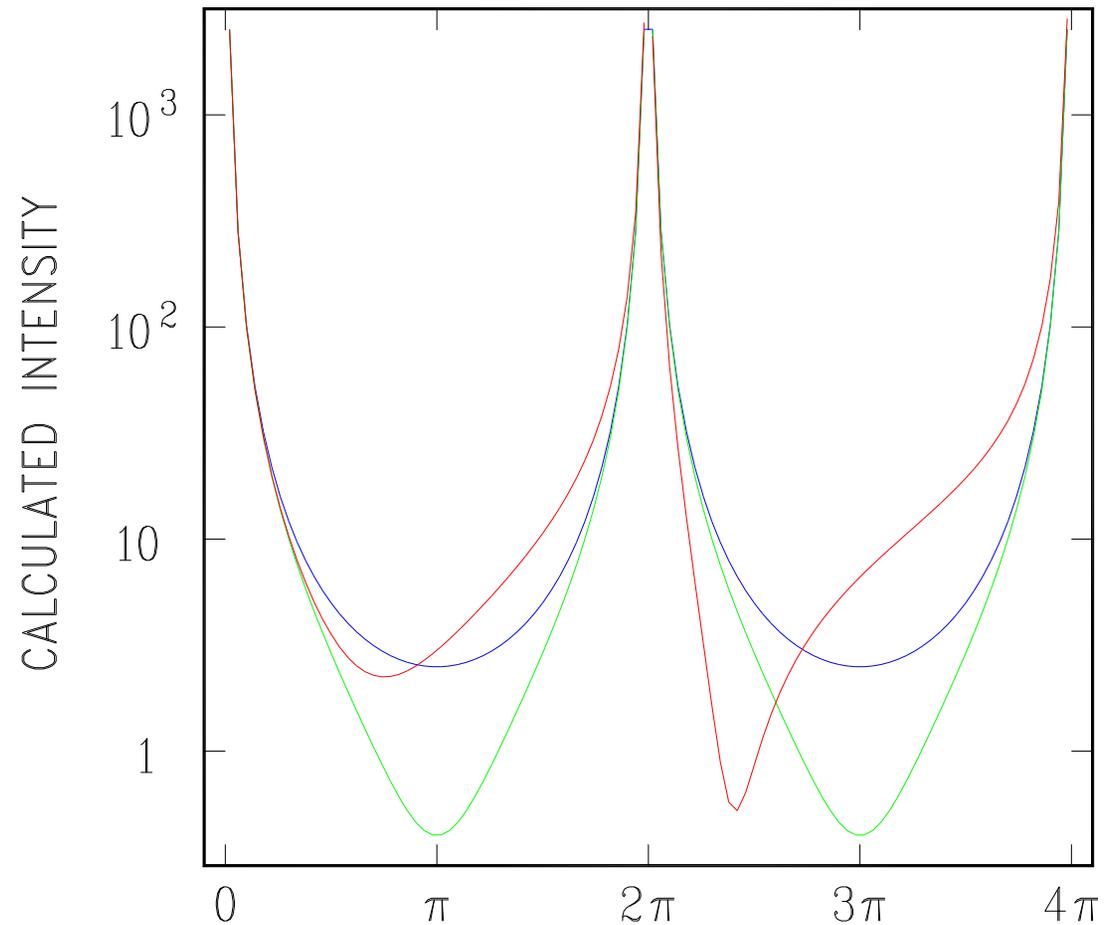
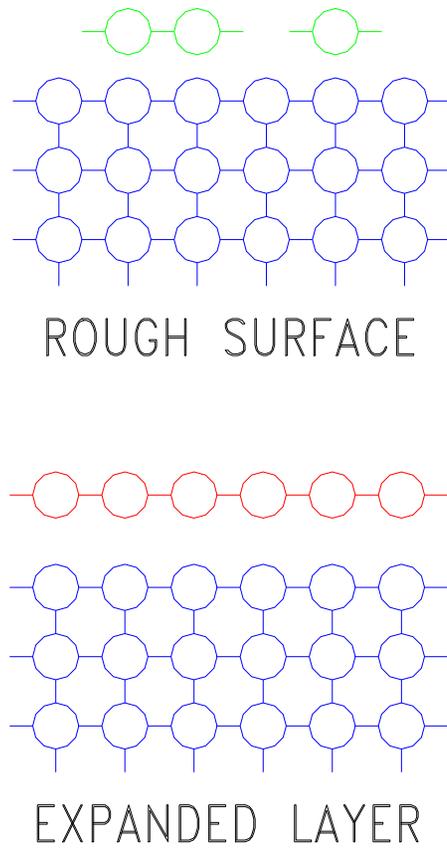
Crystal-Crystal Interface

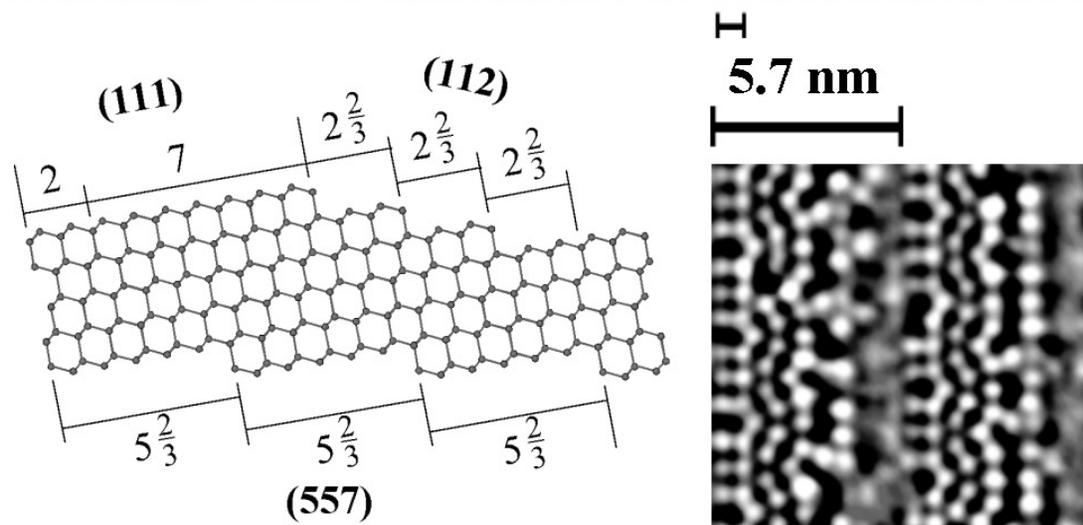
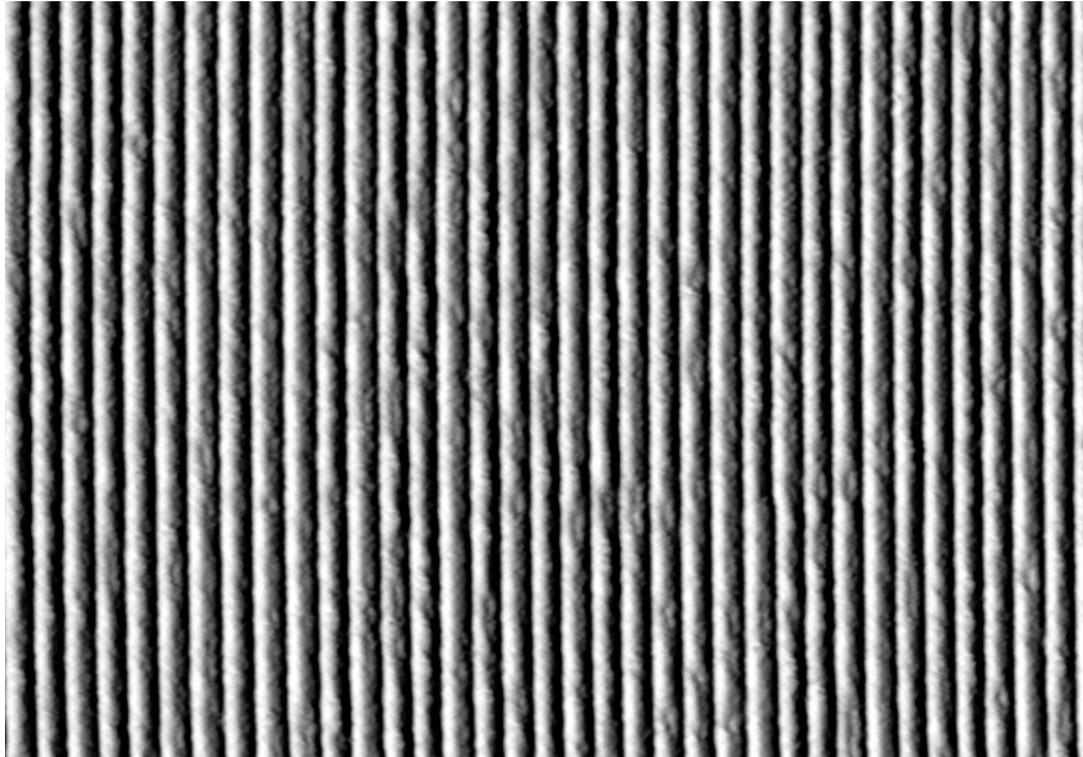
X16A Surface X-ray Diffraction operating since 1987 ...



