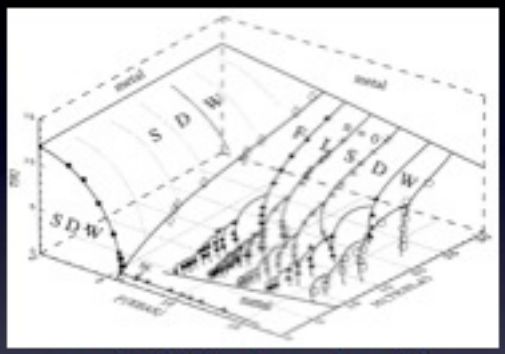
Controlled electron doping into metallic atomic wires; the case of Si(111)4x1-In

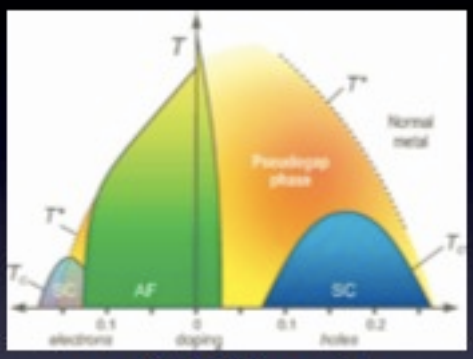
Institute of Physics and Applied Physics
+ Center for Atomic Wires and Layers, Yonsei University

Harumo Morikawa, and H.W.Yeom

Ground states of low dimensional metals



quasi-1D (Beckgaard salt)
Kang et al. PRL 70, 3091



quasi-2D (Cuprate)
Fischer et al. RMP 79, 353

Varieties of ground states depending on electron/hole concentration, pressure, and magnetic field.

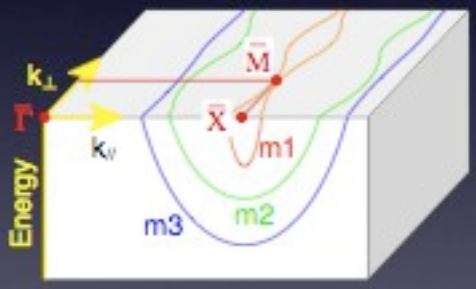
Metallic system on surfaces

1D metals

In/Si(111)-4x1, Au/Si(553), Au/Si(557), Au/Si(5 5 12) etc...

8x2 transition at LT

65 Å x65 Å



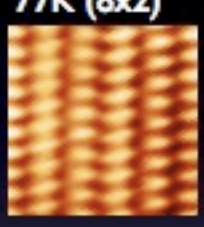
How the ground state is changed when the electron concentration is changed in In/Si(111)-4x1 ?

Phase transition on In/Si(111)

RT (4x1)

cooling

77K (8x2)

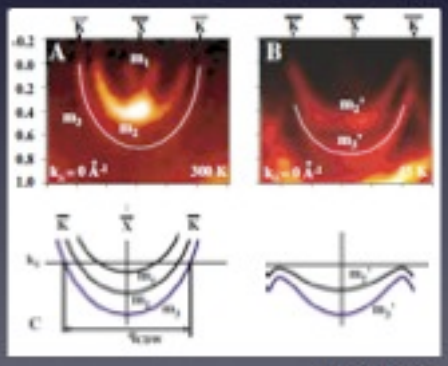


CDW transition

- Metal-insulator behavior
- x2 periodicity of the LT phase

Yeom et al. PRL (1999).

How the ground state is changed when the electron concentration is changed in In/Si(111)-4x1 ?

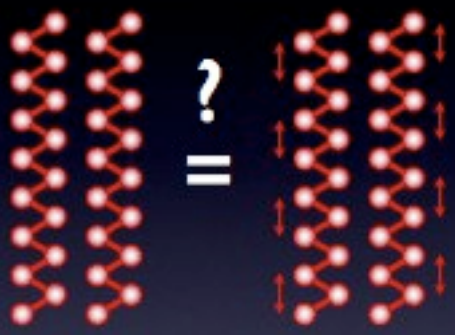


Ahn et al.(2004)

Why electron doping to In/Si(111)-4x1 ?

