H adsorption on Rh(110) Surface

- Experimental data on Rh(110)-H
- Calculations
- Results
- Summary

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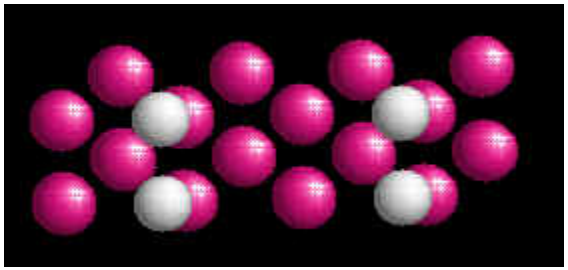
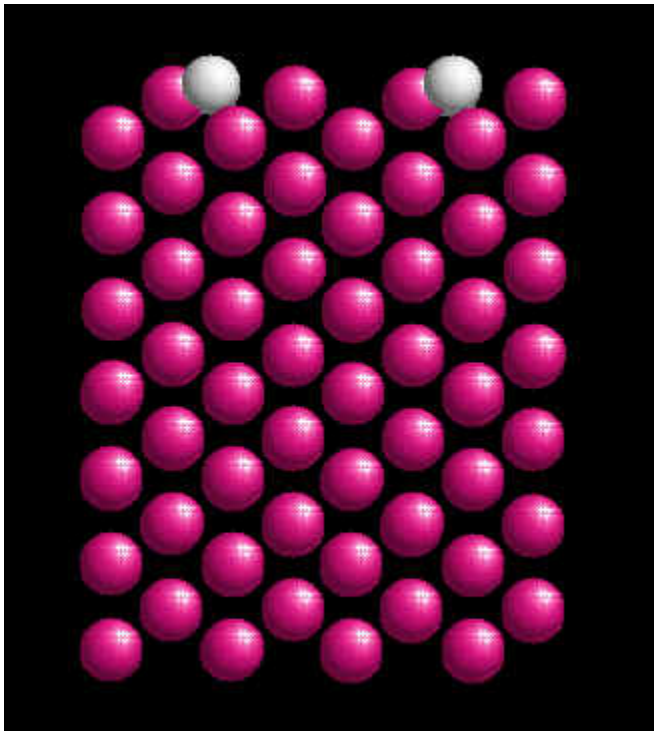
Rh (110) 1x2-H, θ=0.5





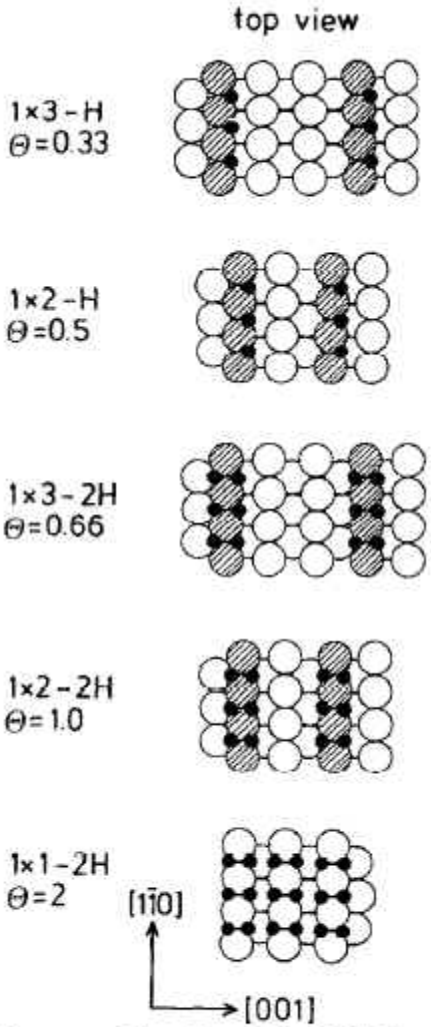


Fig. 3. Real-space configuration of the Rh(110) surface for different hydrogen coverages (top view). Shaded rhodium atoms represent the hydrogen-induced buckling in the first rhodium layer (atomic coordinates are given in detail in refs. [7–11]).