I. K. Robinson, Midwest 50

CTR is Sensitive to Surface Structure

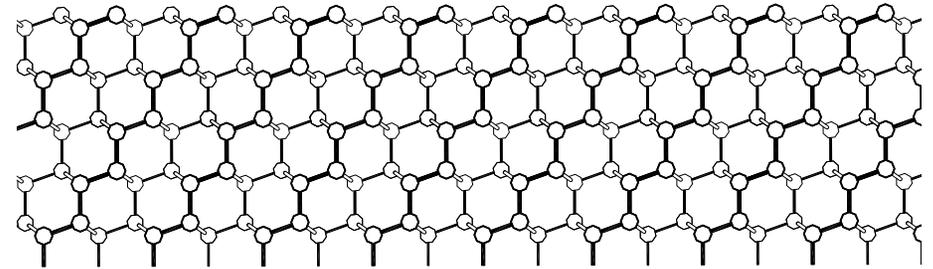




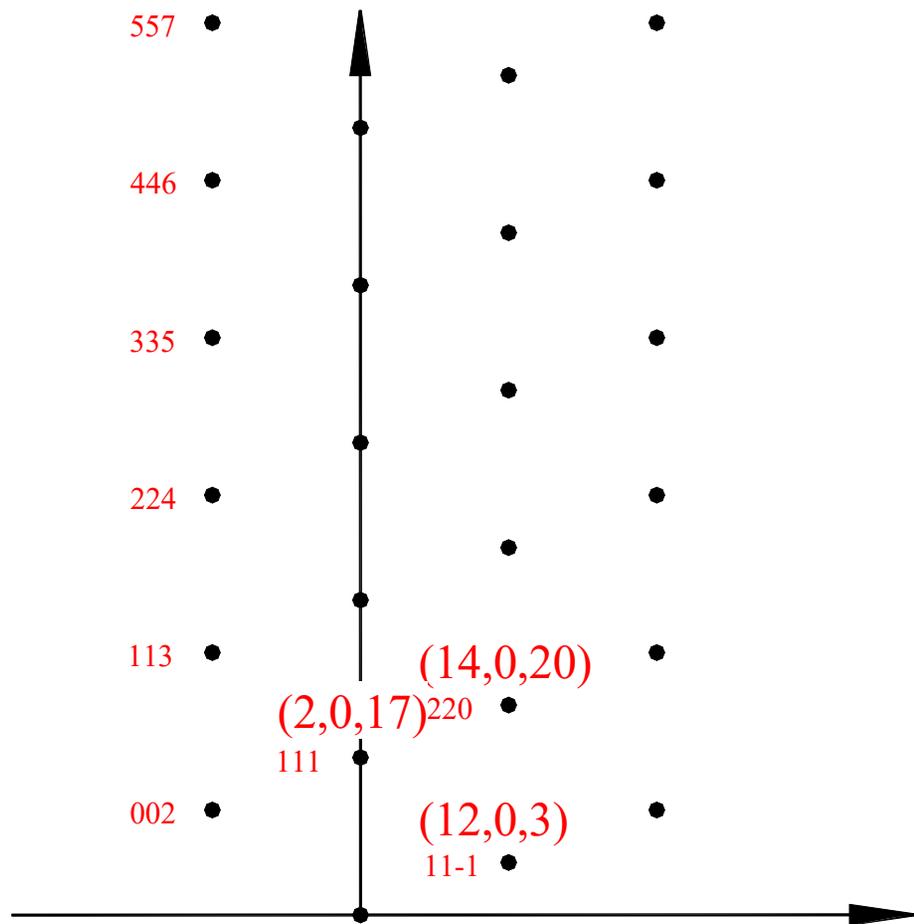
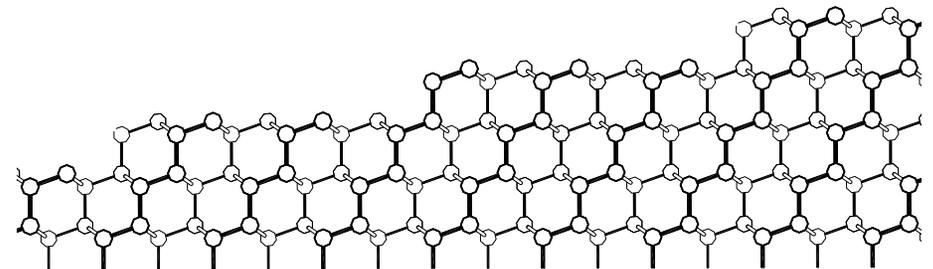
I. K. Robinson, Midwest 50

Crystallography of Stepped Surfaces

Silicon (111)