Another motive...

Order-disorder picture of the transition



4x1 structure
= thermally fluctuating 8x2 structure ??

[Cho et al. PRB (2001), Gonzalez et al. PRL (2006)]

How to distinguish the two models?

Direct method : Check the electronic contribution to the transition.

→ **Doping**

Is the transition electronically driven??

What should be investigated?

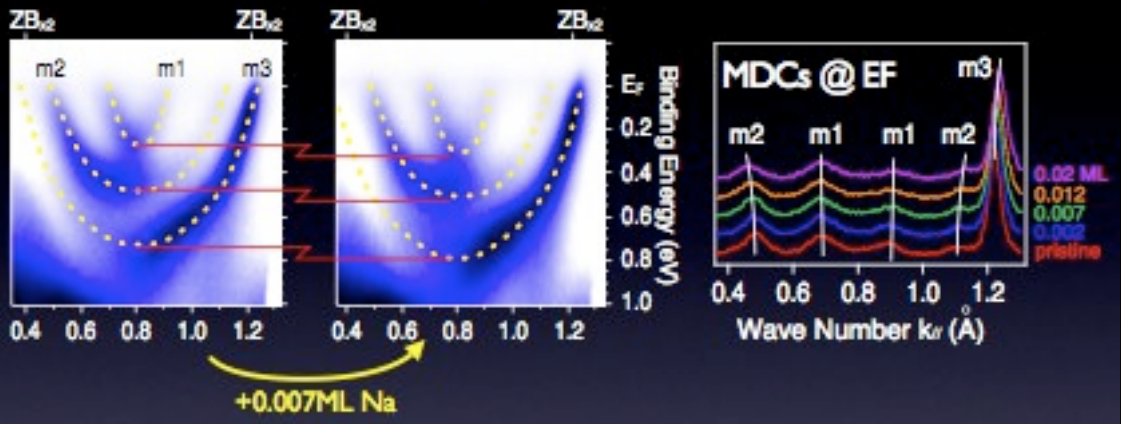
Correlation between the Fermi surface and the transition

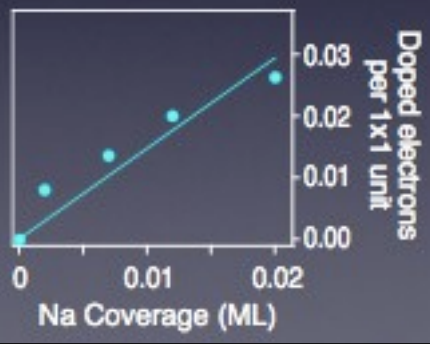
How?

Modify the Fermi surface by electron doping (Na deposition)

Results of the Present Study...

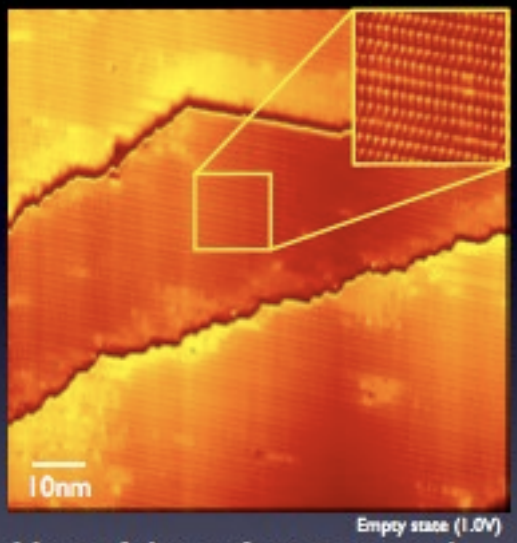
Electron doping to In/Si(111)