W. Nichtl-Pecher et al. Surf. Sci. 249 (1991) 61-74

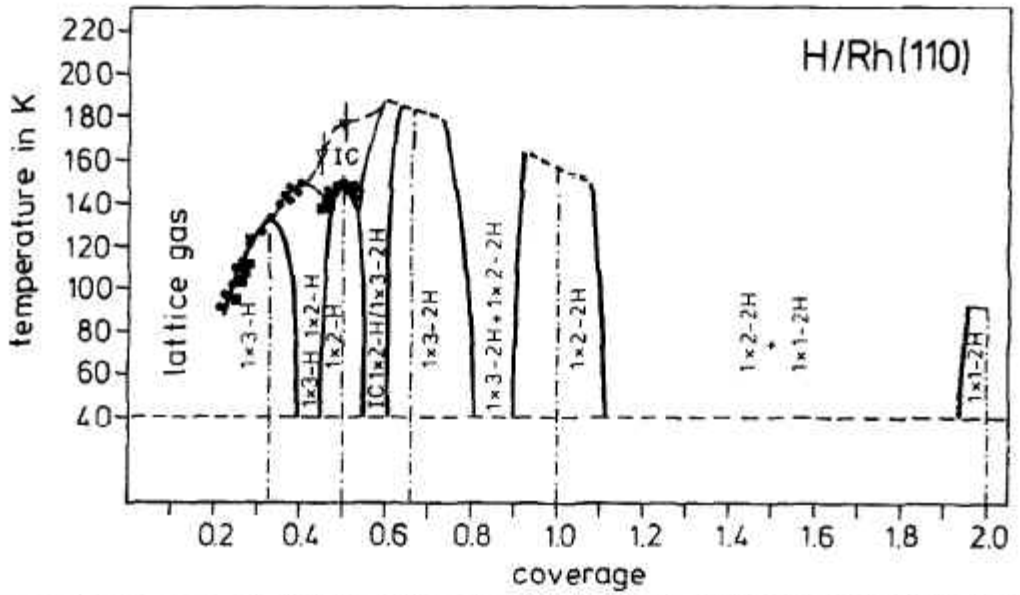


Fig. 5. Phase diagram of hydrogen on Rh(110). For coverages $\theta > 0.5$ the areas of the homogeneous phases are cut off indicating the experimental limitation to observe the respective phase transitions at constant coverage and an operational pressure of $p_{H_2} \sim 1 \times 10^{-10}$ mbar.

W. Nichtl-Pecher et al. Surf. Sci. 249 (1991) 61-74

References

- K. Christmann, Prog. Surf. Sci. 48, 15 (1995)
- H. J. Mussig et al, Surf. Sci. 311, 295 (1994)
- K. Mueller, Prog. Surf. Sci. 42, 245 (1993)
- A. Baraldi et al, Surf. Sci. 293, 246 (1993)
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- E. Kirsten et al, Chem. Phys. Lett. 181, 544 (1991)
- W. Nichtl-Pechner et al, Vacuum, 41, 297 (1990)
- W. Puchta et al, Phys. Rev. B, 39, 1020 (1989)
- W Oed et al, J. Phys. C, 21, 237 (1988)
- K. Christmann et al, Chem. Phys. Lett., 131, 192 (1986)

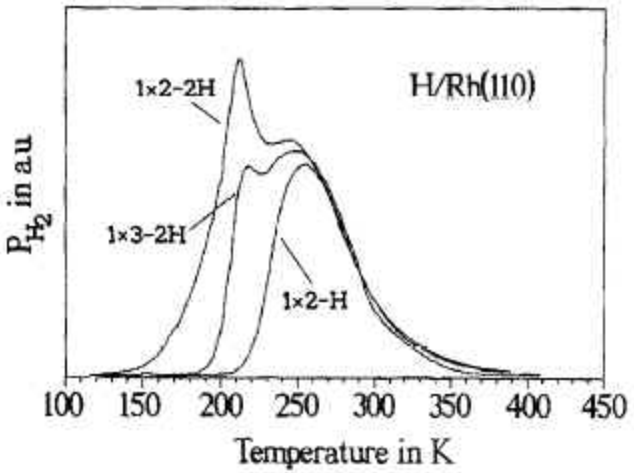


Fig. 4. TD spectra of the corresponding commensurate phases 1×2–H, 1×3–2H and 1×2–2H (heating rate 5 K/s).