Si(557) surface



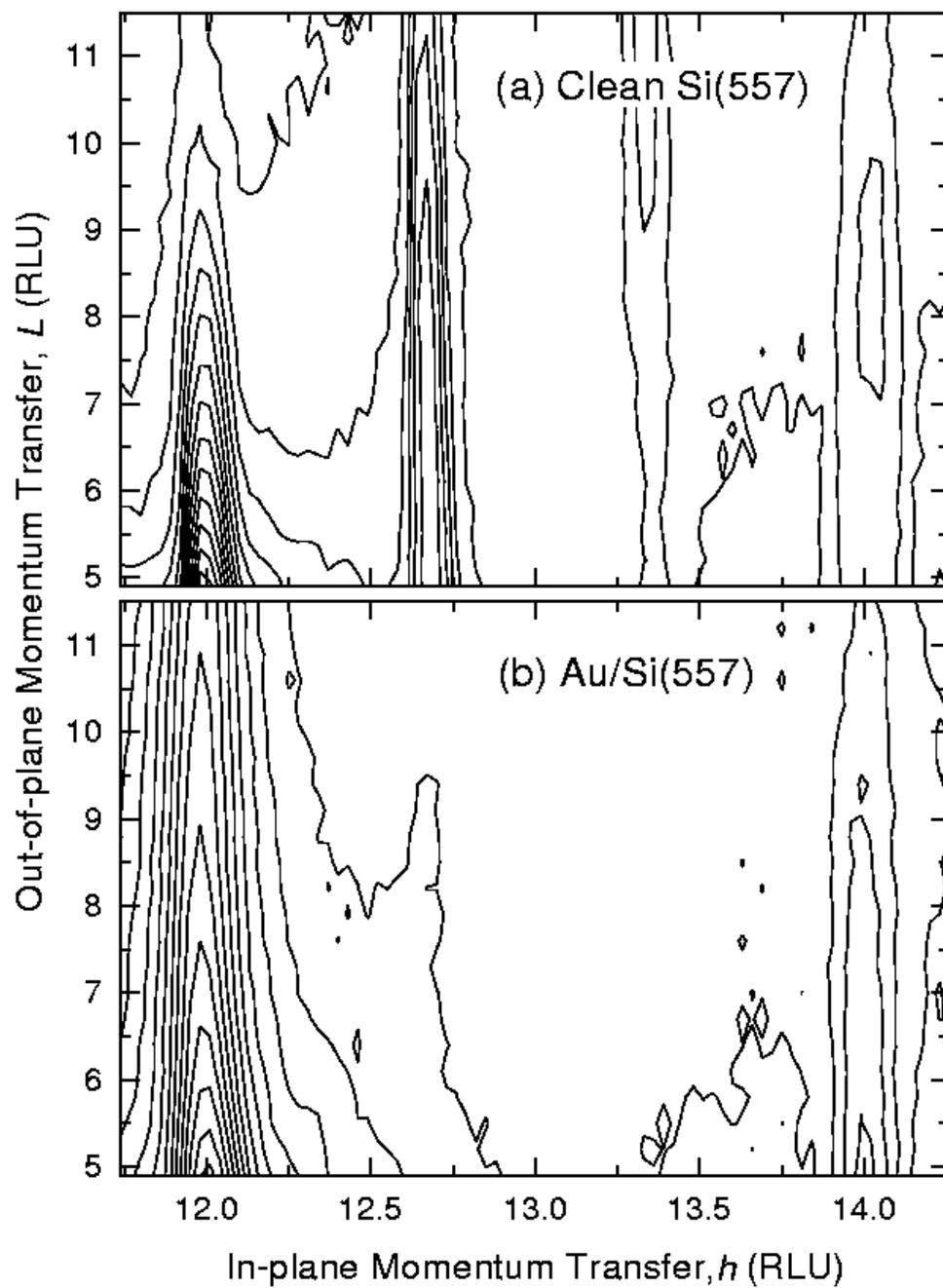
Alignment is Straightforward

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 Å, $wv = 5.19647$, Energy = 10.2542 keV (FIXED)
Five-Circle Mode using alm = 2 and bem = 2:

Centered Orthorhombic unit cell contains two steps.