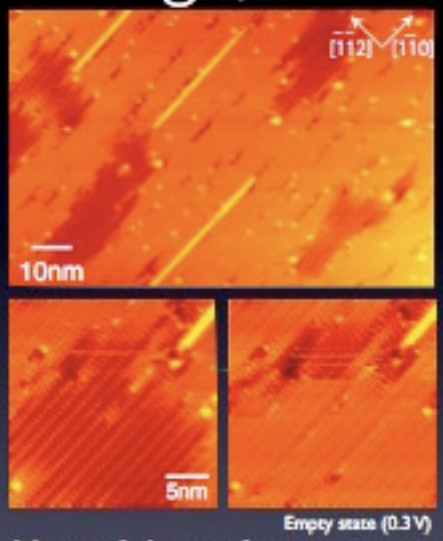
Electrons are successfully doped monotonically with the Na coverage. (Roughly one electron per Na)

Pristine surface @115 K



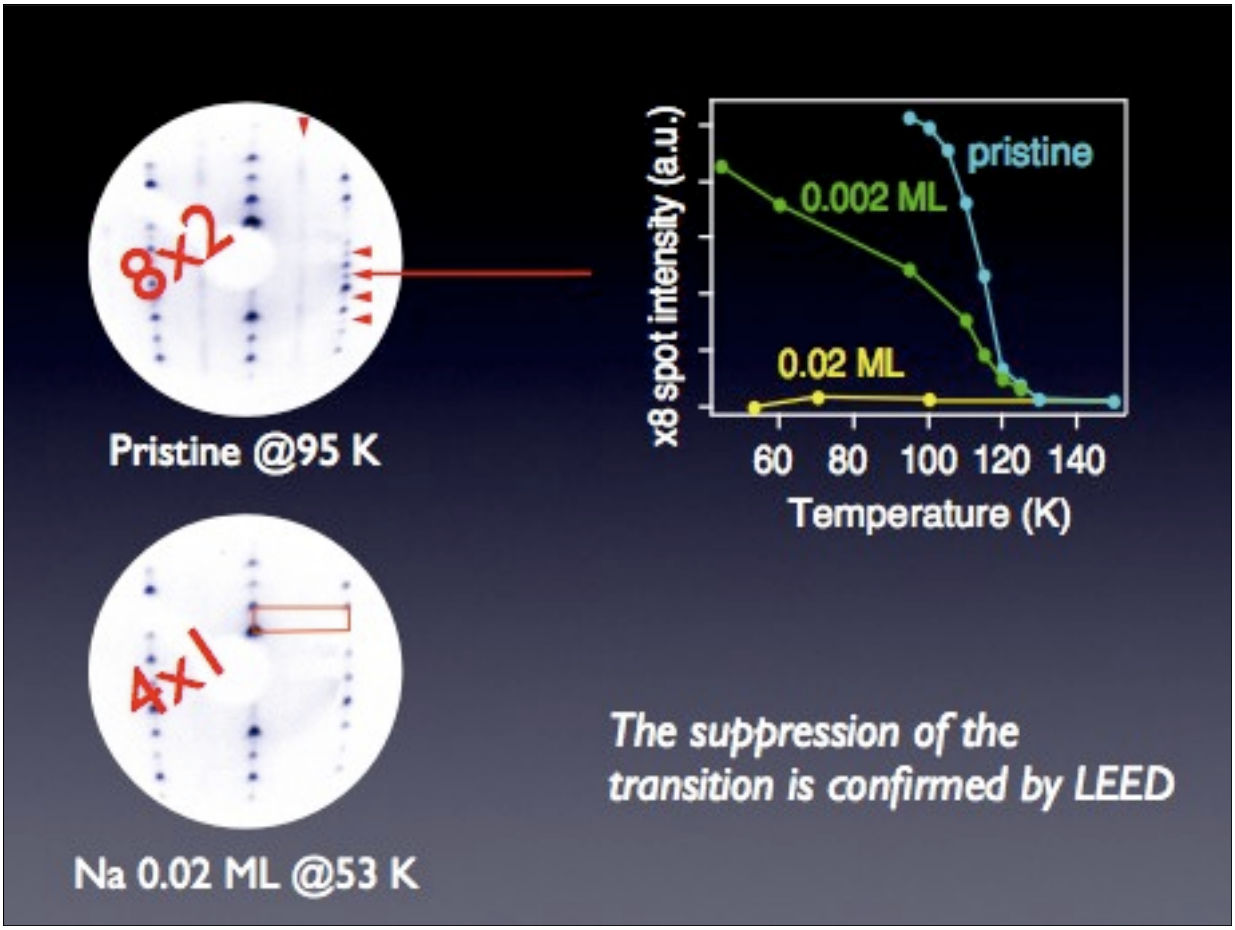
Most of the surface is covered with the 8x2 domain

