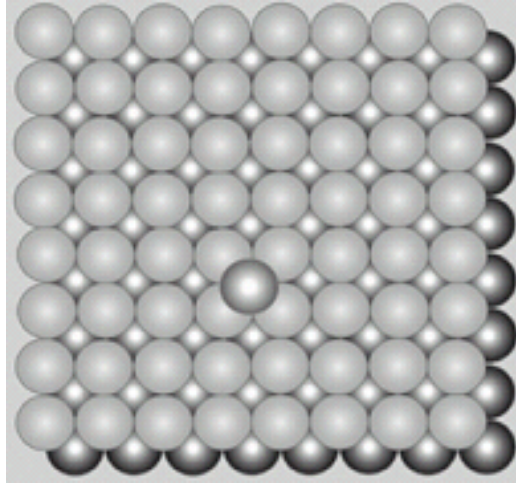


**ЗАКОНОМЕРНОСТИ
ПОВЕРХНОСТНОЙ
ДИФФУЗИИ**

Механизмы Ленгмюра-Хиншельвуда и Или-Ридела

ПРОСТАЯ МОДЕЛЬ



fcc; (100)

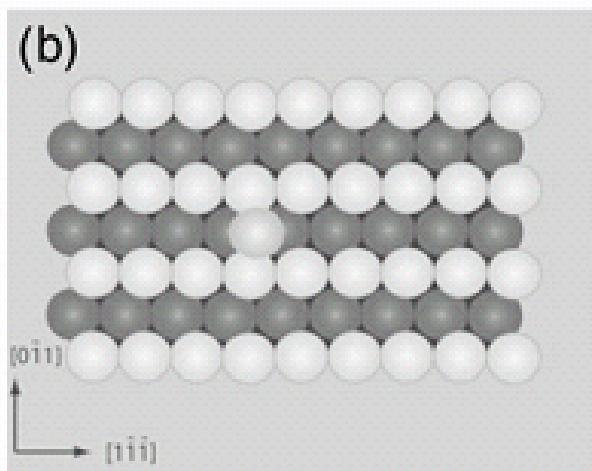
$$D = a^2 / 2\tau \quad \text{Лэнгмюр (1933)}$$

$$\langle \Delta x^2 \rangle = 2Dt \quad \text{Эйнштейн}$$

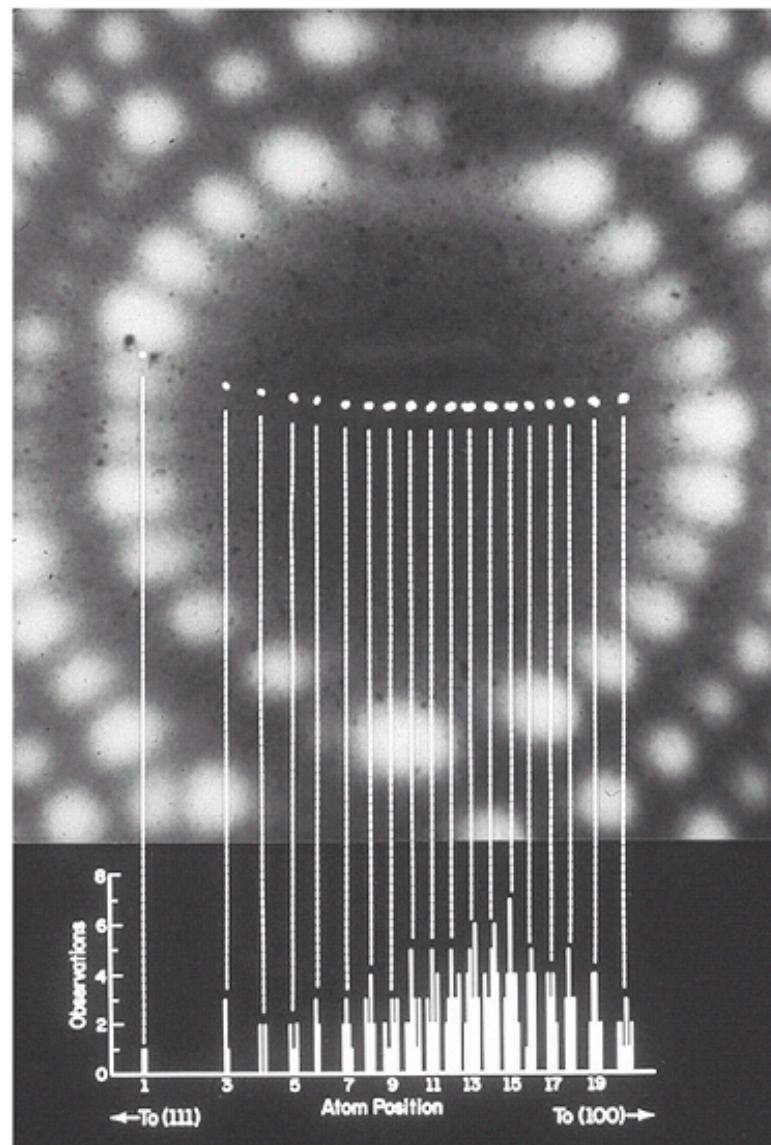
$$D = D_0 \exp\left(-\frac{E_D}{kT}\right)$$