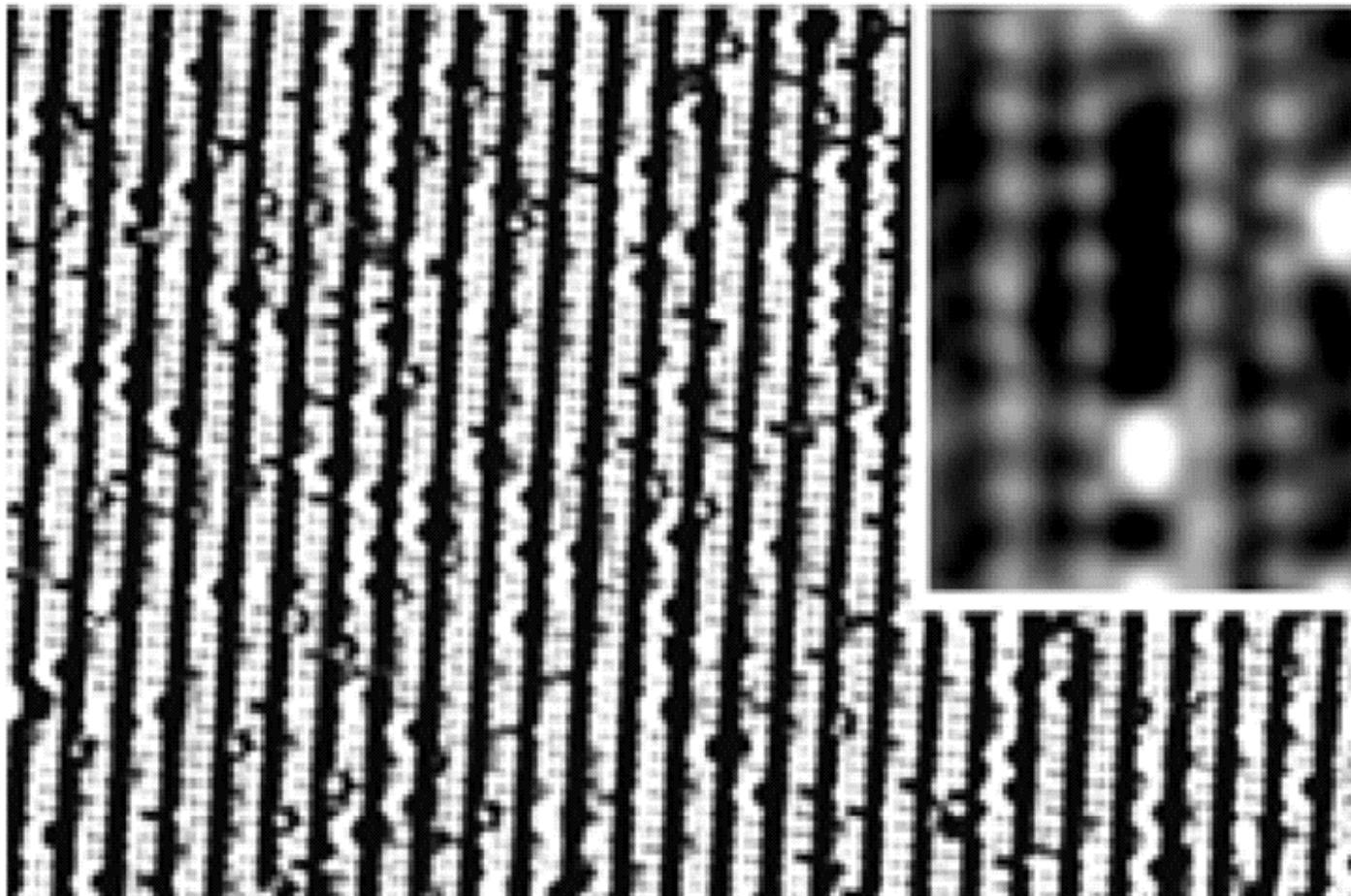
3×1 clean
surface

1×1 surface
with 0.2ML Au
at 600C

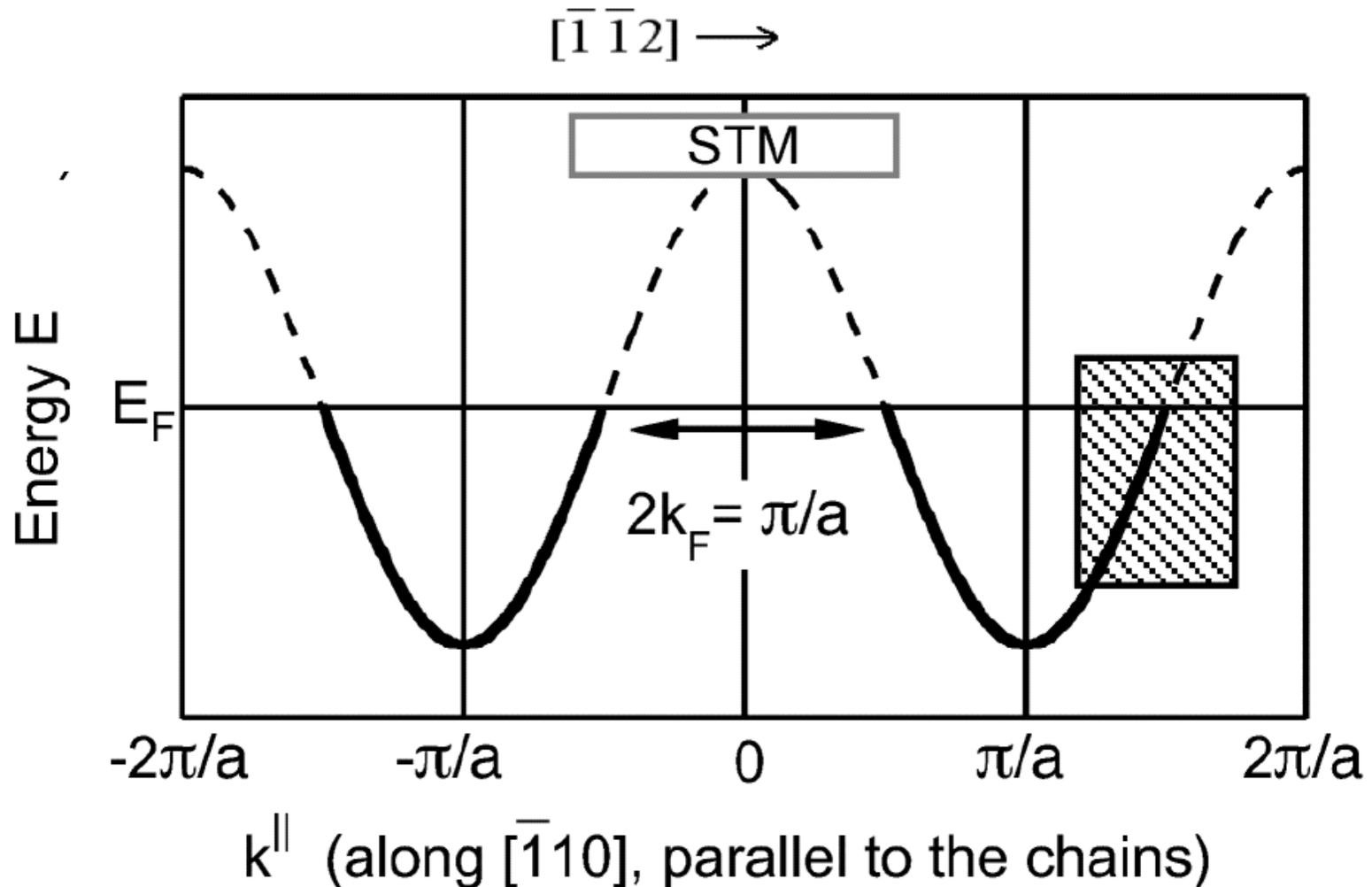
STM of Si(557)/Au

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

1.9 nm



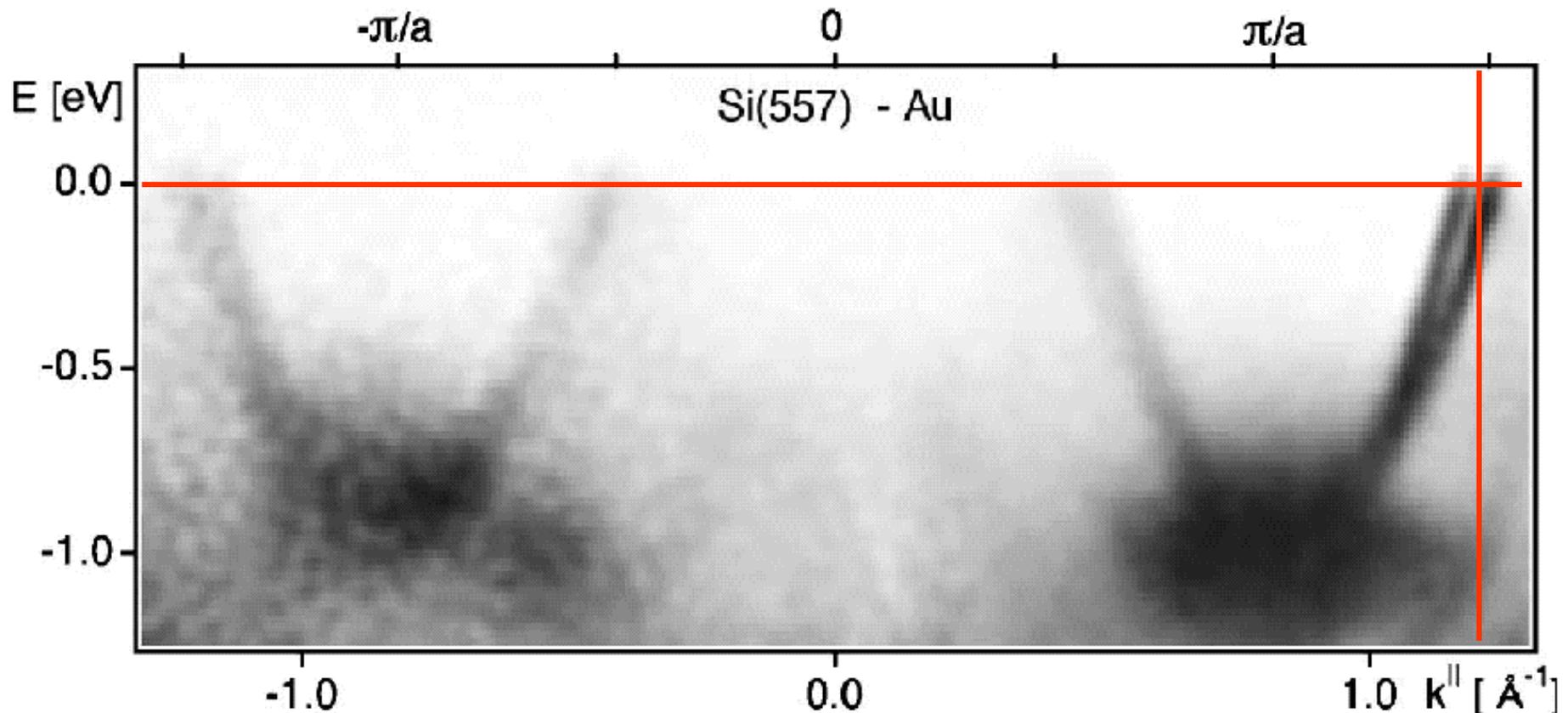
Schematic Band Topology for Au/Si(557)

