Zonghai Hu

Outline

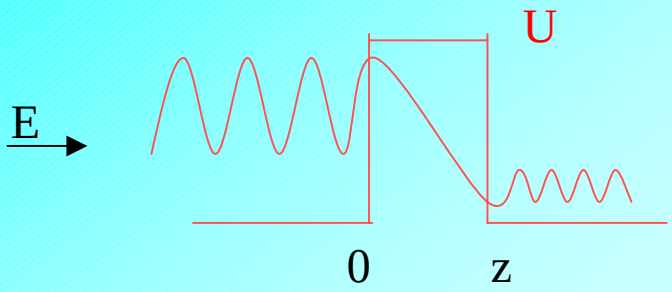
Invention of STM

G. Binnig and H. Rohrer, Helv. Phys. Acta 55, 726 (1982).

(IBM Zurich)

Noble Prize 1986 (photo by C.Chen)

One Dimensional Square Barrier – Tunneling Effect



$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial z^2}+U\Psi=E\Psi$$

$$T \sim e^{-2\kappa Z}$$

where

$$\kappa=\sqrt{\frac{2m(U-E)}{\hbar^2}}$$

Φ **κ**

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Quantitative Description – Modified Bardeen's method

Fermi's Golden Rule

$$T = \frac{2\pi}{\hbar}\left|M_{\mu\nu}\right|^2 \delta(E_\mu - E_\nu) \quad \text{where} \quad M_{\mu\nu} = -\frac{\hbar^2}{2m}\oiint_\Sigma (\chi_\nu^* \nabla\Psi_\mu - \Psi_\mu \nabla\chi_\nu^*)\,dS$$

$$I = \frac{2\pi e}{\hbar}\sum_{\mu\nu}\left\{f(E_\mu)[1 - f(E_\nu + eV)] \bullet \left|M_{\mu\nu}\right|^2 \delta(E_\mu - E_\nu)\right\}$$

In the limit of small bias voltage and low temperature :

$$I = \frac{2\pi e^2 V}{\hbar}\sum_{\mu\nu}\left\{\delta(E_\mu - E_\nu)\left|M_{\mu\nu}\right|^2\right\}$$

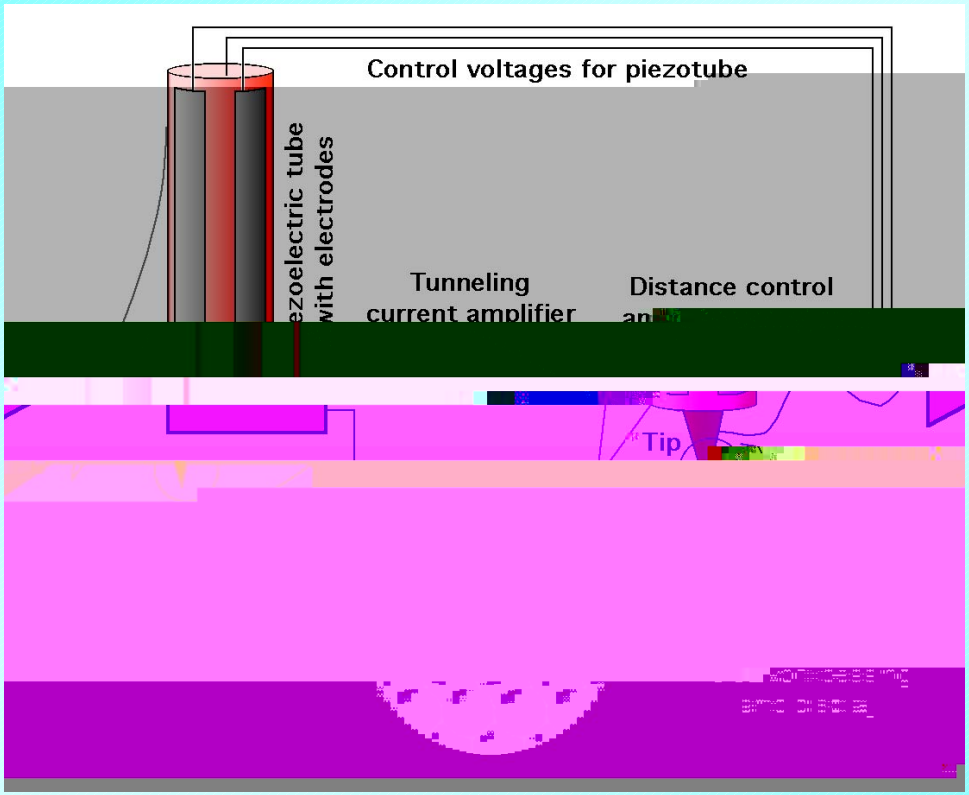
Assuming spherical tip and s wave function of tip:

$$\frac{dI}{dV} \propto \sum_{E_f - eV}^{E_f}\left|\Psi_\nu(r_0)\right|^2 \propto \rho_s(r_0, E_f - eV) \longrightarrow$$

J. Bardeen, Phys. Rev. Lett. 6, 57 (1961).

J. Tersoff and D. R. Hamann, Phys. Rev. B 31, 805 (1995).

STM Instrumentation and Operation



STM Applications

Motivations to study H/Si(001)

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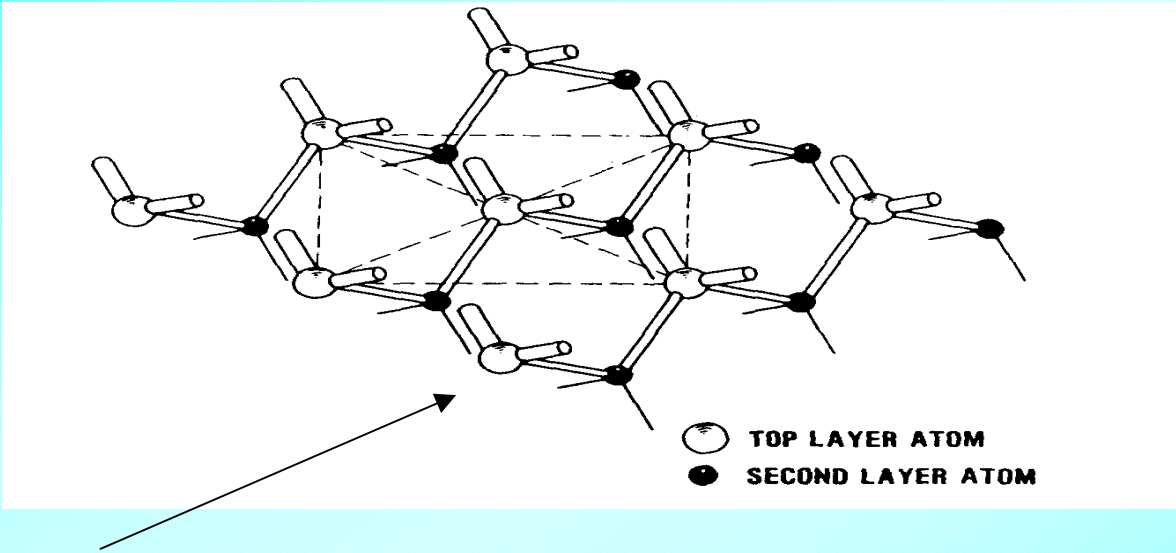
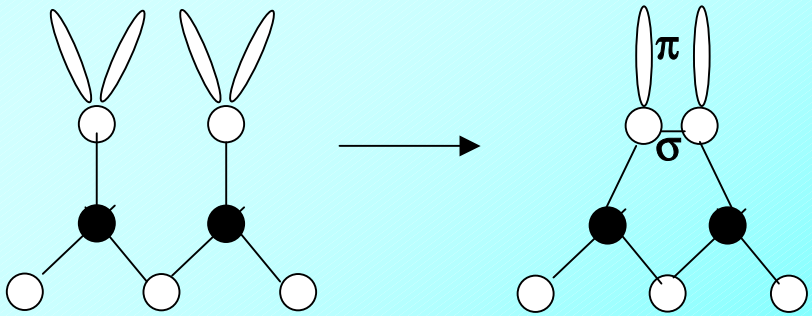
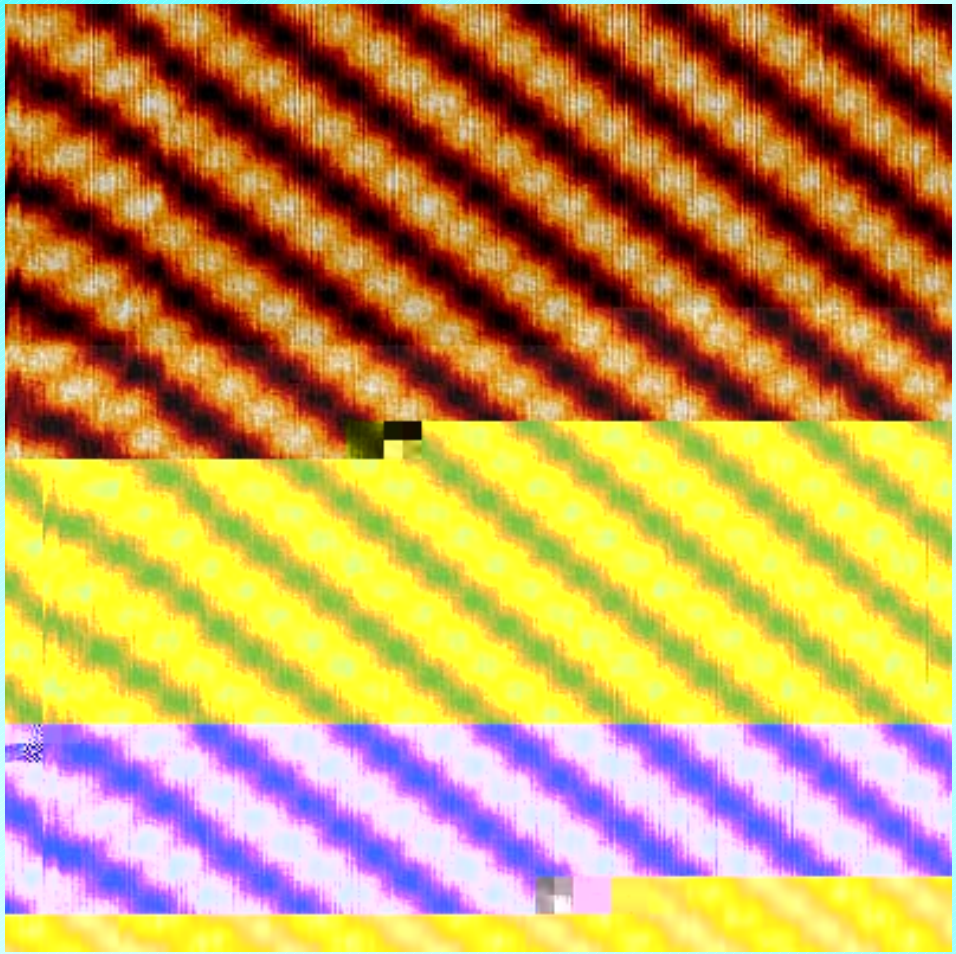
Si(001) surface reconstruction