W. Nichtl-Pecher et al. Surf. Sci. 249 (1991) 61-74

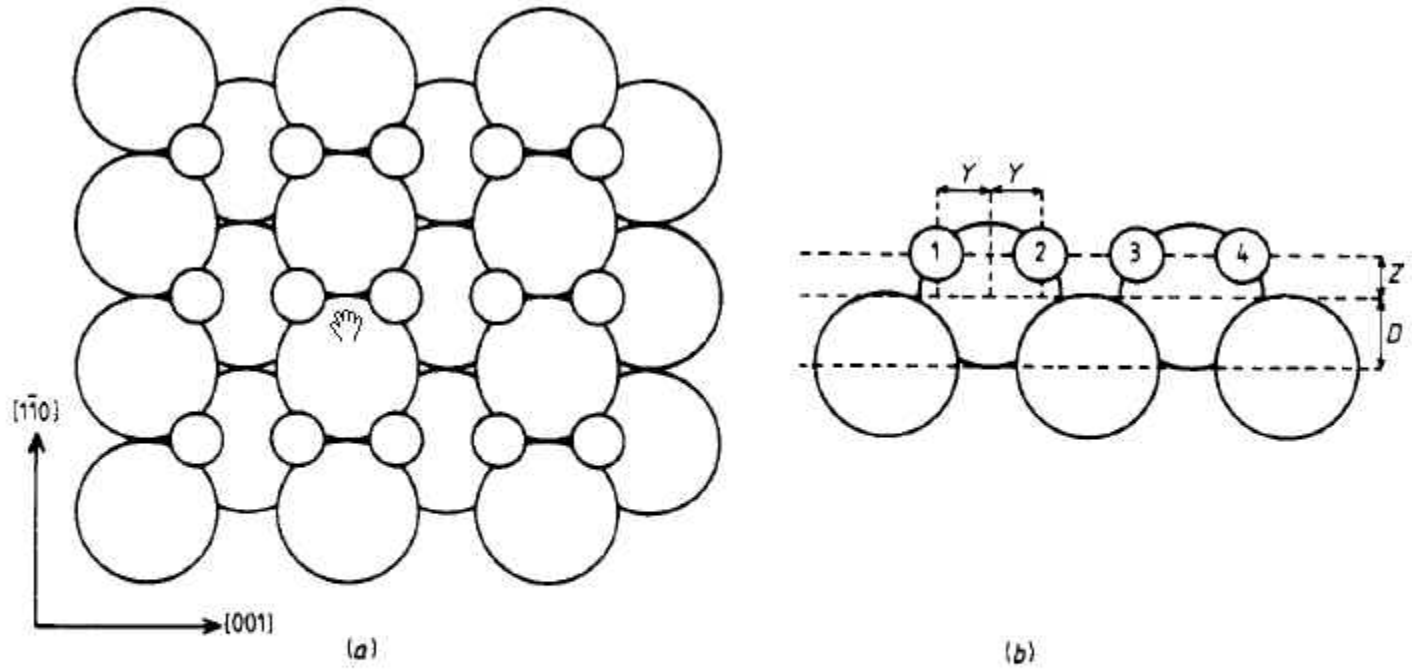
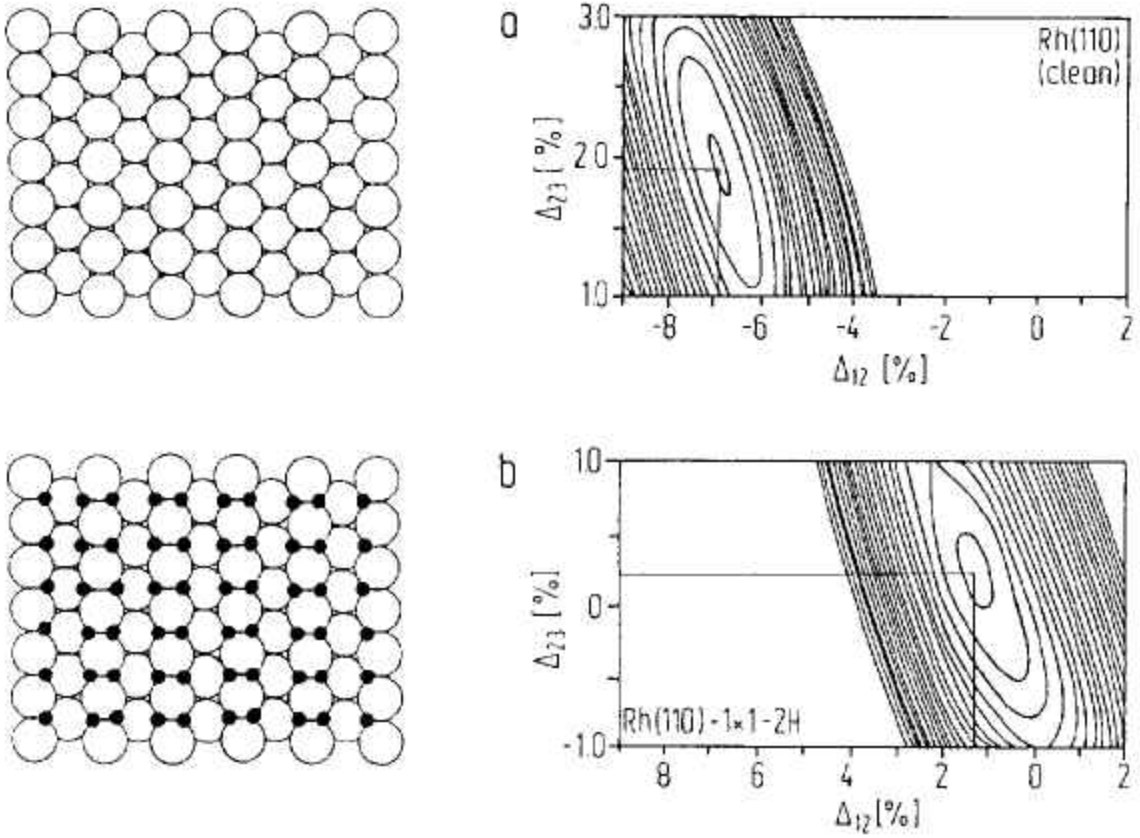