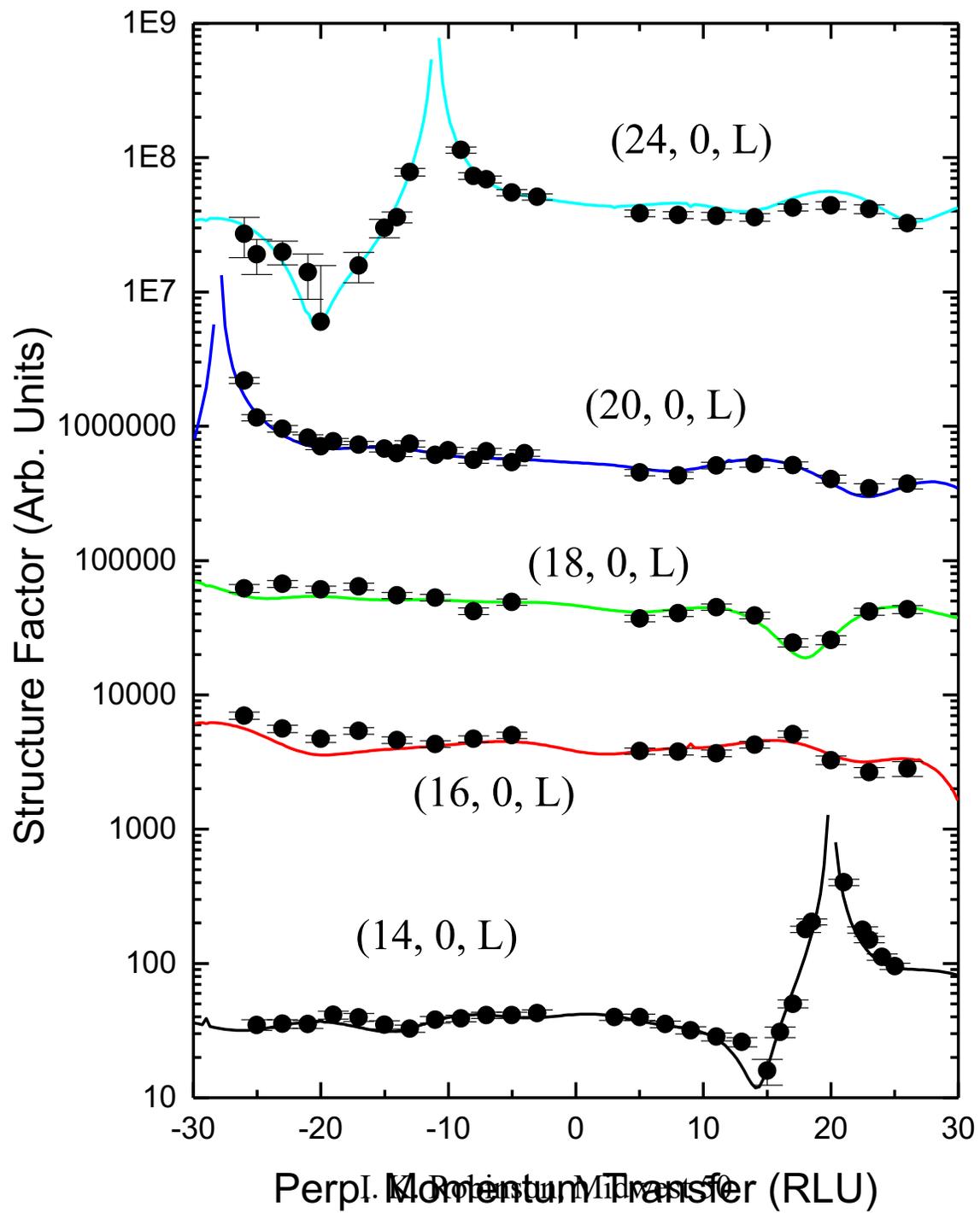


Photoemission from Surface States

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

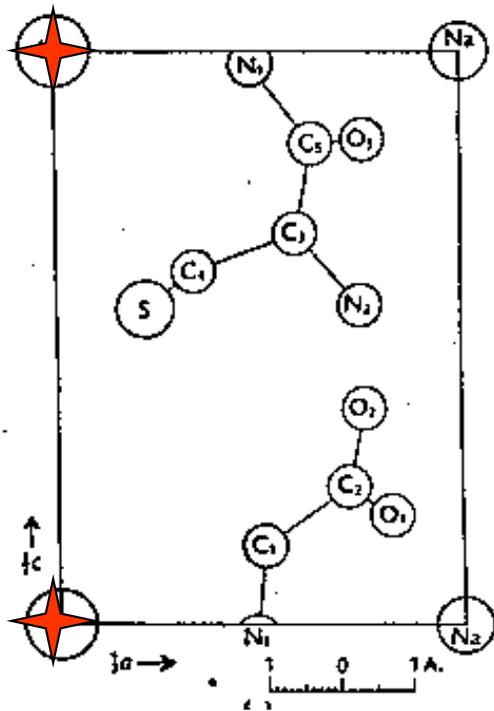
K. N. Altmann et. al. Phys Rev B 64 035406 (2001)



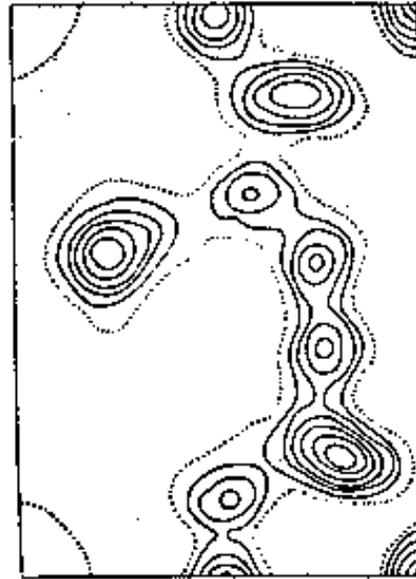


Phasing by a Single Heavy Atom

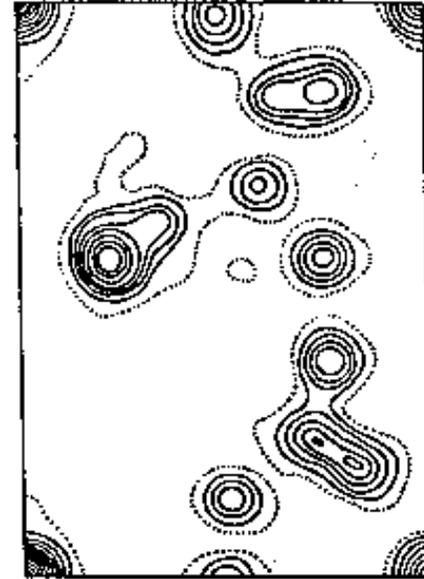
H. B. Dyer, Acta Cryst. 4 42 (1951)