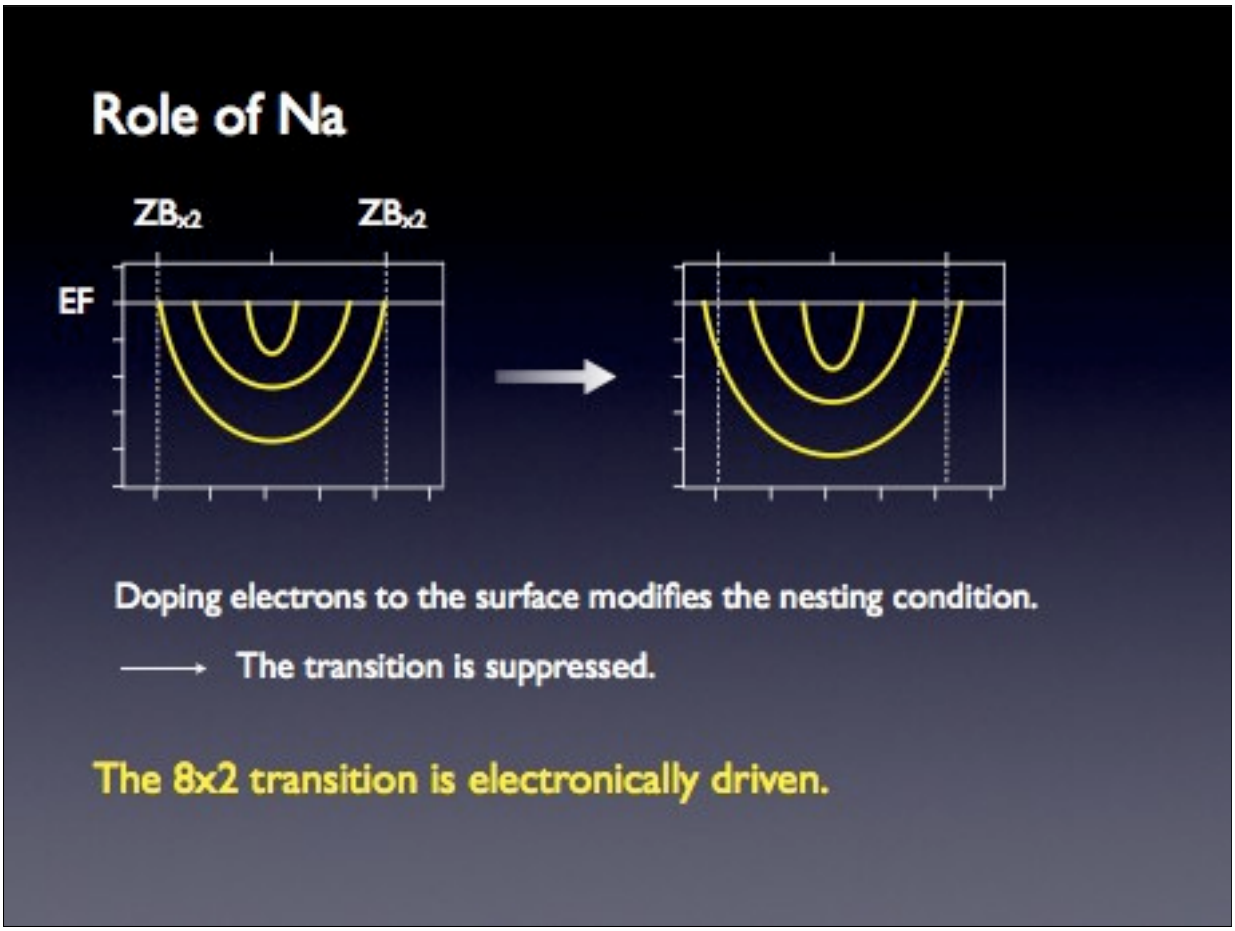
Na-deposited (0.002ML) surface @110 K



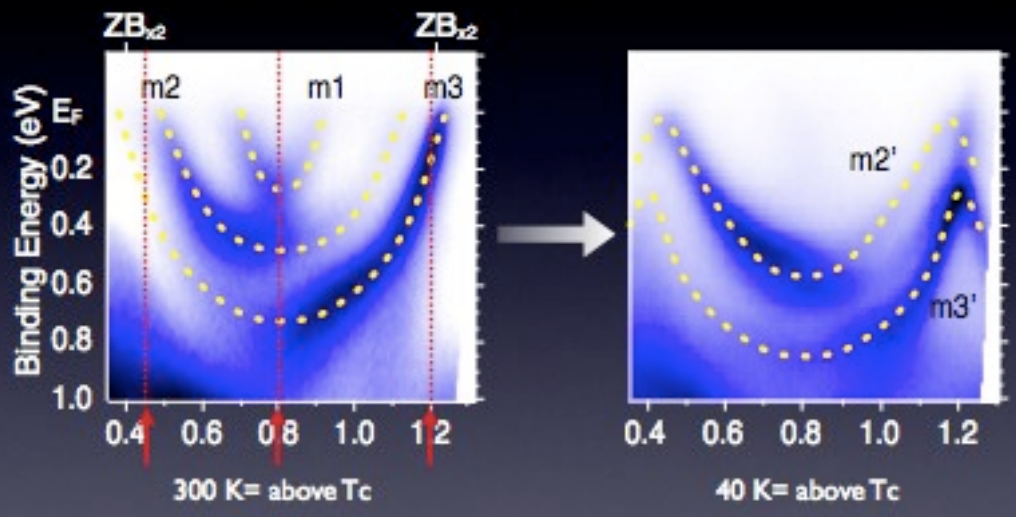
Most of the surface is covered with the 4x1 domain with a x2 modulation around Na.

The 8x2 transition is suppressed by Na.


8x2
Pristine @95 K
4x1
Na 0.02 ML @53 K
x8 spot intensity (a.u.)
pristine
0.002 ML
0.02 ML
60 80 100 120 140
Temperature (K)
The suppression of the transition is confirmed by LEED