Si(001) × dimer row structure



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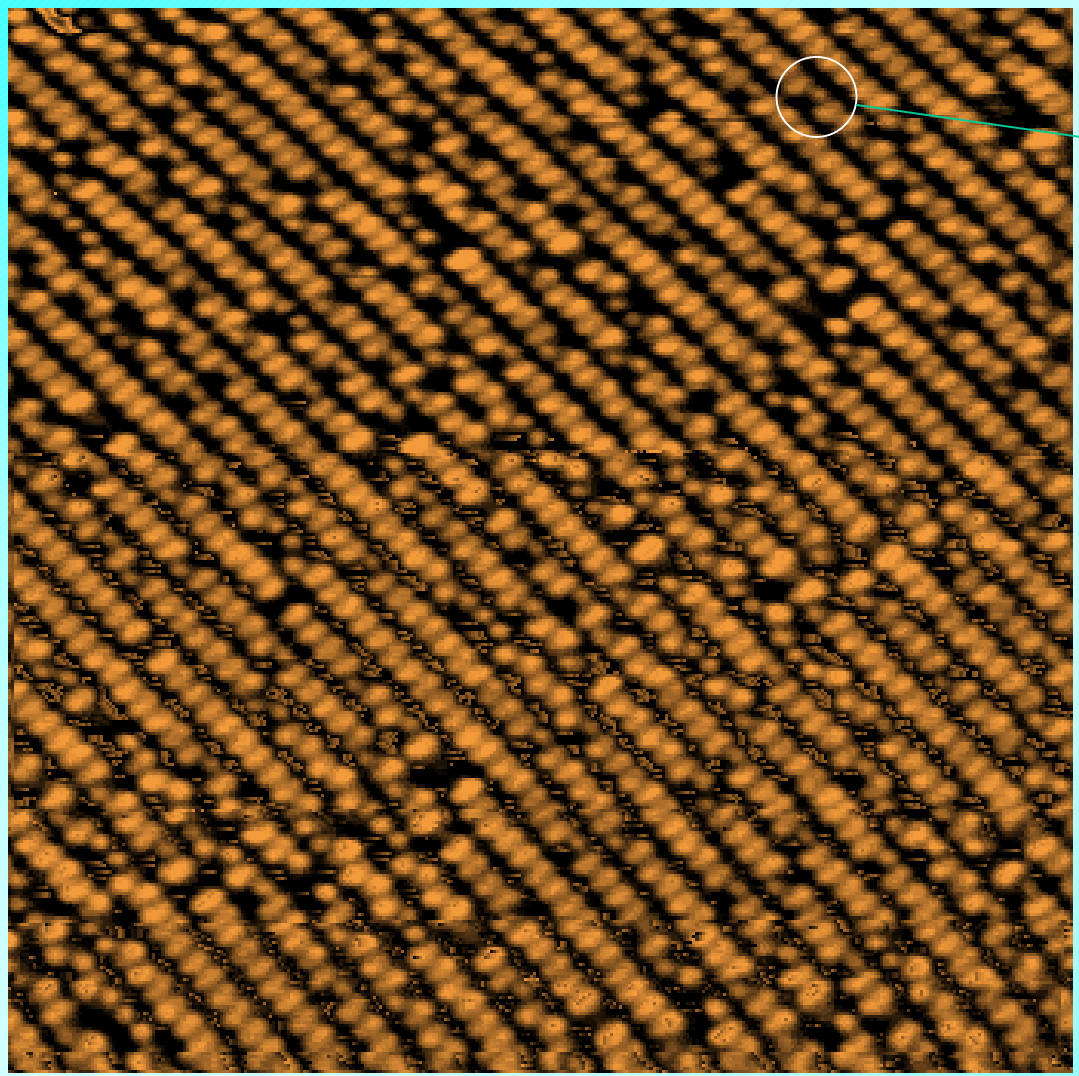
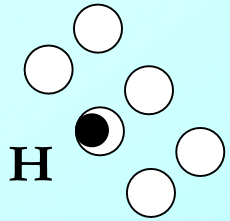
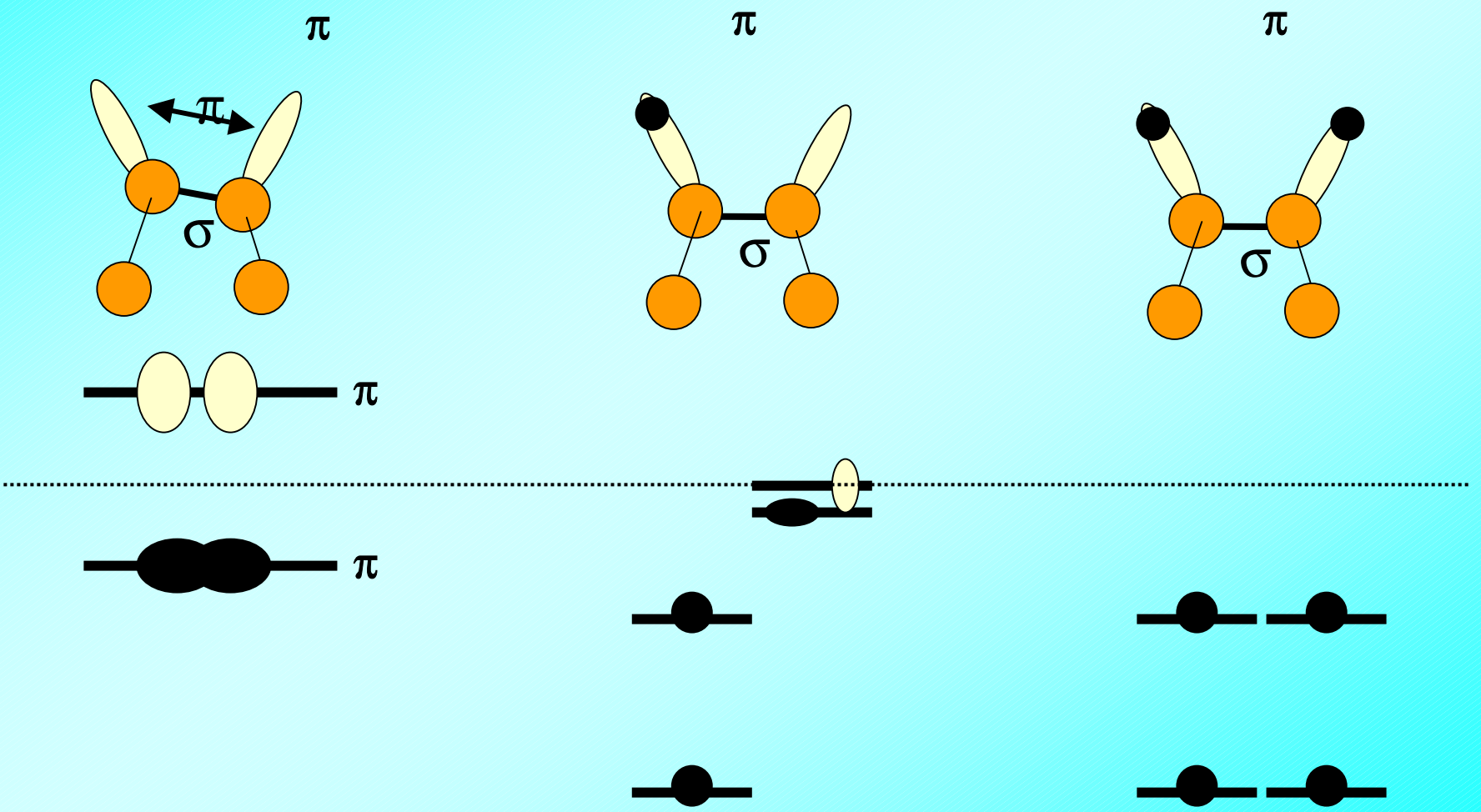
Si(001) surface after atomic H adsorption at RT

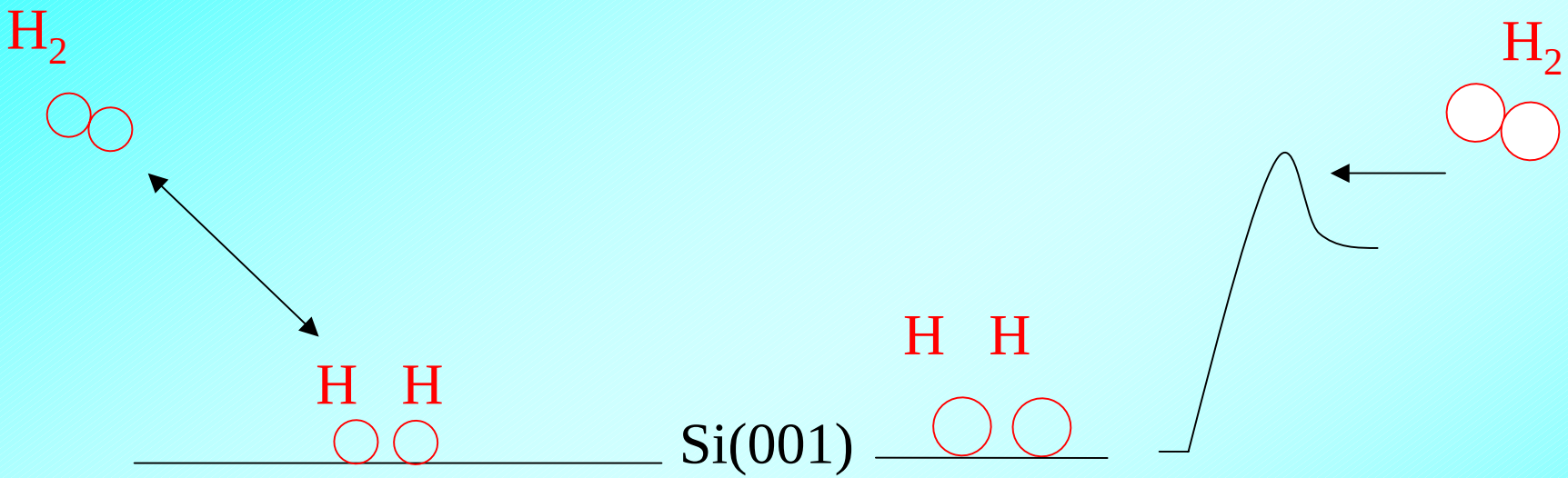




Changes in geometric and electronic structures upon adsorption of hydrogen



Unusual behavior of H_2 - Si(001) interaction



≡ θ ≈ θ θ θ

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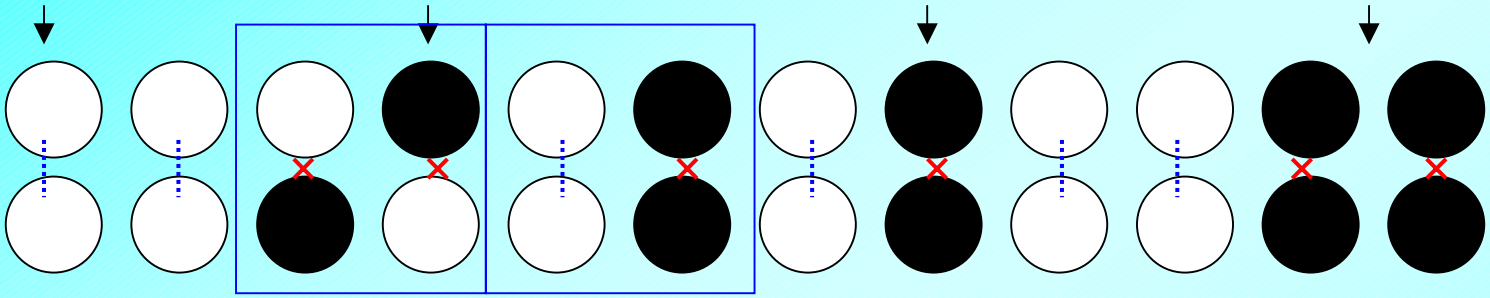
Relevant surface configurations and interactions