Cysteinylglycine
sodium iodide

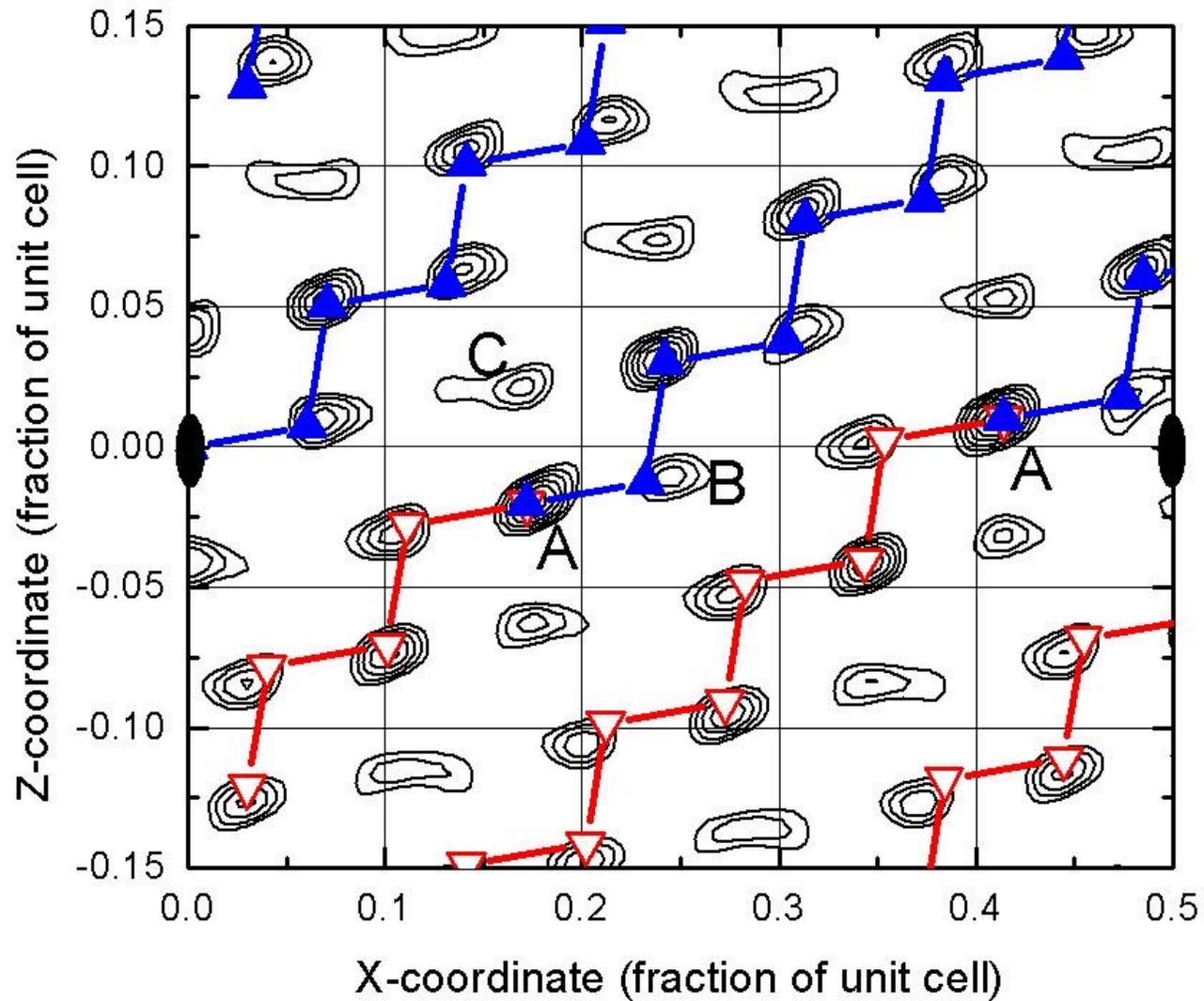


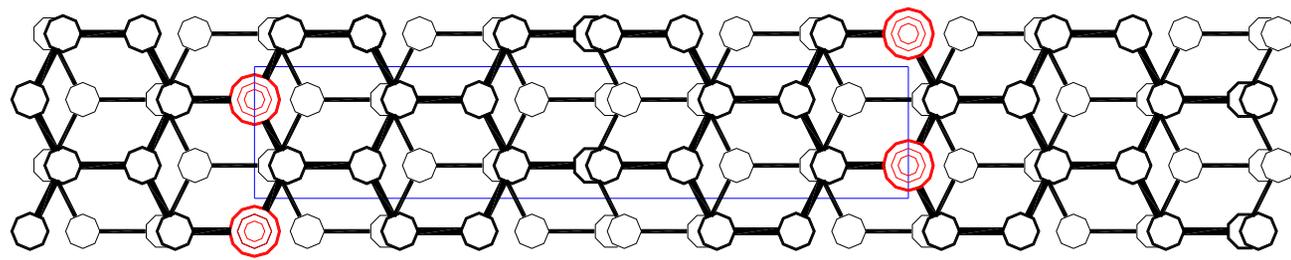
Patterson



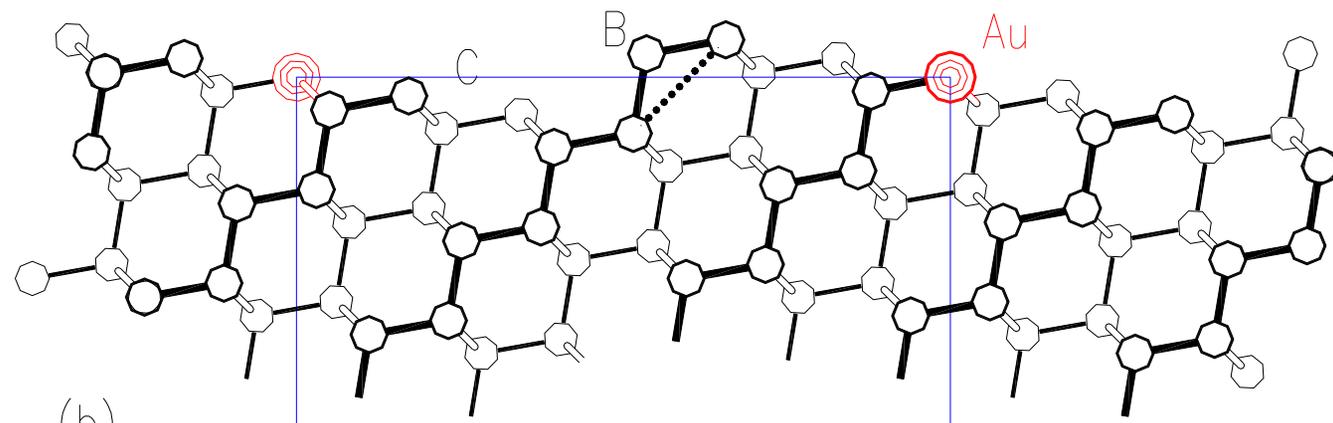
Electron density

X-Z Patterson of Au/Si(557)

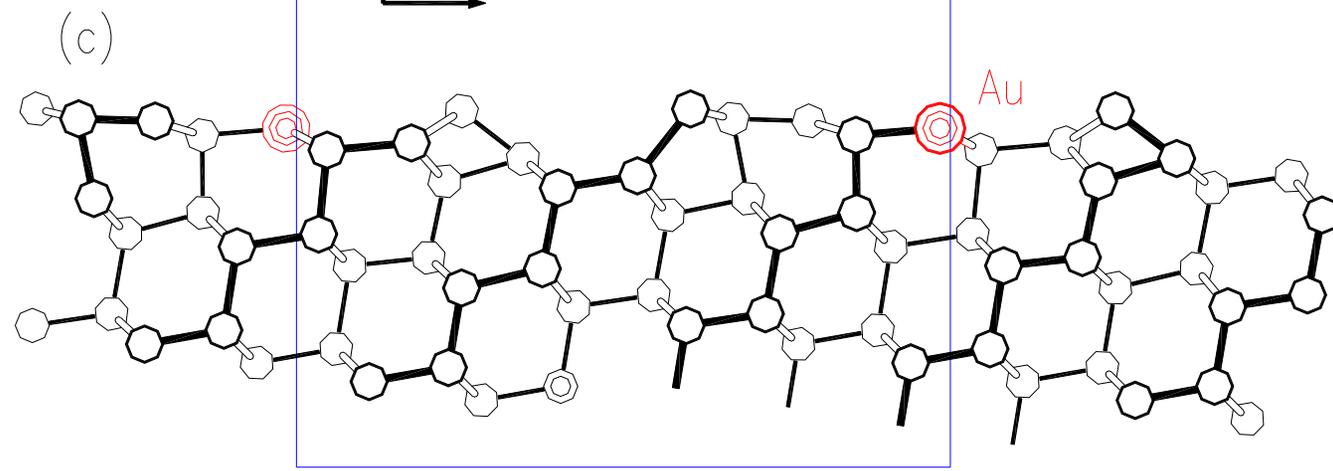




(a) A coordinate system with a vertical y-axis and a horizontal x-axis.