Figure 1. Structural model of H adsorption on Rh(110), (*a*) top view and (*b*) side view, with a first to second Rh layer distance D and vertical and horizontal H distances Z and Y respectively.

W Oed et al. J. Phys. C: Solid State Phys. 21 (1988) 237-243

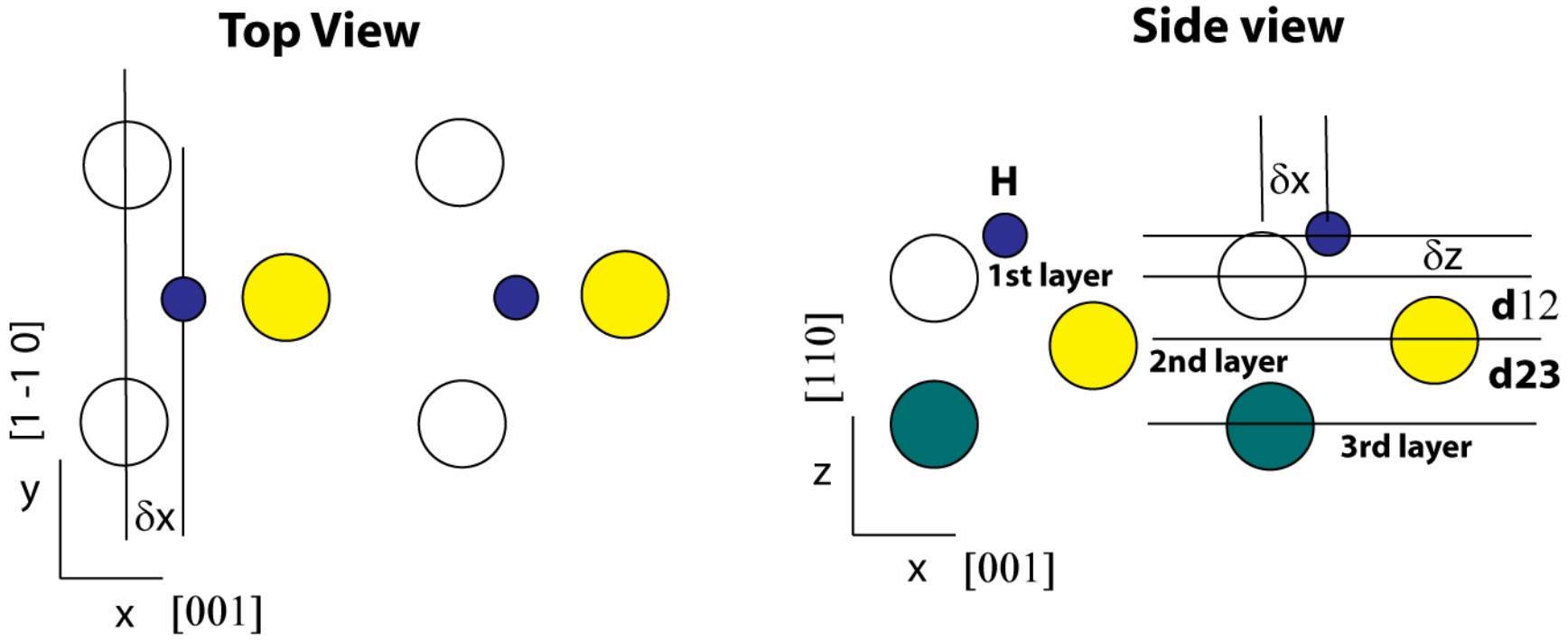


K. Christmann, Prog. Surf. Sci. 48 (1995) 15.

Calculations

- Density Functional Theory (DFT)
- Projector Augmented Wave (PAW)
- 32 -45 atom slab
- Periodic boundary conditions

FCC (110) Surface



H adsorption sites

- Atop site: -3.12 eV
- [001] Long Bridge site: -3.68 eV
- [1 -1 0] Short bridge site: -4.08 eV

(3-fold coordinated, but not at equal distances)

H_2 binding energy 3.30 eV/H atom

Structural comparisons

1x1-2H, θ = 2: substrate not relaxed

3-fold coordinated sites (☺)

δx = 0.93Å (0.98±0.3 Expt.*)(0.97±0.1#)

δz = 0.60Å (0.78±0.14*) (0.82±0.1#)

$R_{\text{H-Rh(1st L.)}}$ = 1.75Å (1.84±0.2*)(1.85±0.1#)

$R_{\text{H-Rh(2nd L.)}}$ = 2.20Å (2.30±0.2*)

* W Oed et al J. Phys. C, 21, 237 (1988), LEED, fixed 2nd layer

E. Kirsten et al, Chem. Phys. Lett. 181, 544 (1991), 1x2-H

Structural comparisons

1x1-2H, θ = 2: 2 layers relaxed

3-fold coordinated sites (☺)

δx = 0.92Å (0.98±0.3 Expt.*)