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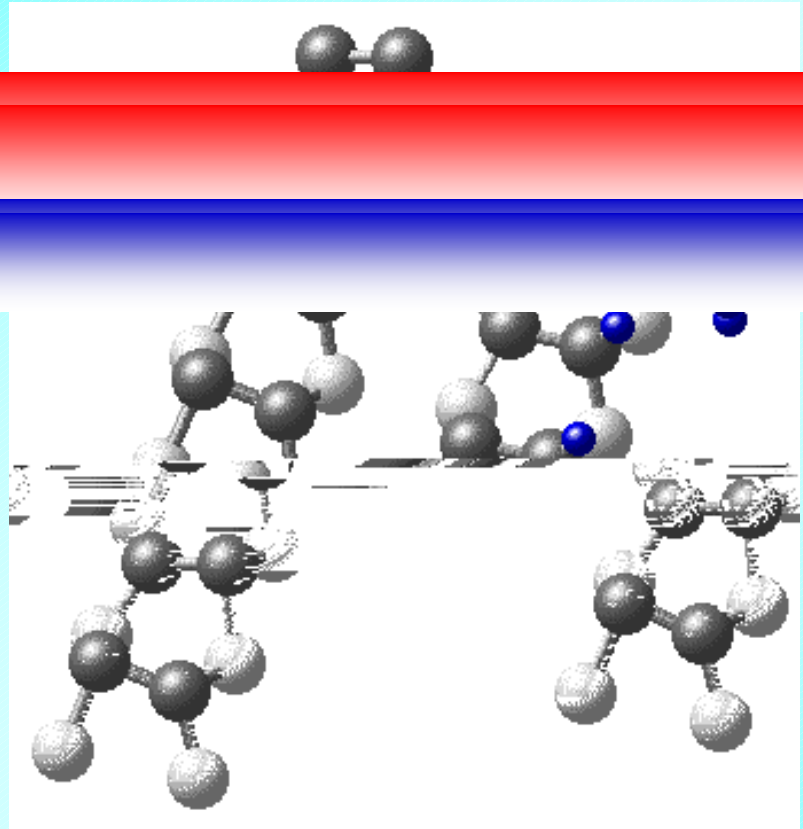
Desorption pathways in controversy



Experimental

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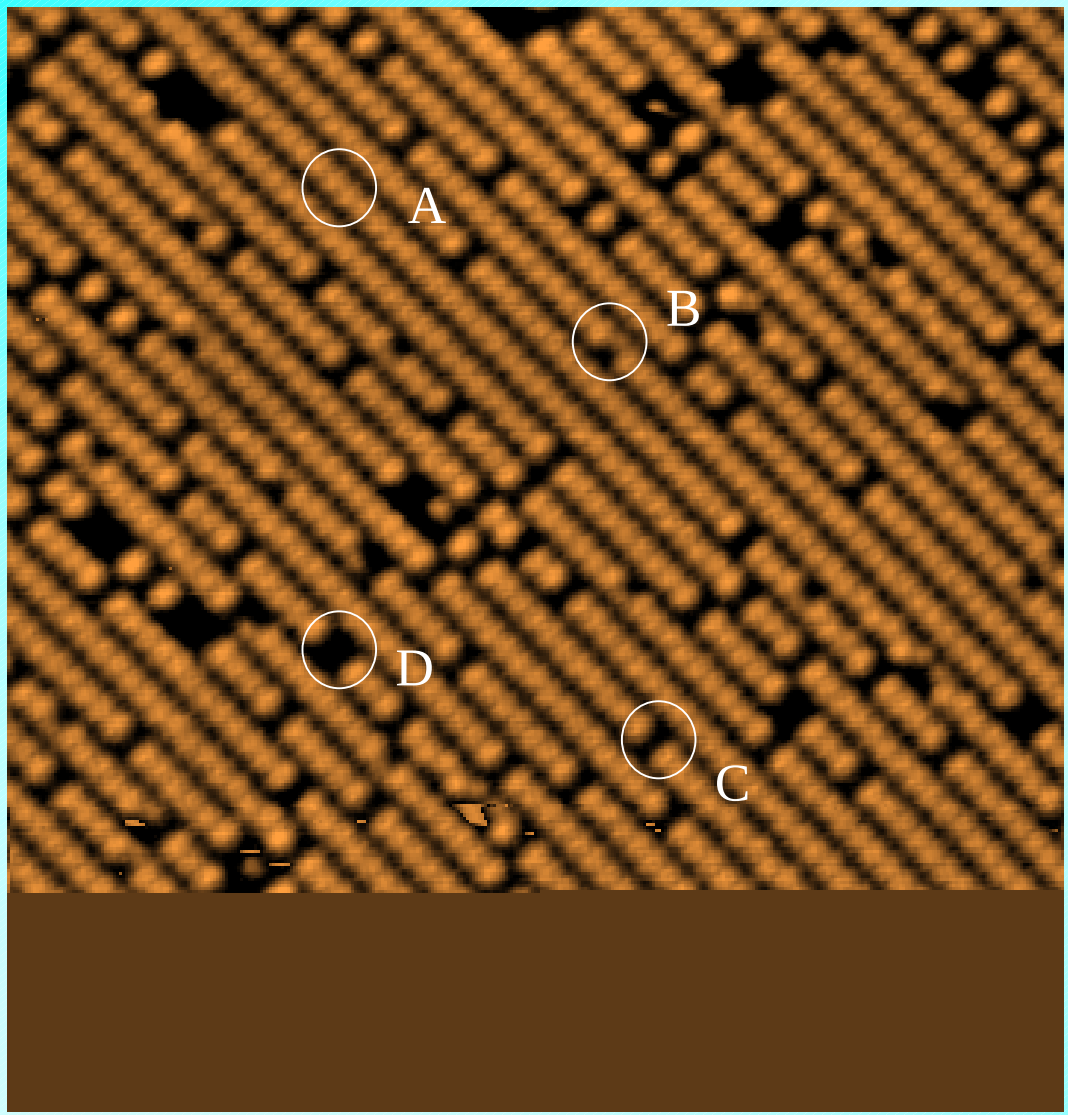
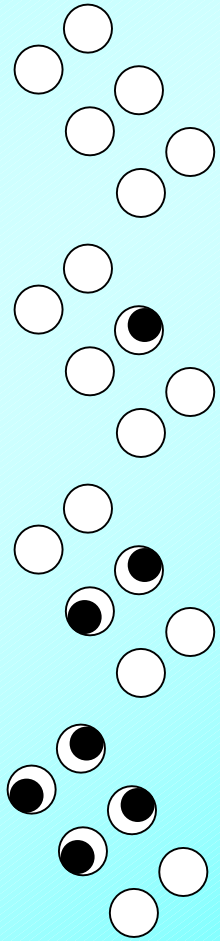
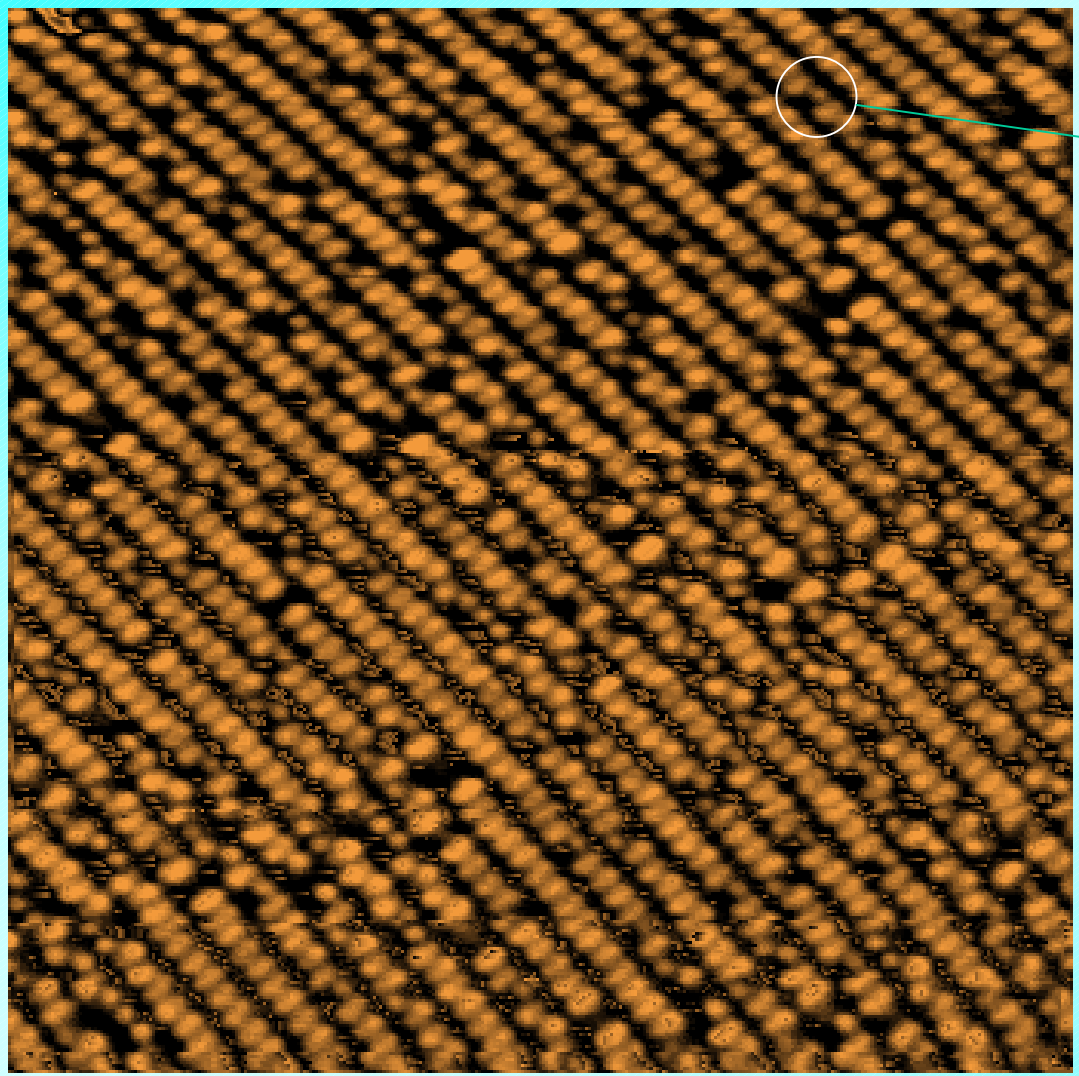
Experimental set-up