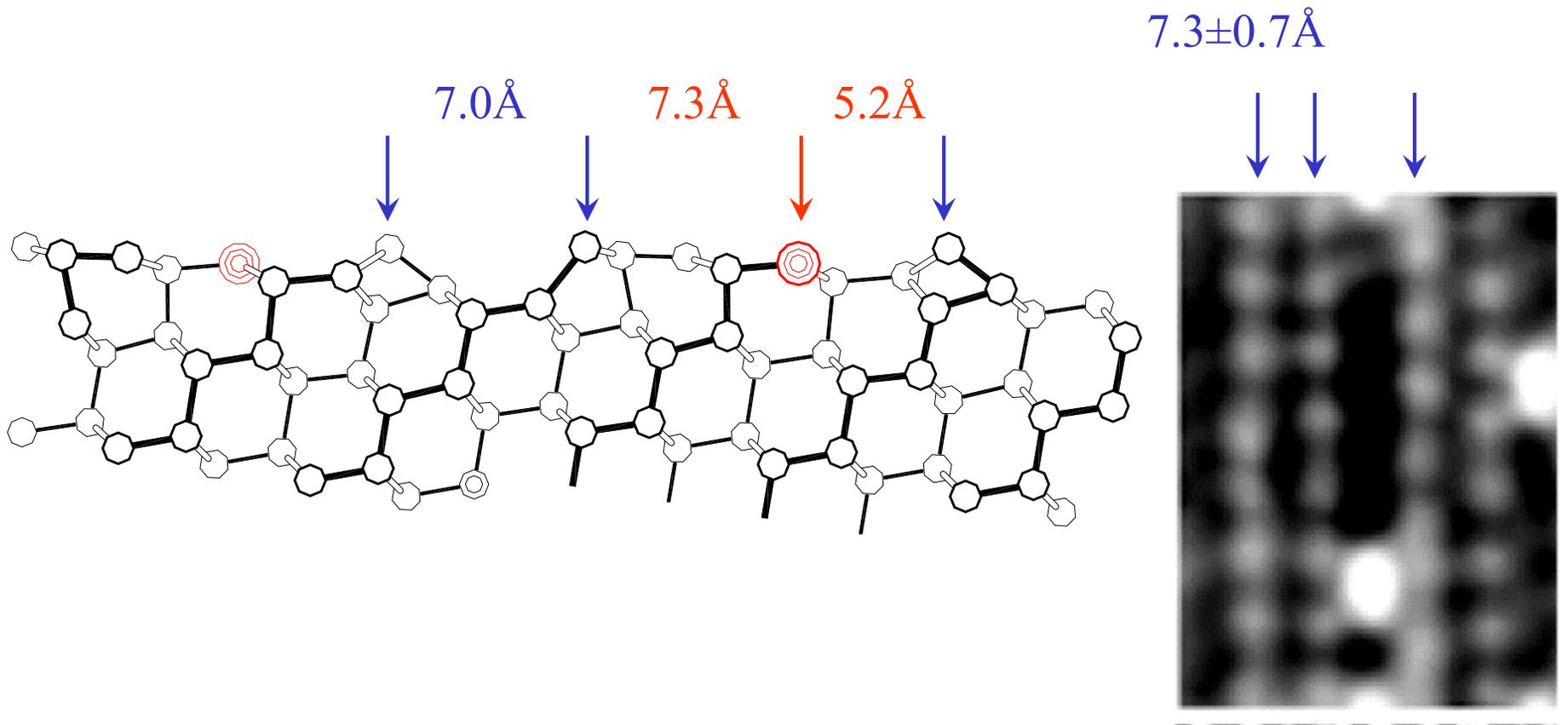


(b) A coordinate system with a vertical z-axis and a horizontal x-axis.



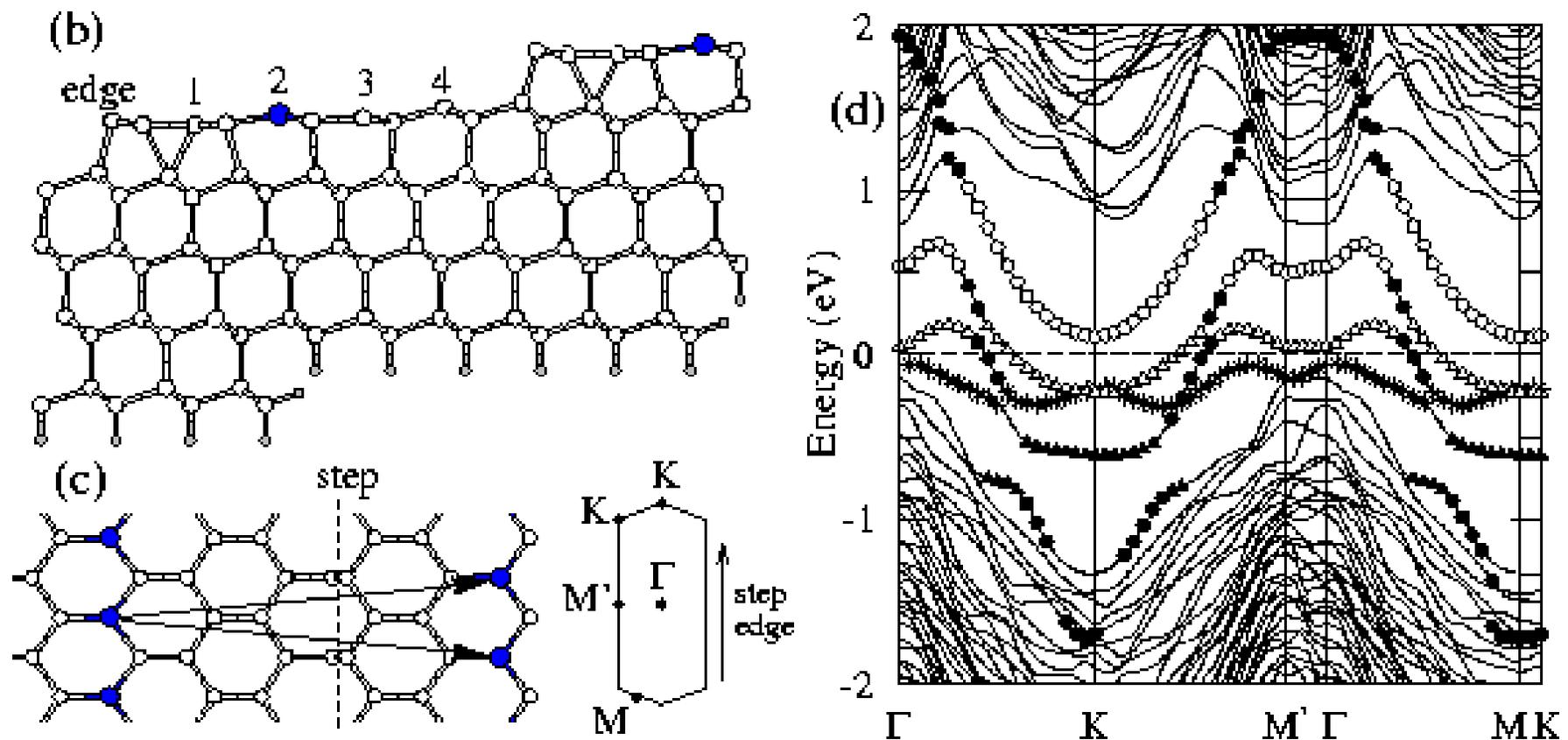
(c)

Comparison with STM



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

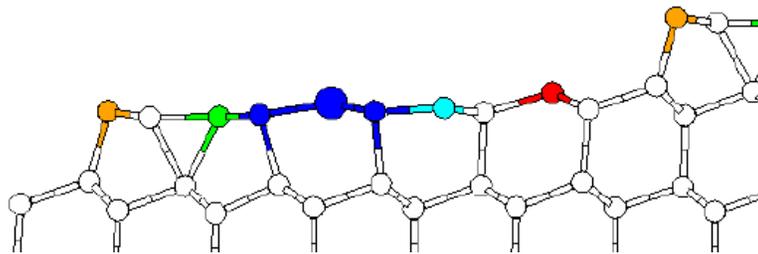
D. Sanchez-Portal et. al. Phys. Rev. B **65**, 081401 (2002)