δz = 0.59Å (0.78±0.14)

$R_{\text{H-Rh(1st L.)}}$ = 1.74Å (1.84±0.2)

$R_{\text{H-Rh(2nd L.)}}$ = 2.28Å (2.30±0.2)

* W Oed et al J. Phys. C, 21, 237 (1988), LEED, fixed 2nd layer

Structural comparisons

1x1-2H, θ = 2: fully relaxed

3-fold coordinated sites (☺)

δx = 0.92Å (0.98±0.3 Expt.*)(0.97±0.1#)

δz = 0.59Å (0.78±0.14) (0.82±0.1#)

$R_{H\text{-}Rh(1st\ L.)}$ = 1.74Å (1.84±0.2)(1.85±0.1#)

$R_{H\text{-}Rh(2nd\ L.)}$ = 2.28Å (2.30±0.2)

*W Oed et al J. Phys. C, 21, 237 (1988), LEED, fixed 2nd layer

E. Kirsten et al, Chem. Phys. Lett. 181, 544 (1991), 1x2-H

1x1-2H, θ = 2: 1 layer relaxed

d_{12} = 1.38Å (1.33±0.1, if neglects H)

(1.32±0.05, if considers H)

d_{23} = 1.359Å (1.34)

d_{34} = 1.359Å (? fixed)

$d_{\mathbf{bulk}}$ = 1.359Å (1.345)

* W Nichtl-Pecher et al. Vacuum, 41 (1990) 297-300

1x1-2H, θ = 2: 2 layers relaxed

d_{12} = 1.454Å (1.33±0.1, if neglects H)

(1.32±0.05, if considers H)

d_{23} = 1.283Å (1.34)

d_{34} = 1.359Å (? fixed)

$d_{\mathbf{bulk}}$ = 1.359Å (1.345)

* W Nichtl-Pecher et al. Vacuum, 41 (1990) 297-300

1x1-2H, θ = 2: fully relaxed

d_{12} = 1.47Å (1.33±0.1, if neglects H)

(1.32±0.05, if considers H)

d_{23} = 1.30Å (1.34)

d_{34} = 1.33Å (? fixed)