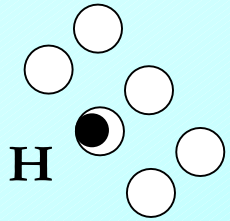
H distribution after annealing to 640 K



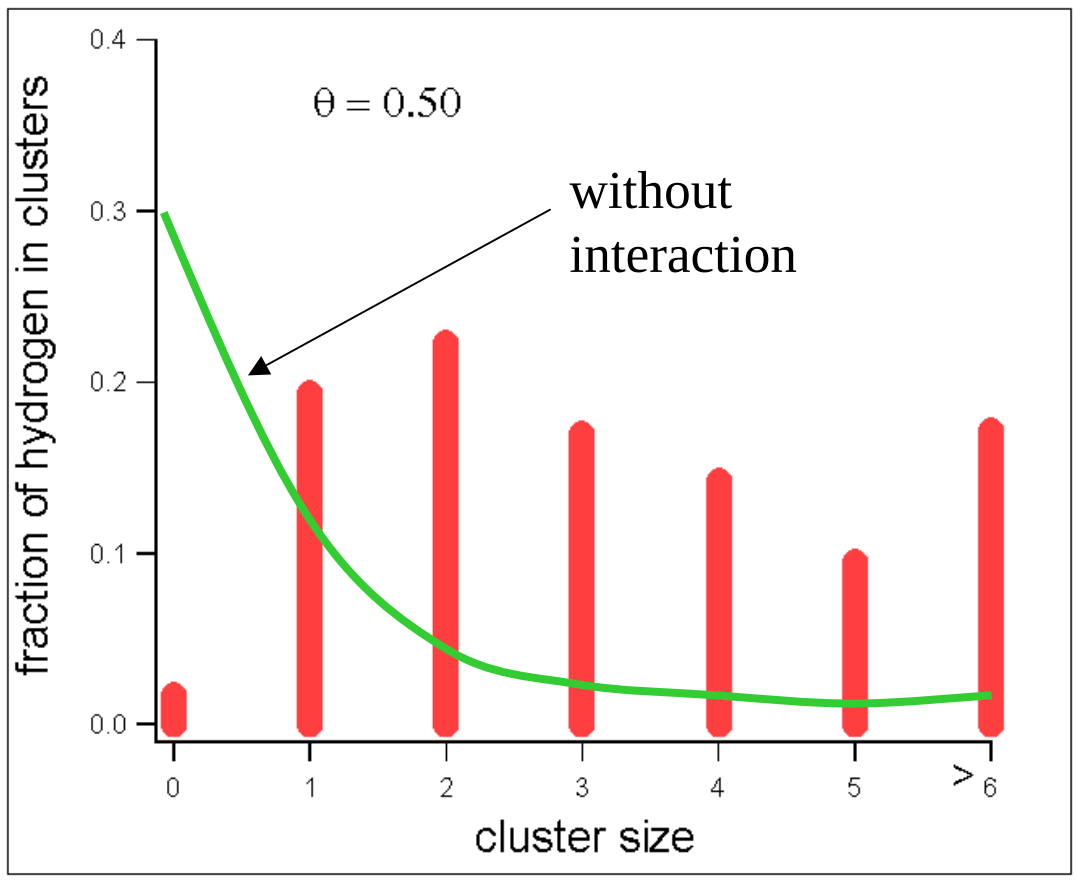


Si(001) surface after atomic H adsorption at RT





Counting results of H configurations



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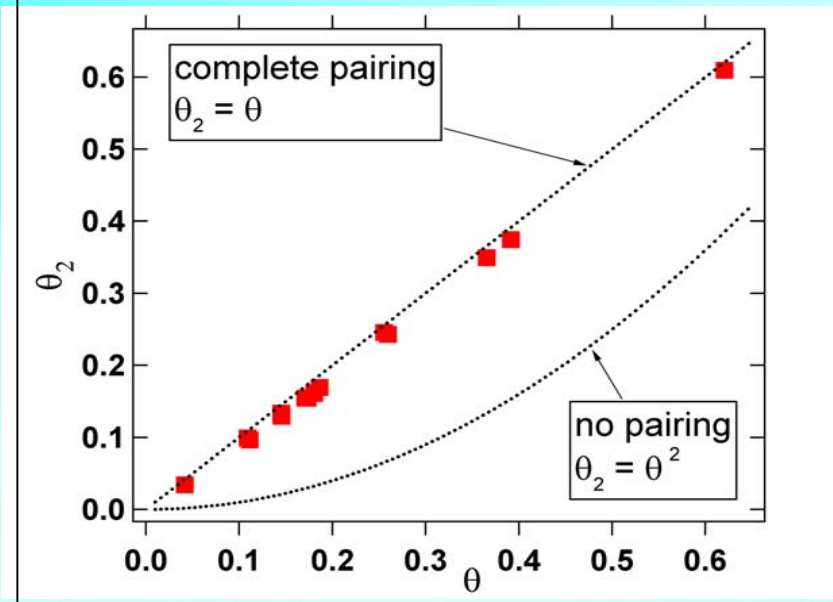
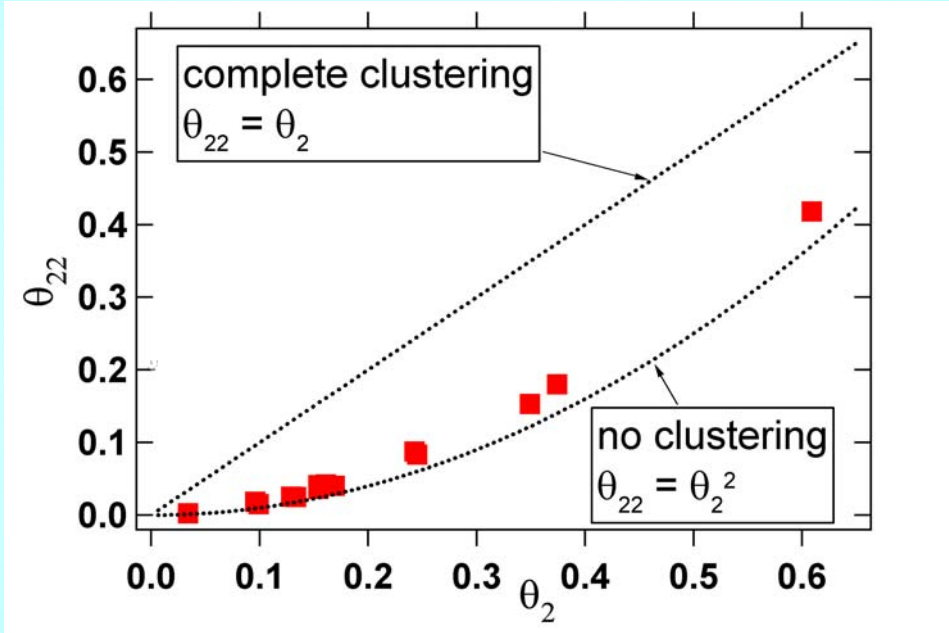
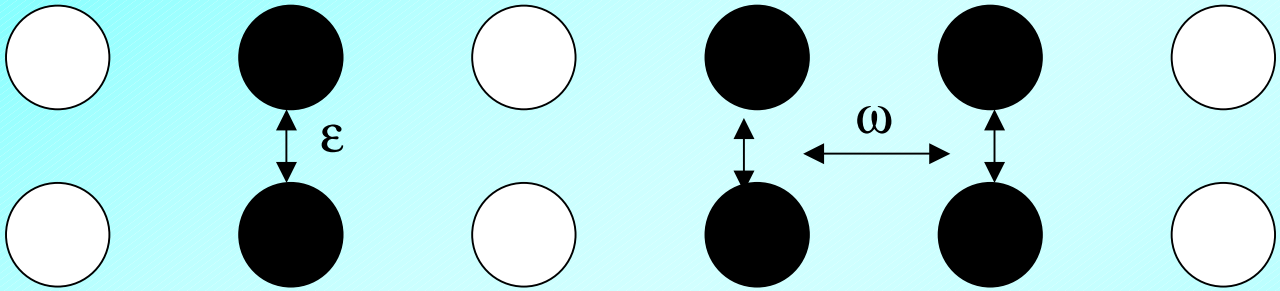
Qualitative analysis