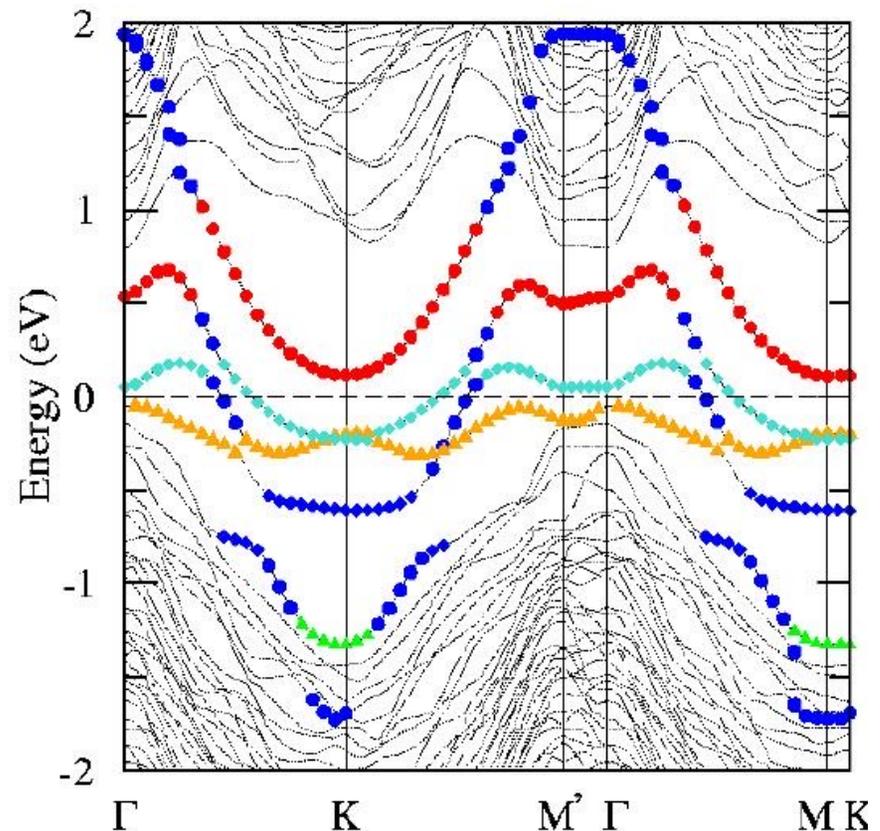
Si(557)-Au: calculated band structure

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

Mulliken populations allow to identify the origin of each band



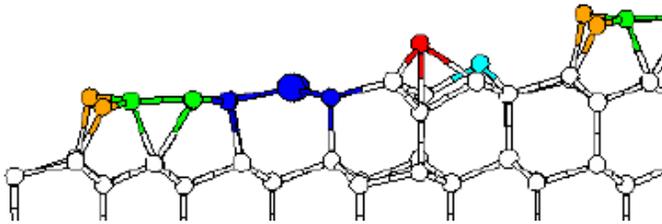
- Directions Γ - K - M' and Γ - M are parallel to the gold chains
- “Gold bands” (blue) are strongly hybridized with the Si neighboring atoms
- Orange band corresponds to the step edge
- Red and cyan bands are due to dangling bonds in the terraces
- The inclusion of adatoms saturating some of the Si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



Si(557)-Au: role of adatoms

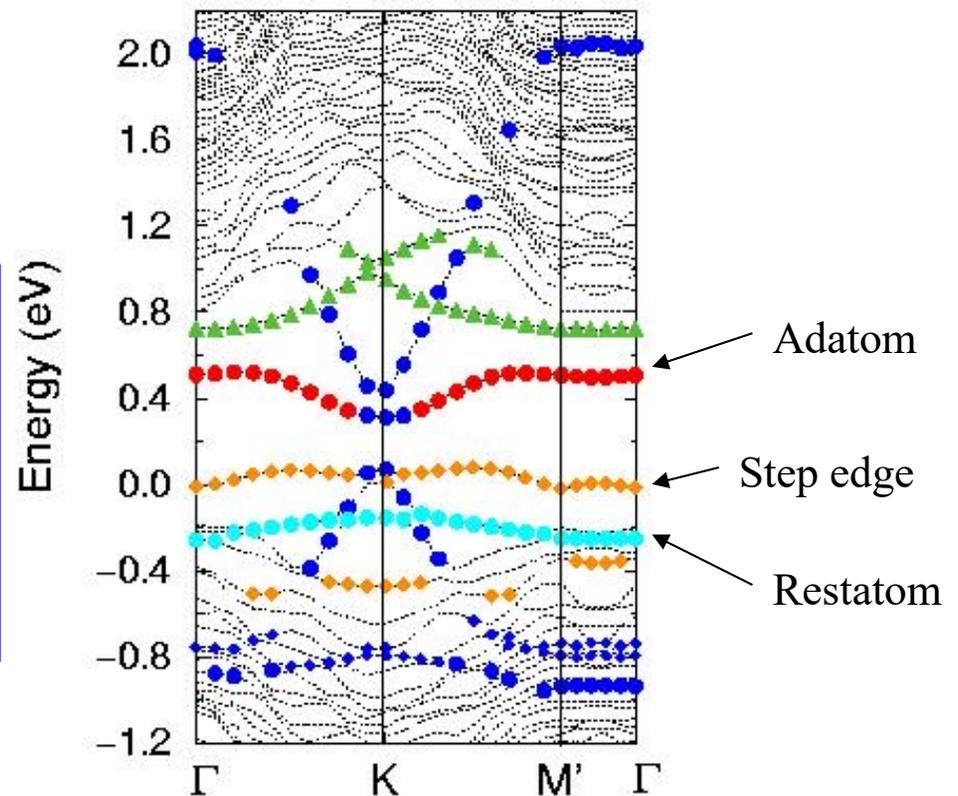
D. Sanchez-Portal et. al. (to be published)

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



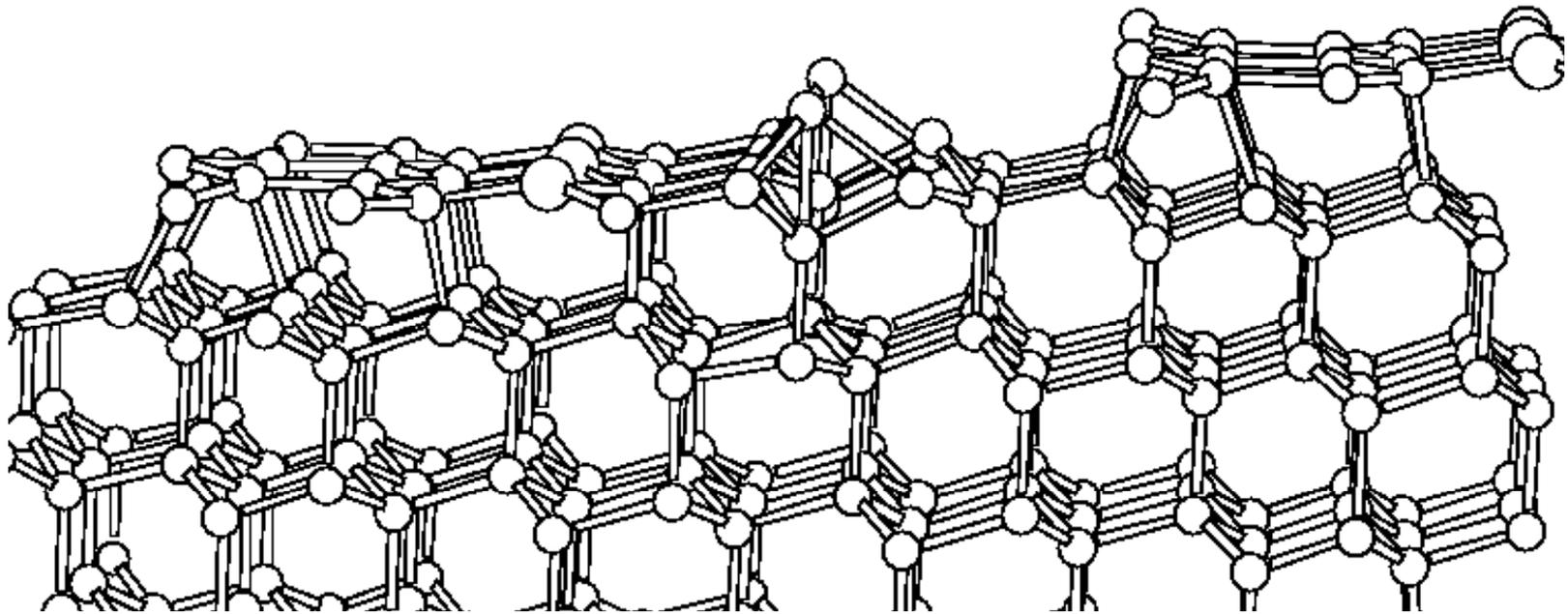
- The **step-edge band** (orange) is located precisely at the Fermi energy
- Still **two bands*** (blue symbols) associated to the gold chain.

*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