$d_{\mathbf{bulk}}$ = 1.359Å (1.345)

$R_{H\text{-}H}$ = 1.84 & 2.01 Å

* W Nichtl-Pecher et al. Vacuum, 41 (1990) 297-300

Change in work function

- Clean 1x1 Rh(110) → 4.55 eV
- Rh (110) 1x1-2H, θ=2.0 → 5.31 eV
- Change in work fuction 0.76 eV (0.93 eV)*

* M. Ehsasi and K. Chhristmann, Surf. Sci. 194, 172 (1988)

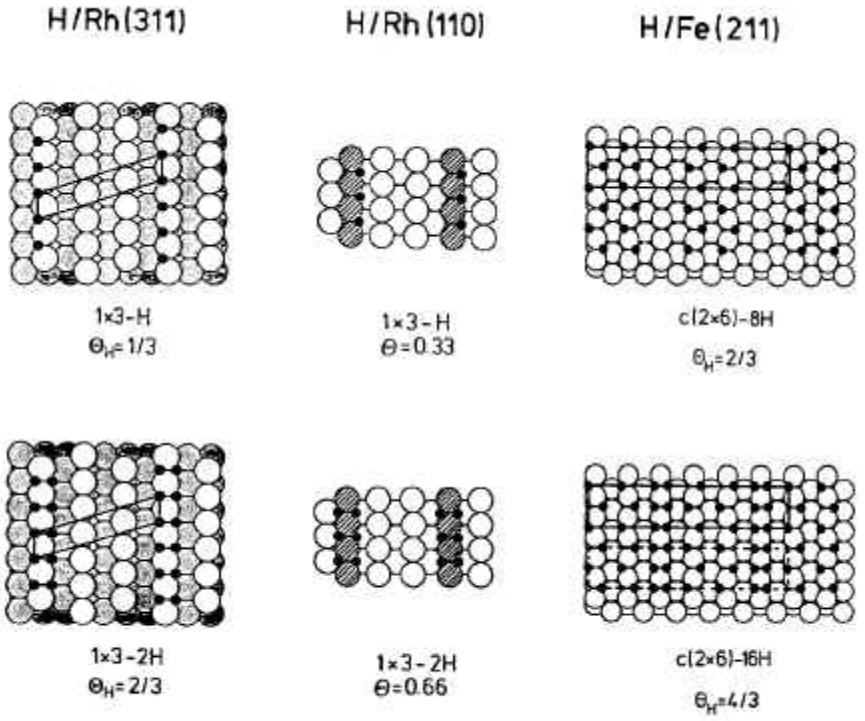
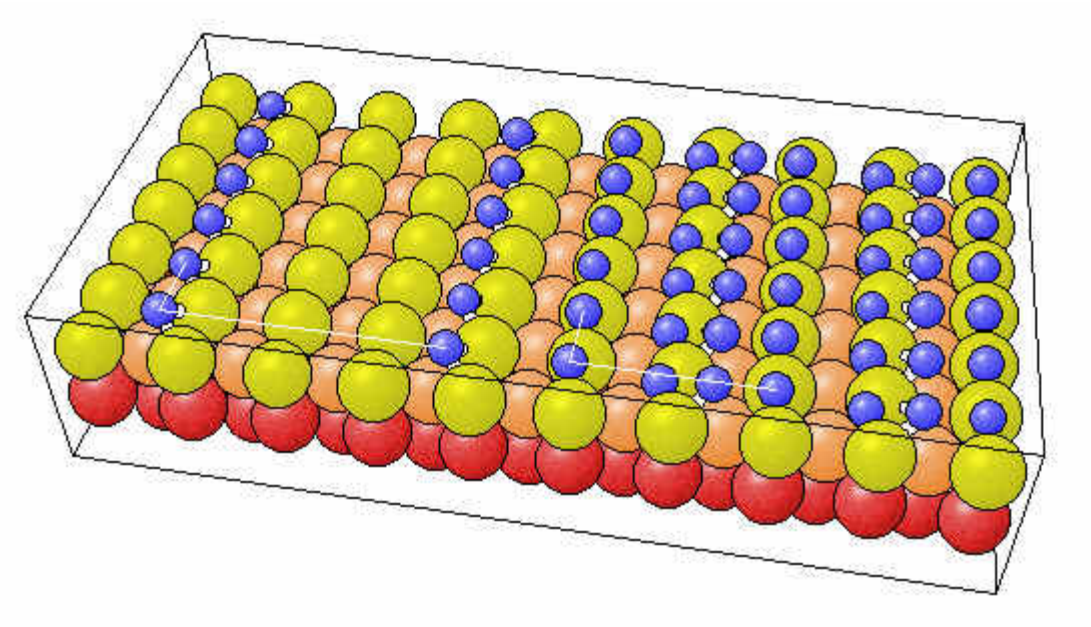


Fig. 3. Real space configuration models for selected ordered phases. Full dots mark adsorption sites.