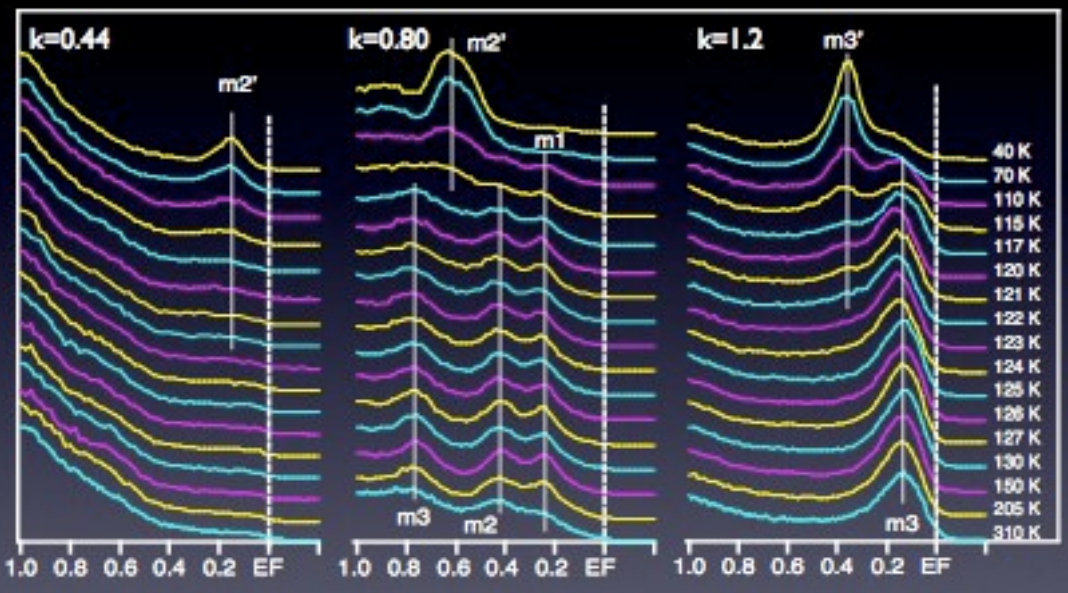

Role of Na
ZBx2
ZBx2
EF
Doping electrons to the surface modifies the nesting condition.
The transition is suppressed.
The 8x2 transition is electronically driven.

Detailed temperature dependence of the bands



How do the gapped bands (m2' and m3') develop?

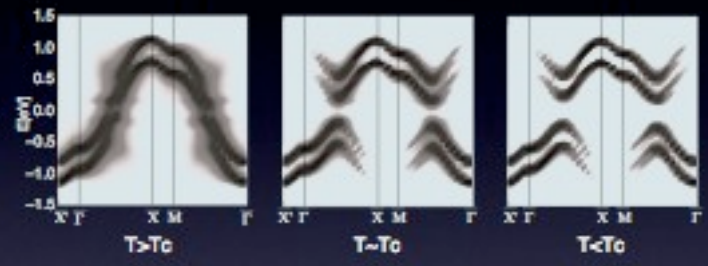
Detailed temperature dependence of the bands



The gapped bands suddenly appears.
No temperature dependence for the gap size.

The transition is a first-order type.

- *Contradictory to the order-disorder picture (2nd order transition).*



Simulated m2 and m3 bands based on the Ising model
Yagi et al. (2008)

- *Contradictory also to the weak-coupling CDW picture.*

BCS theory

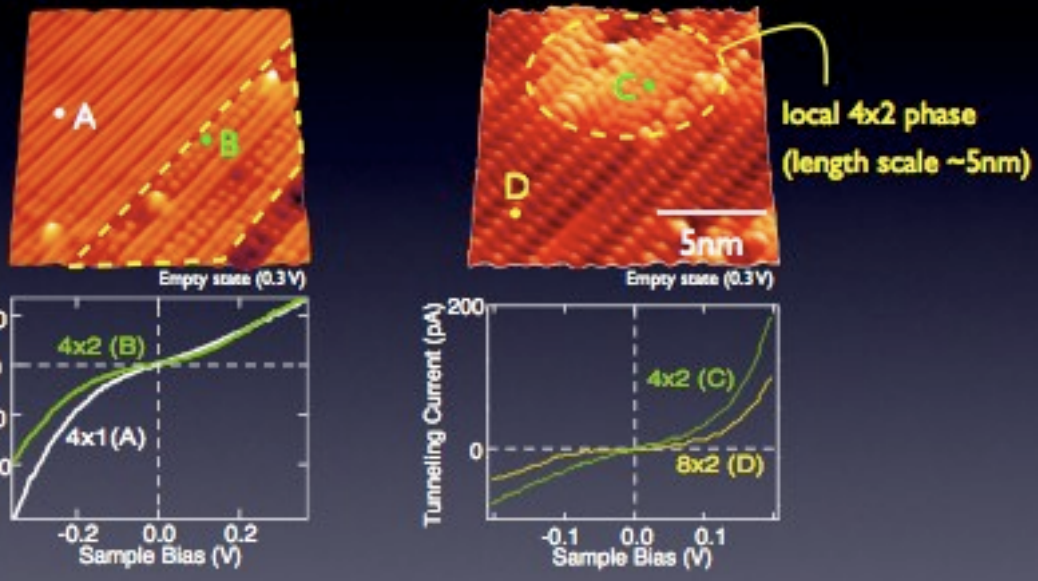
$$\frac{\Delta(T)}{\Delta(0)} = \left(1 - \frac{T}{T_c}\right)^{1/2}$$