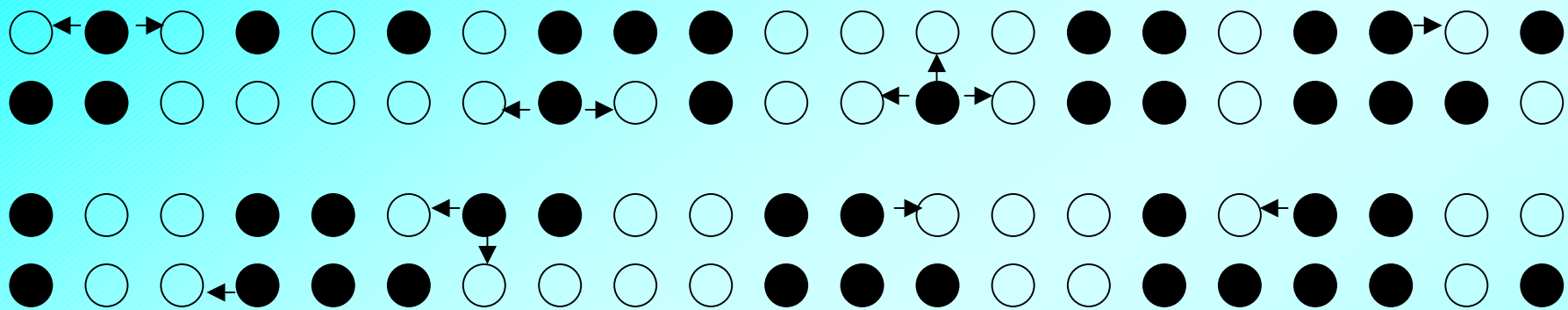


Pairing and clustering interactions



θ θ θ

Monte Carlo simulation



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Δ

Δ ≥

Δ ≤

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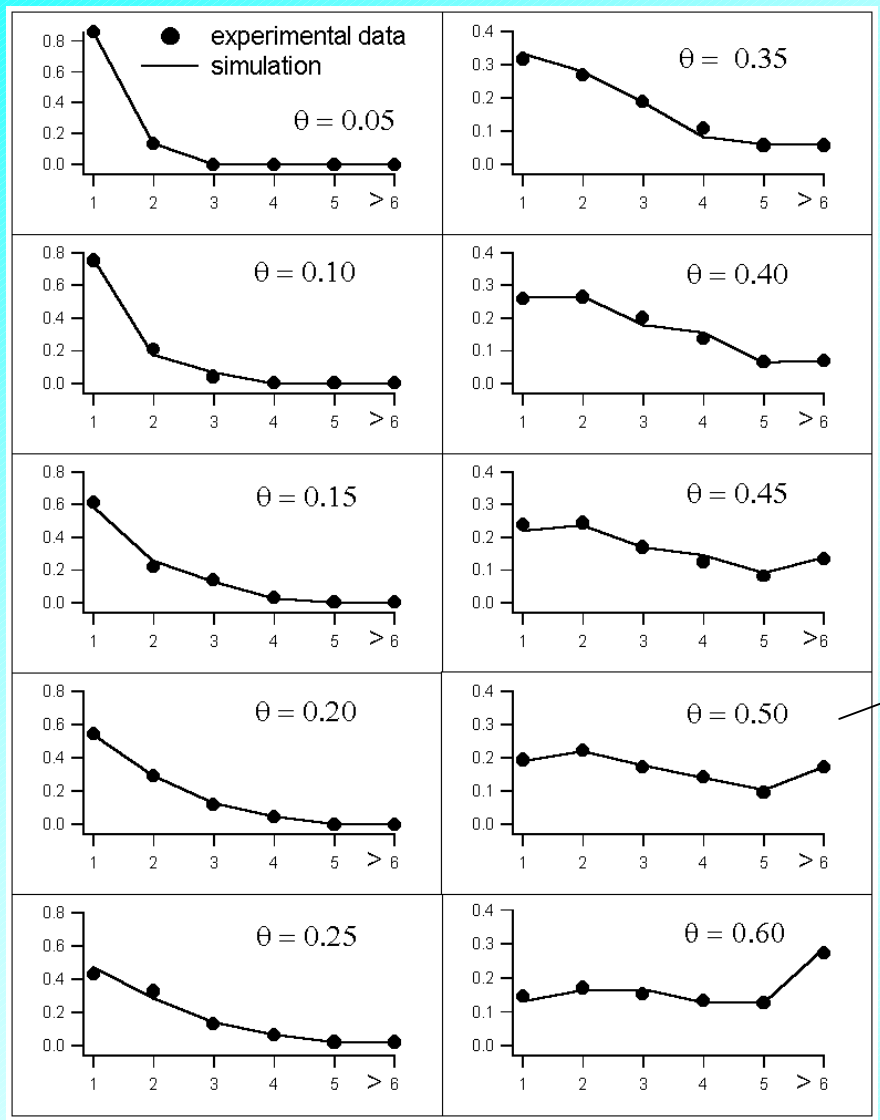
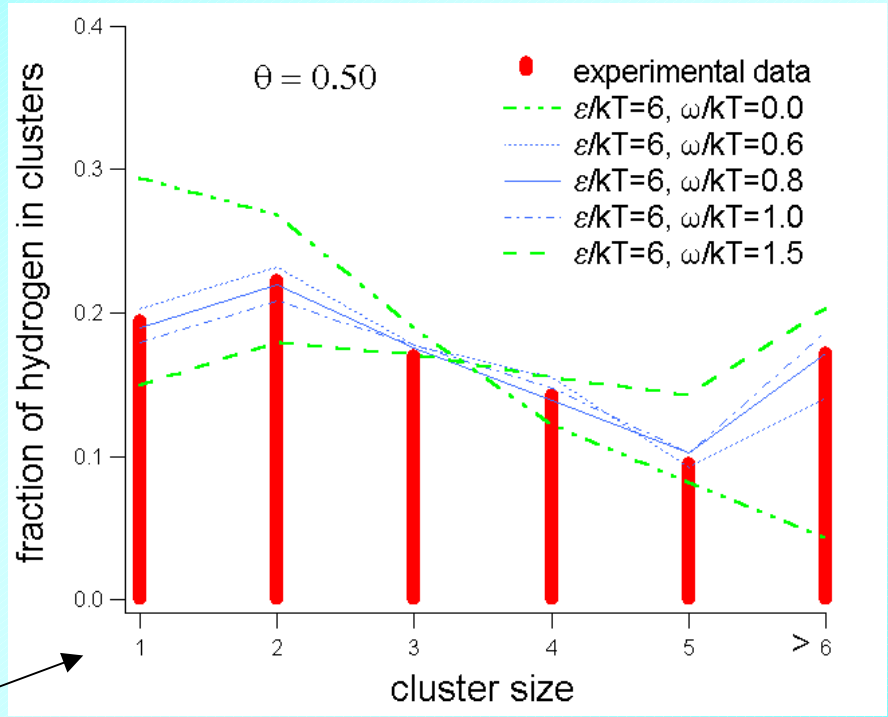
Comparison of MC simulation results and experimental data



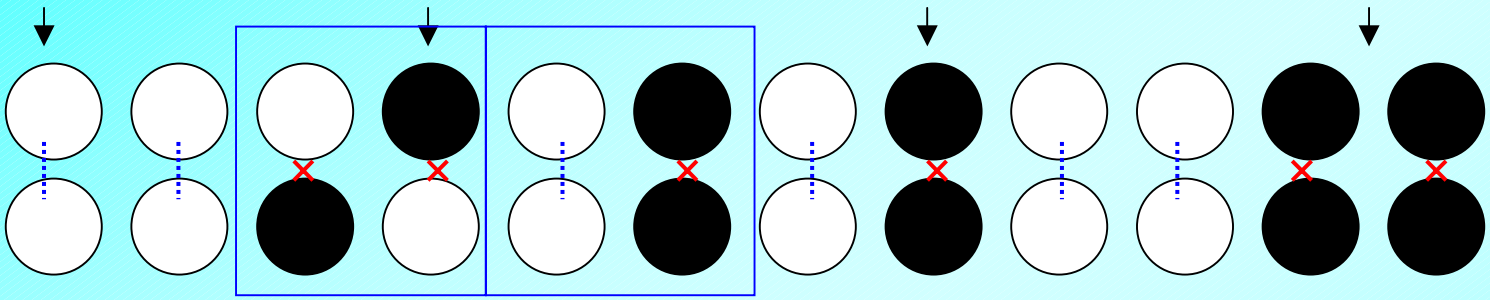


ε ±

ω ±

Intradimer and interdimer interactions of H on Si

Relevant surface configurations and interactions



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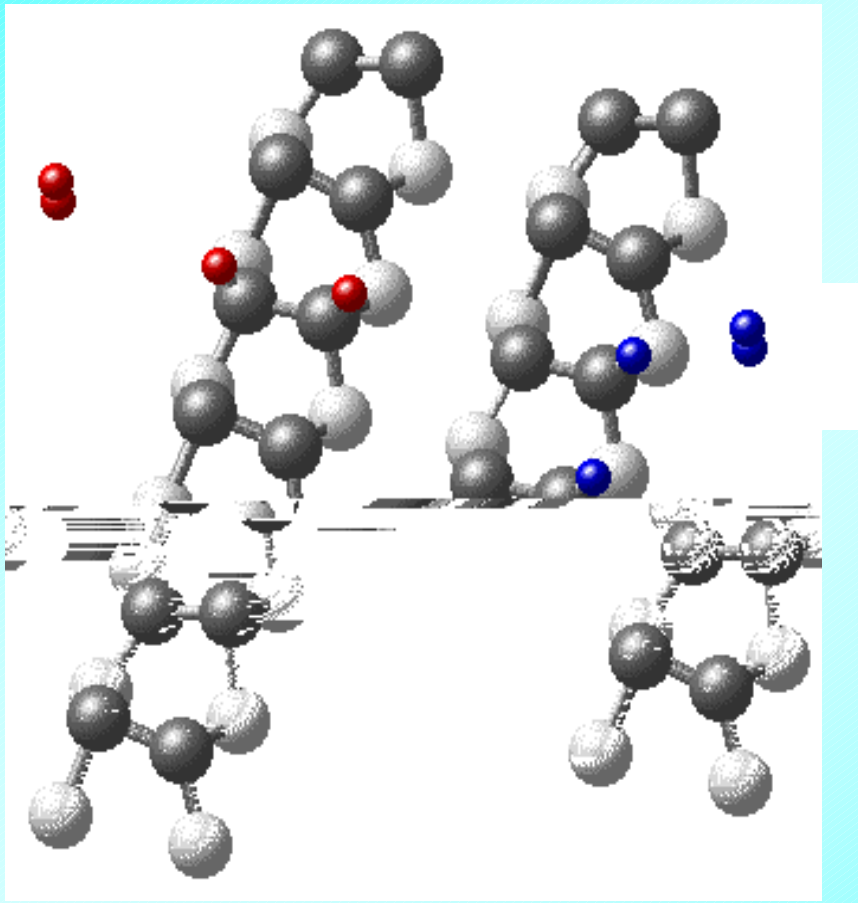
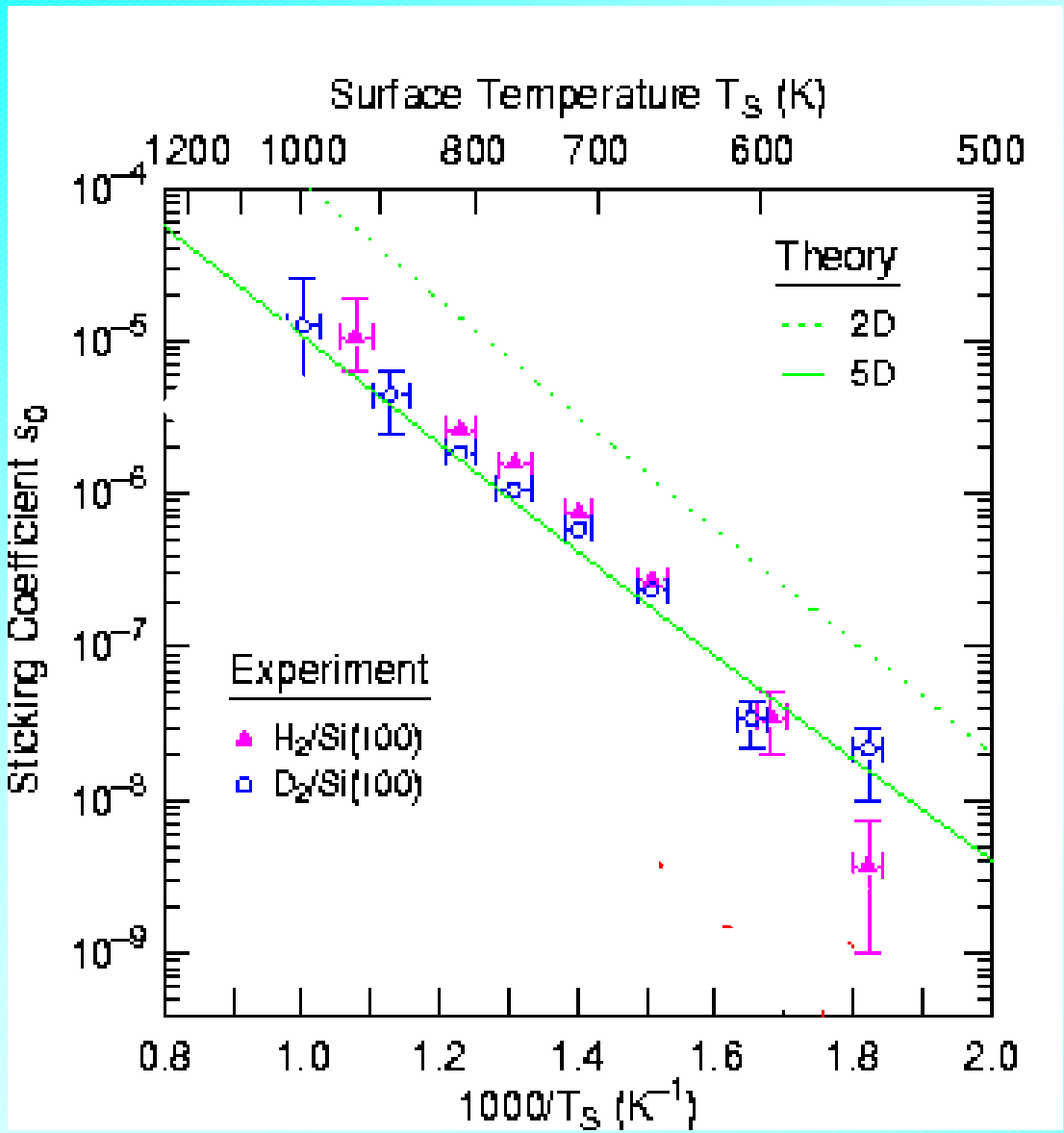
Desorption/adsorption pathways in controversy