K. Mueller, Prog. Surf. Sci. 42 (1993) 245-255

Picture from the NIST Surface Structure Database (SSD)*



Geometry of Rh(110)+(1x3)-H; Rh(110)+(1x2)-3H

* SSD is the NIST Standard Reference Database no. 42 by P. R. Watson, M. A. Van Hove, and K. Hermann. The pictures have been prepared from NIST SSD output and processed with BALSAC by K. Hermann.

1x3-2H cases, θ = 0.66

- Case A: 0.0 eV (proposed from LEED)
- Case B: +1.26 eV
- Case C: +1.24 eV
- Case D: +1.25 eV

(Only H atoms were relaxed)

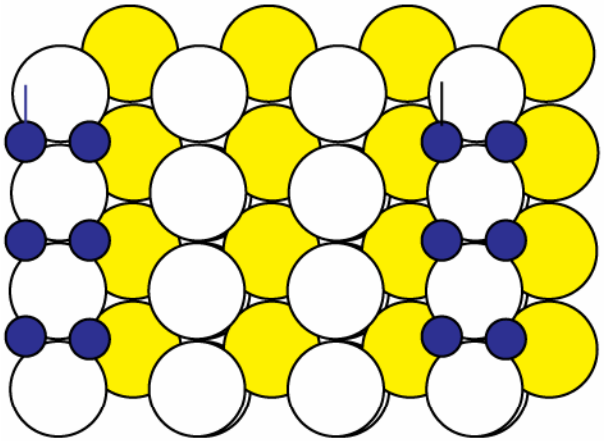
1x3-2H cases, θ = 0.66

- Case A: 0.0 eV (proposed from LEED)
- Case B: -0.371 eV
- Case C: -0.367 eV
- Case D: -0.347 eV

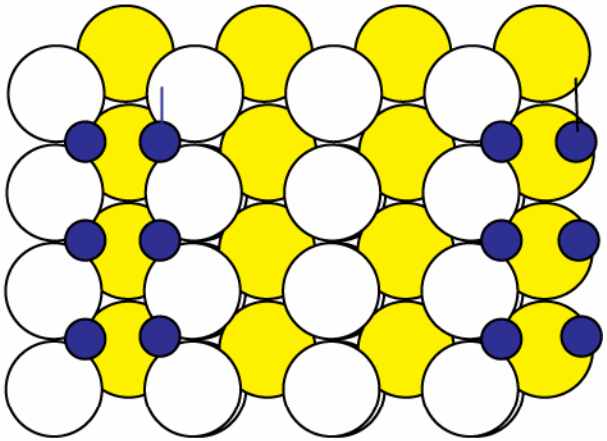
(H and 3 layers of Rh atoms were relaxed)