Although the transition is electronically driven, it is not a simple weak-coupling CDW type. More complicated mechanism should be considered.

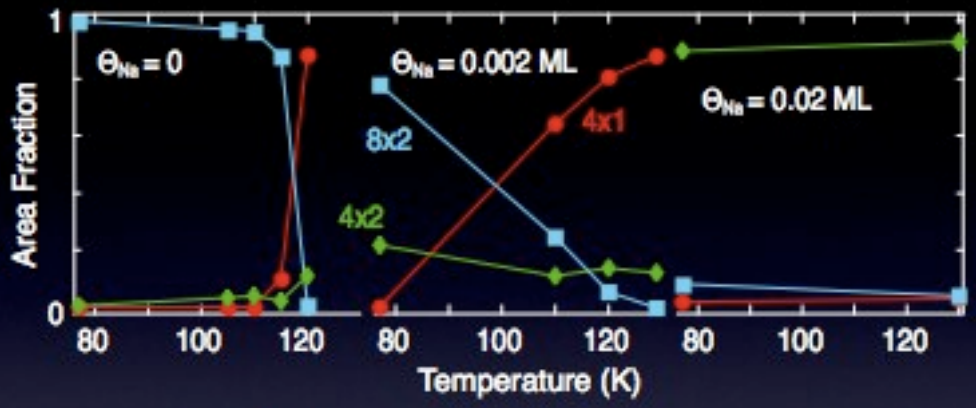
Local action of Na

130 K: 4x1 + local 4x2

77 K: 8x2 + local 4x2



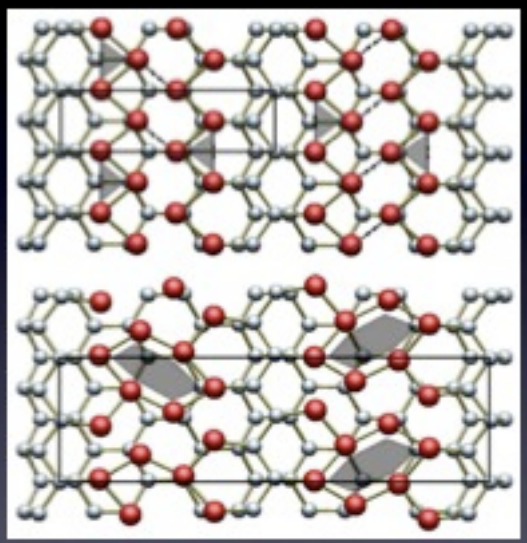
Na makes local 4x2 structure with metallic DOS.
The 4x2 structure is less metallic than the 4x1 phase.



The metallic 4x2 phase does not show the temperature dependence.

The metallic 4x2 phase is the local ground state around Na.
The 4x2 structure would be energetically close to the 8x2 phase,
and induced by the weak perturbation by Na.

Two different structure models for In/Si(111)-8x2



Trimer model
Cho et al. PRB (2001)

Hexagon model
Gonzalez et al. PRL (2006)

Energy difference between the two is extremely small (<12 meV per 4x1 unit)
Stekolnikov et al. PRL (2007)

Summary : Role of Na on In/Si(111)-4x1

Global action : electron doping

Break the commensurate nesting condition and suppress the 8x2 transition.

↓

The 8x2 transition is electronically driven, not an order-disorder type.

Local action : local 4x2 phase

Metallic and independent of the temperature.

↓

The surface can take two energetically close x2 structures, one of which is induced locally by the adsorbates.