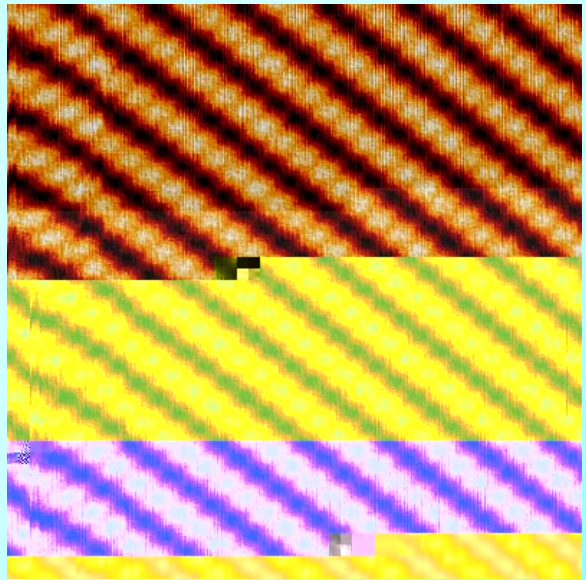


Strong dependence of surface temperature



U. Hofer *et al.* Phys. Rev. B , 5978 (1996)

Experimental



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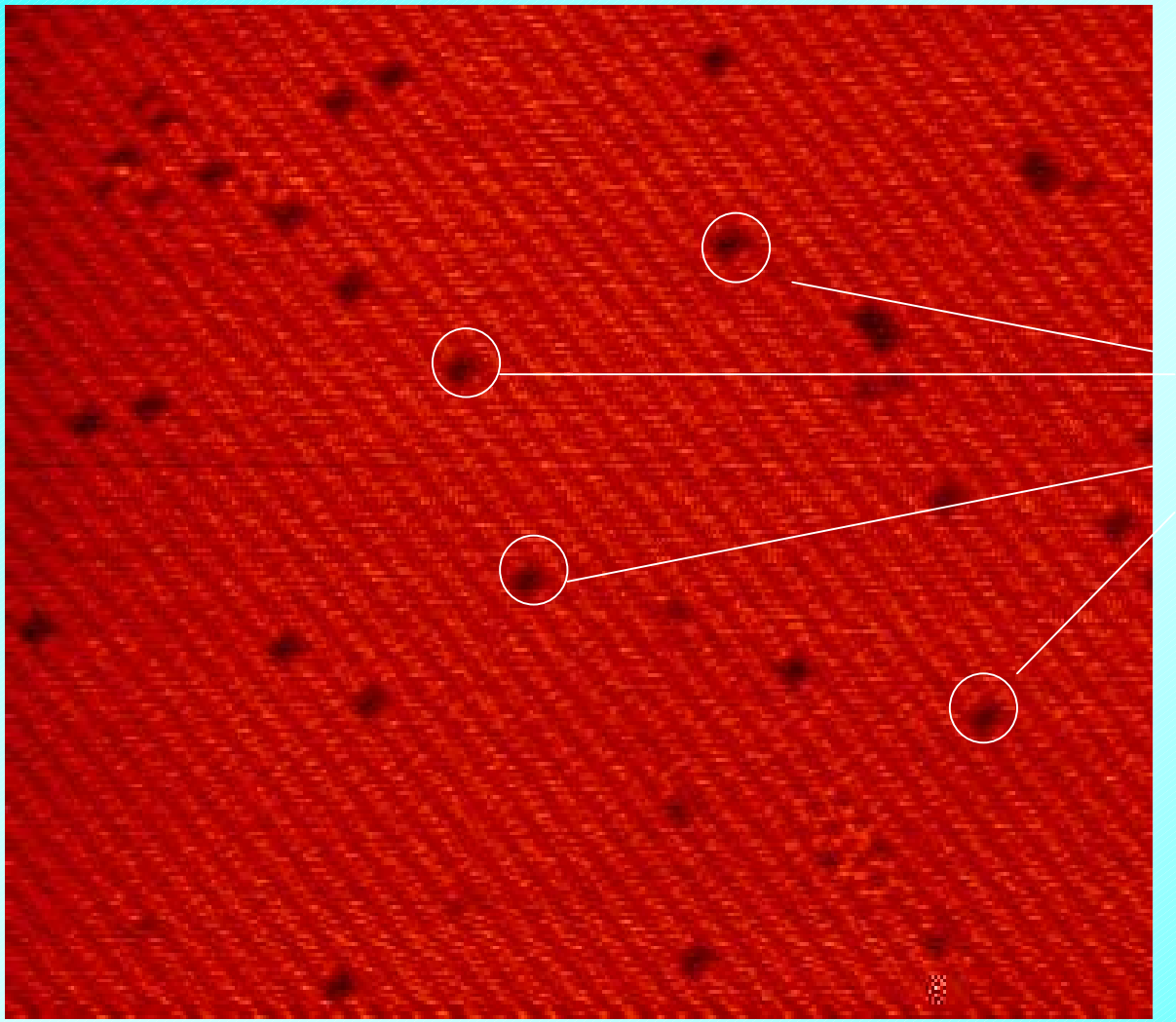
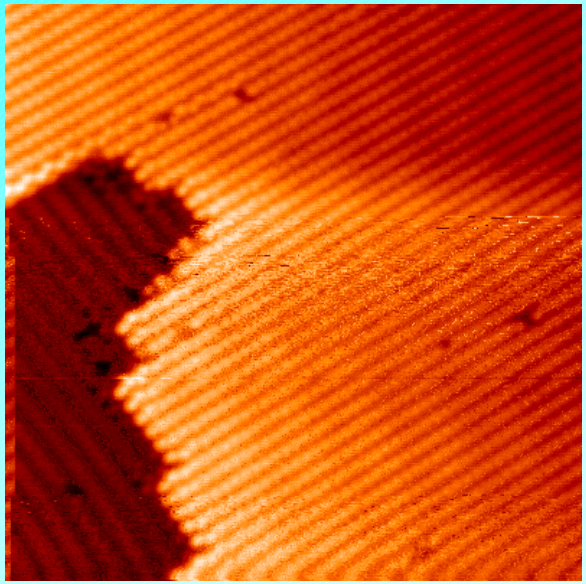
STM image of H_2 adsorption on clean Si(001) at 450K



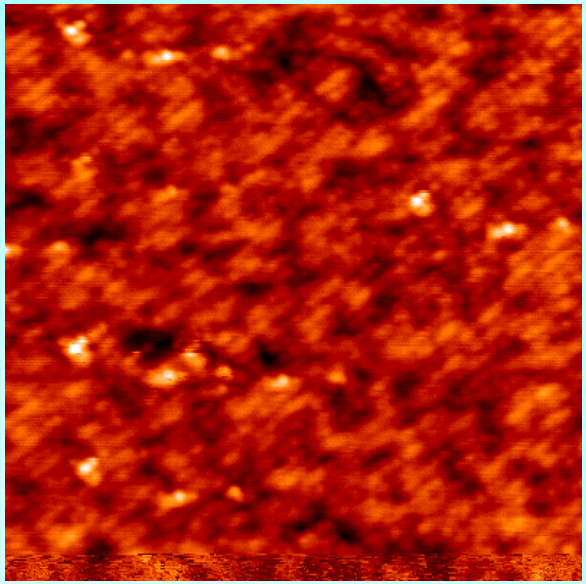
TPD confirmation of adsorbed species



clean Si(001) before ads.