1x3-2H, θ=0.66

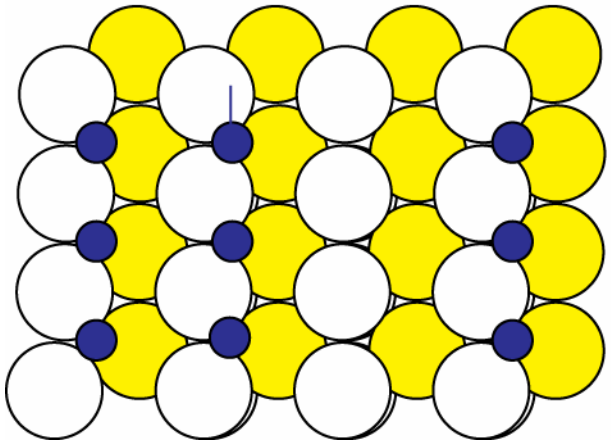
A 0.0 eV



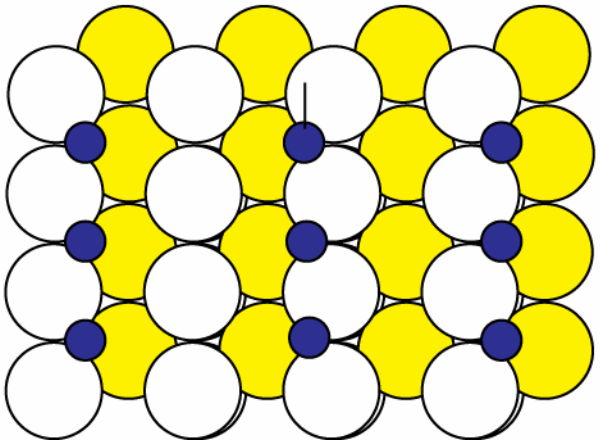
B -0.371 eV



C -0.367 eV



D -0.347 eV



1x2-2H cases, θ = 1.0

- Case A: 0.0 eV (proposed from LEED)
- Case B: +1.28eV
- Case C: +1.26eV

(H relaxation only)

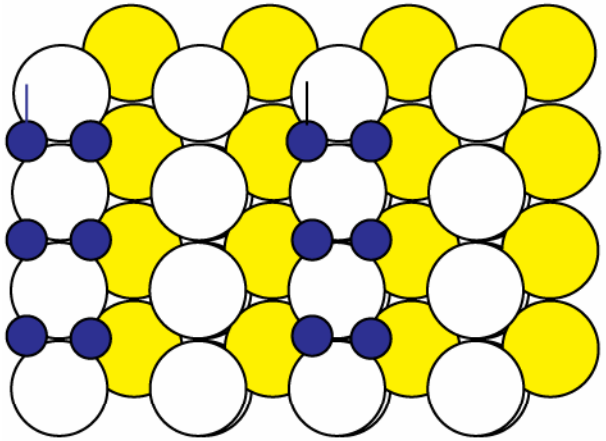
1x2-2H cases, θ = 1.0

- Case A: 0.0 eV (proposed from LEED)
- Case B: -0.326 eV
- Case C: -0.349eV (same as 1x1-H, θ=1.0)

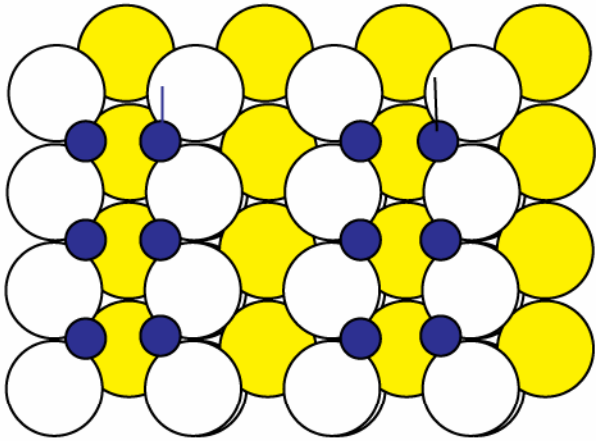
(H and 3 layers of Rh atoms were relaxed)

1x2-2H, θ=1.0, Full relaxation

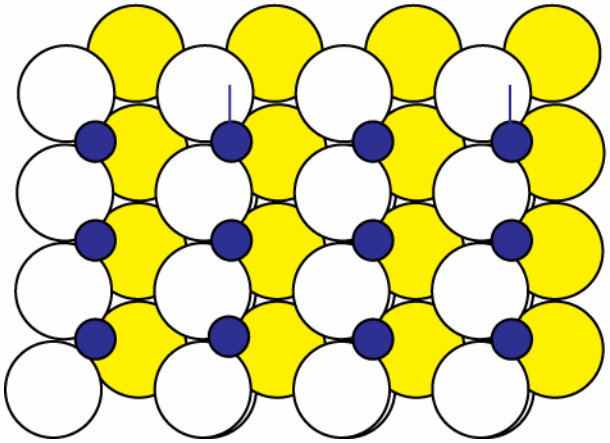
A 0.0 eV



B -0.326eV



C -0.349eV (same as 1x1-H, θ=1.0)



Summary

- H_2 will dissociate into H atoms on Rh(110).
- H atom will occupy a quasi 3-fold site.
- Very good agreement on H arrangement and positions. Θ from 0.33 to 2.0
- New arrangement for 1x3-2H, 1x2-2H was found.
- Detailed structures need to be refined.