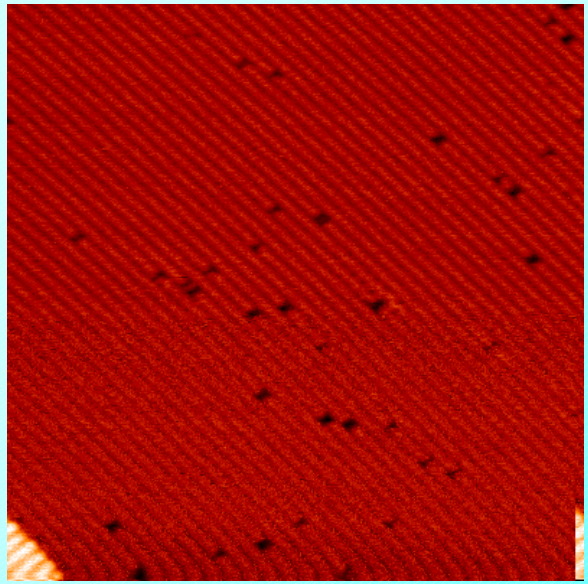
defect/contamination

~ 0.6%



ads. to ~1ML under same

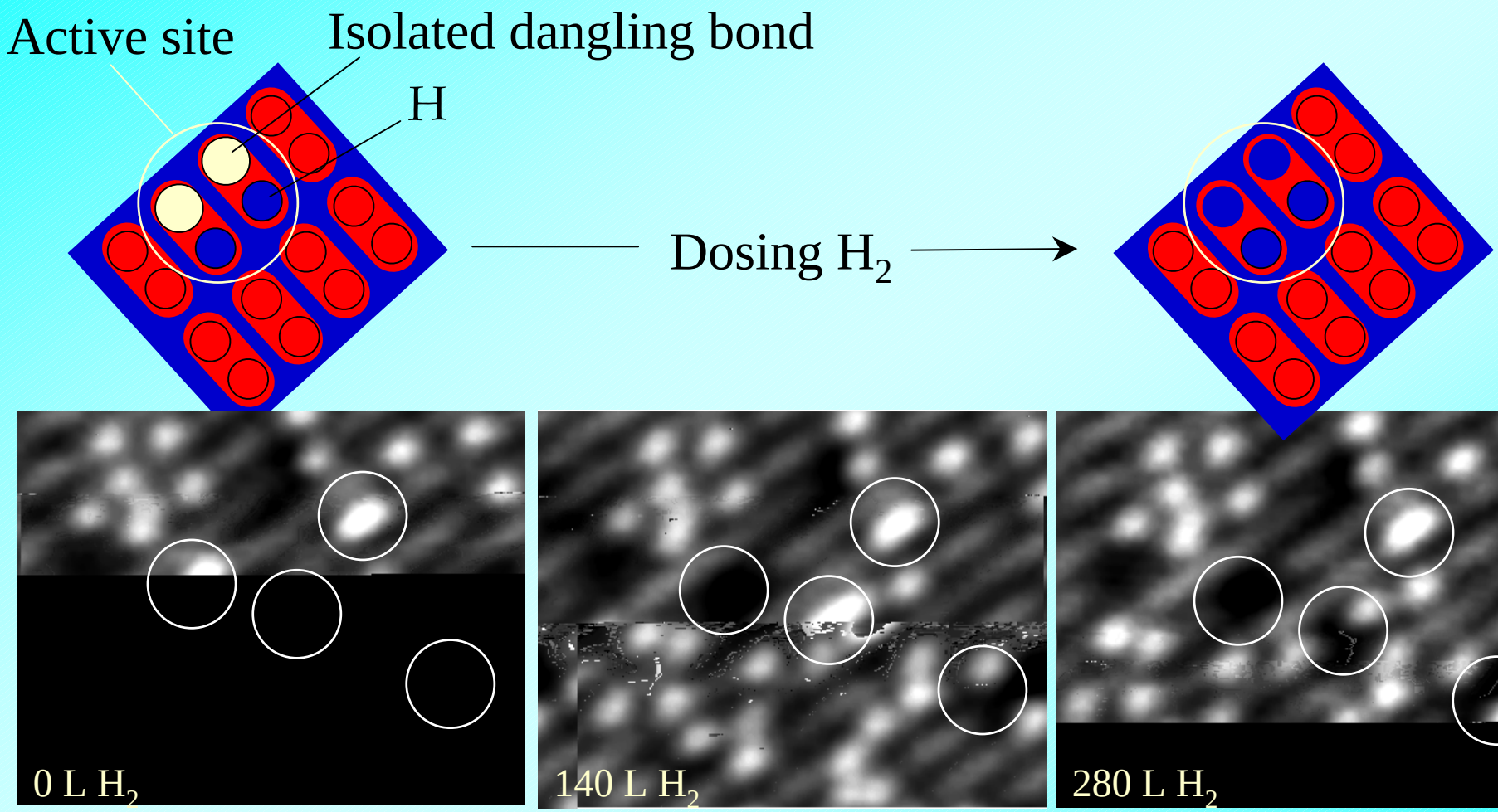
dosing condition



after TPD to 780K

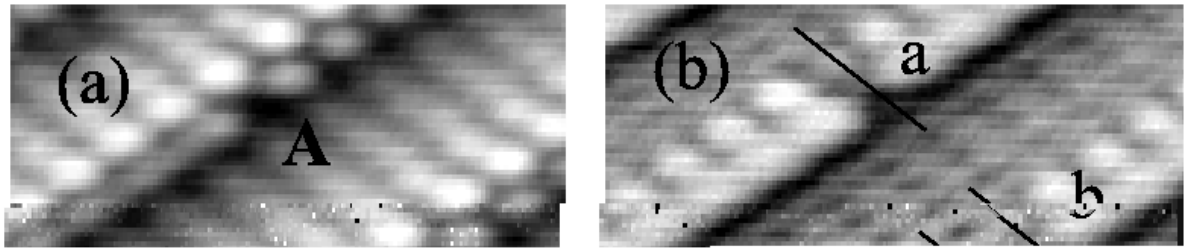
defect/contamination ~ 0.8%

Enhanced H_2 adsorption at specific sites on H/Si(001)

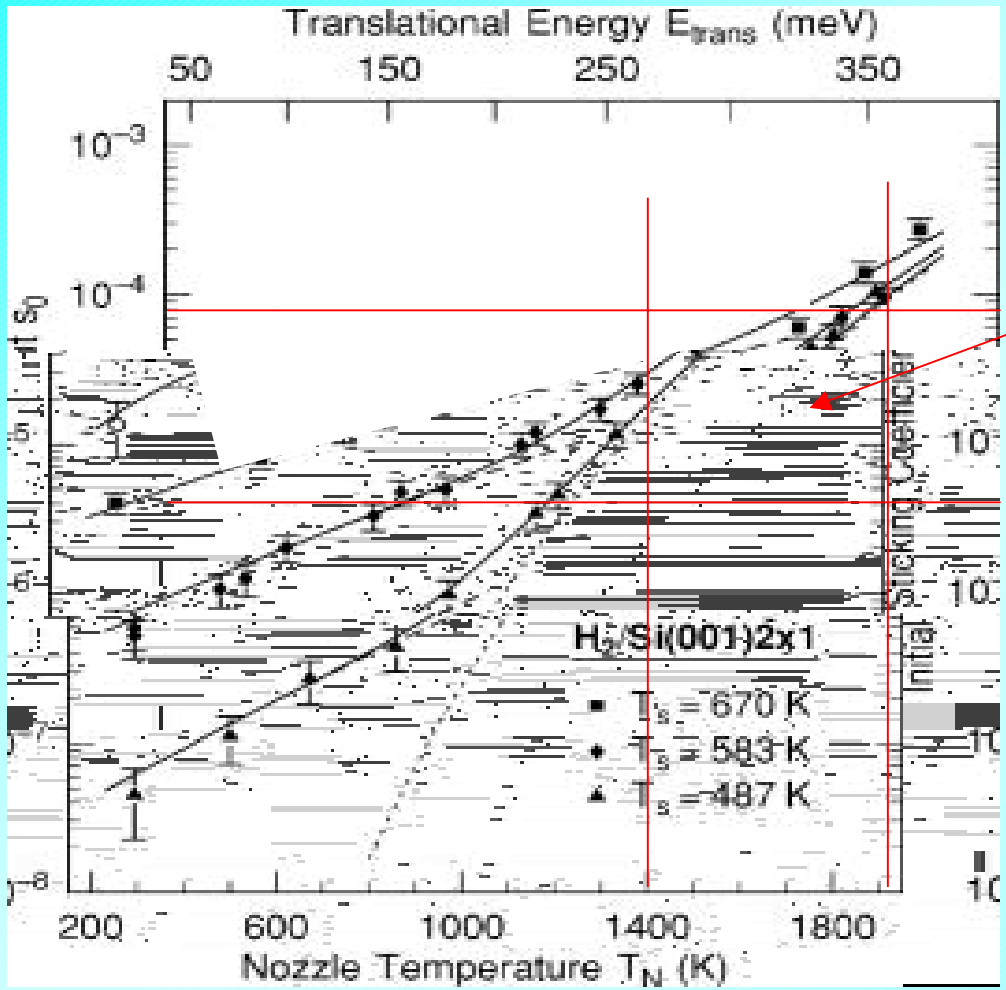


$S_{enh} \sim 8 \times 10^{-4} >> S_{1st}$

images showing H_2 adsorption on D_B step sites



Considerations about nozzle temperature



area having a chance

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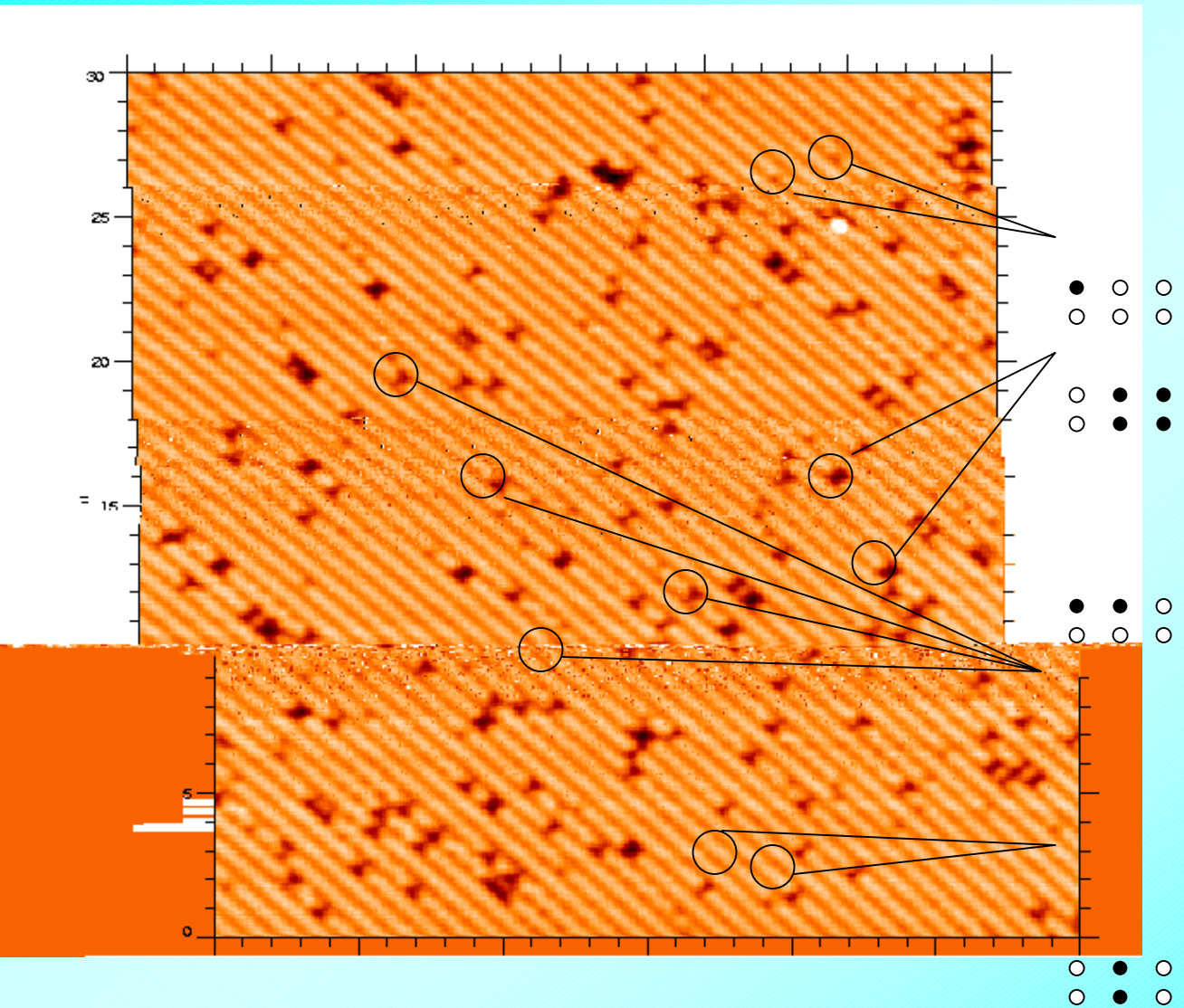
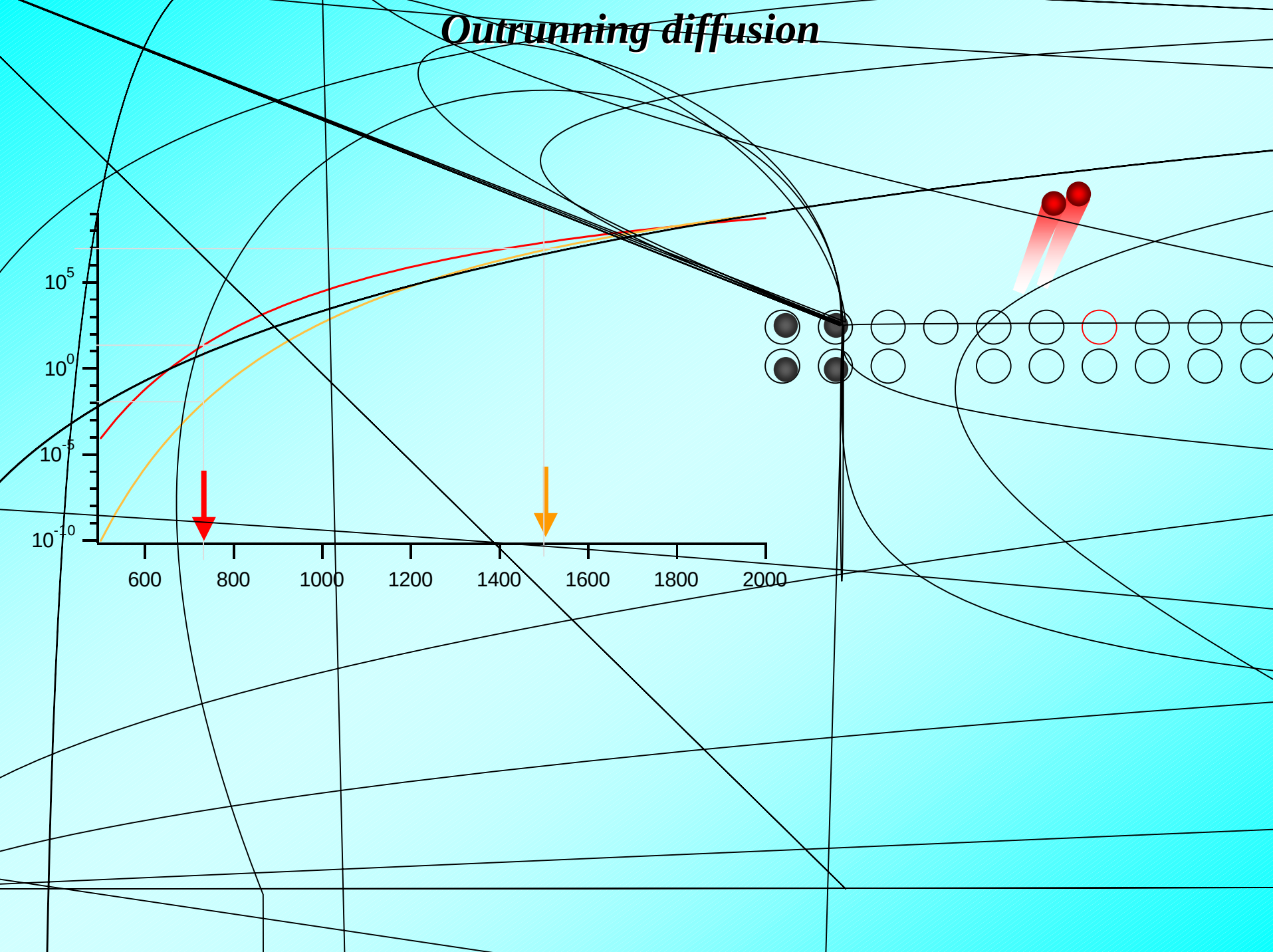
θ θ

et. al.

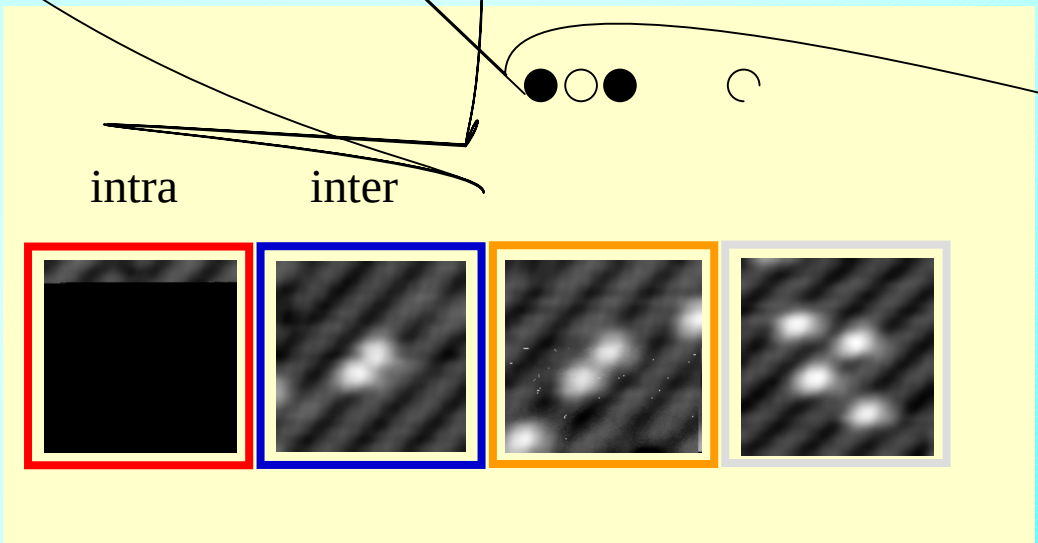
Initial sticking configuration of H_2 on clean Si(001)



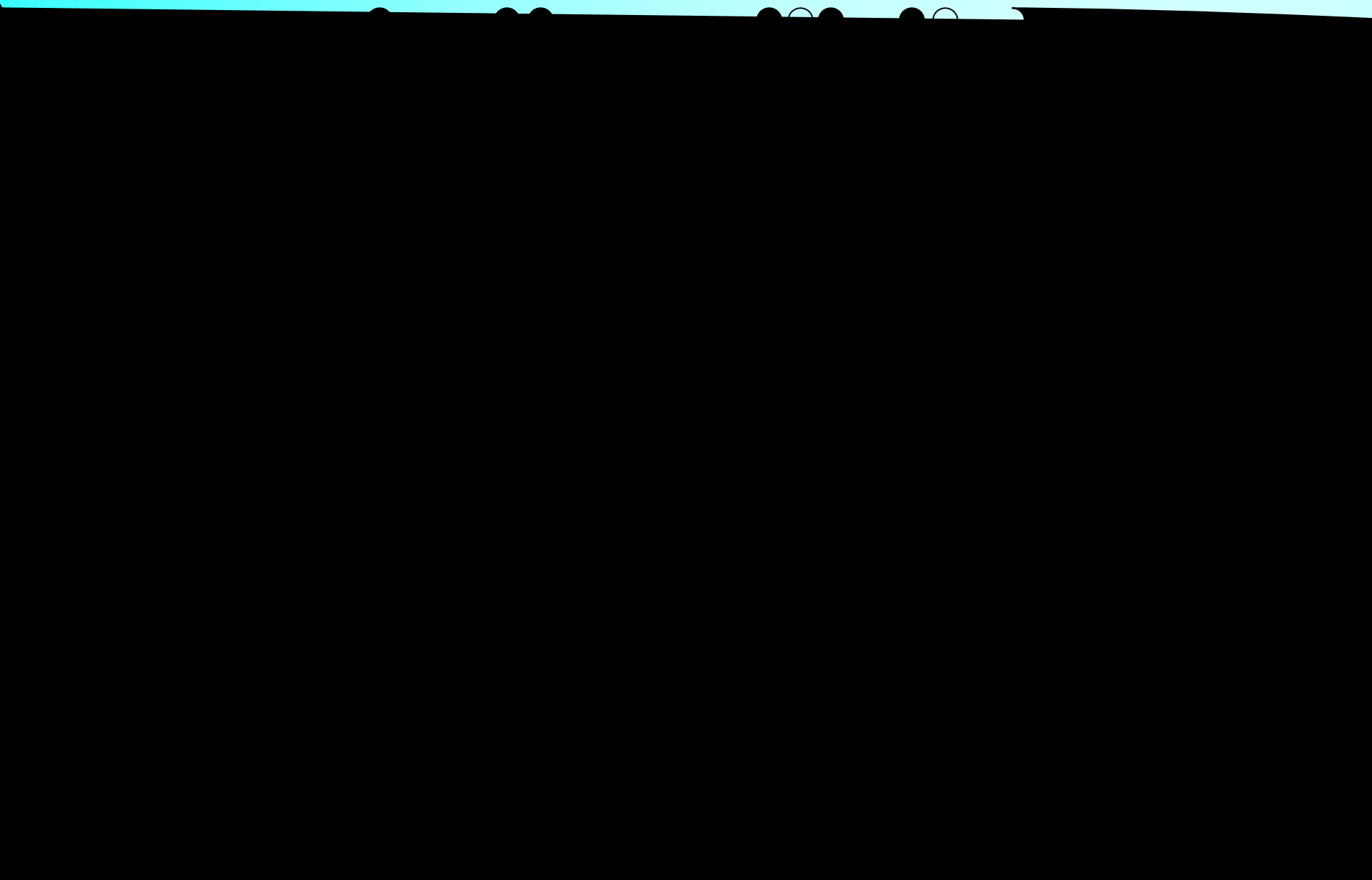
Outrunning diffusion



Surface before and after pulse



Direct counting and quantitative evaluation results



Conclusions

Dynamics of interaction between H_2 and Si(001) surface

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Acknowledgements

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Daejin Eom

Ernst Knoesel

Kwang Rim

Michael Duerr

George Flynn

Tony Heinz

Thank you for your attention!