$$D_0 = va^2 \exp\left(\frac{S_D}{k}\right)$$

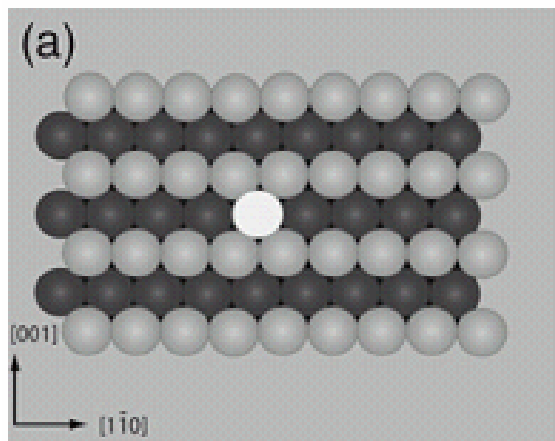
Rh / W(211); 197 K



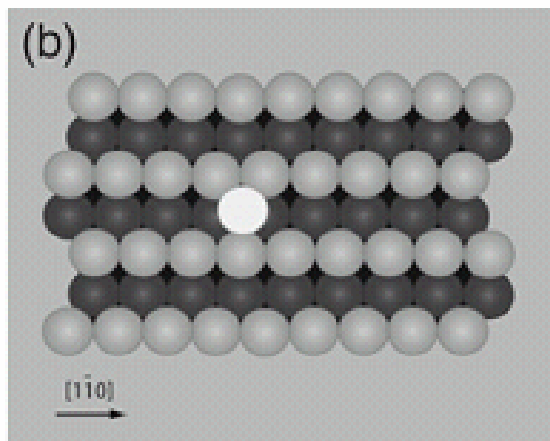
Строго одномерная диффузия →



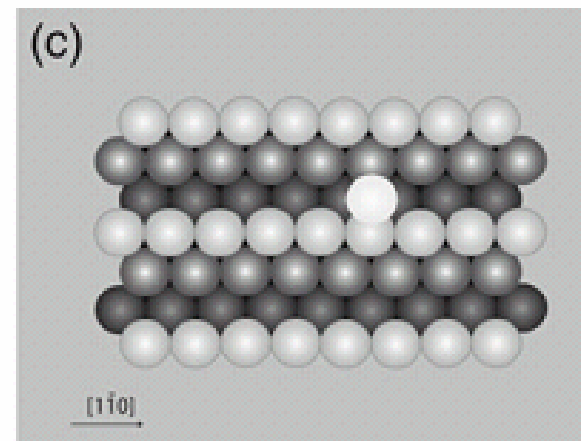
Ir / Pt (fcc)



(110)



(311)



(331)

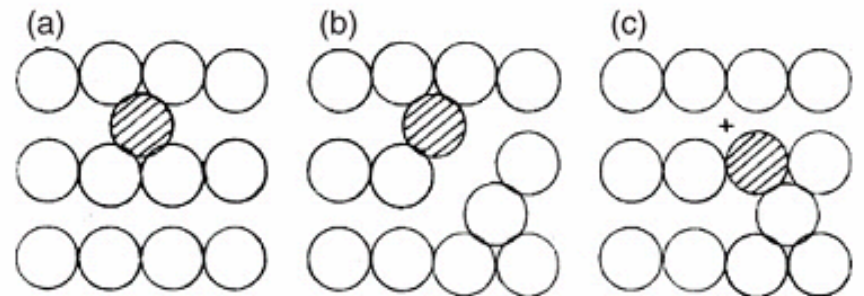
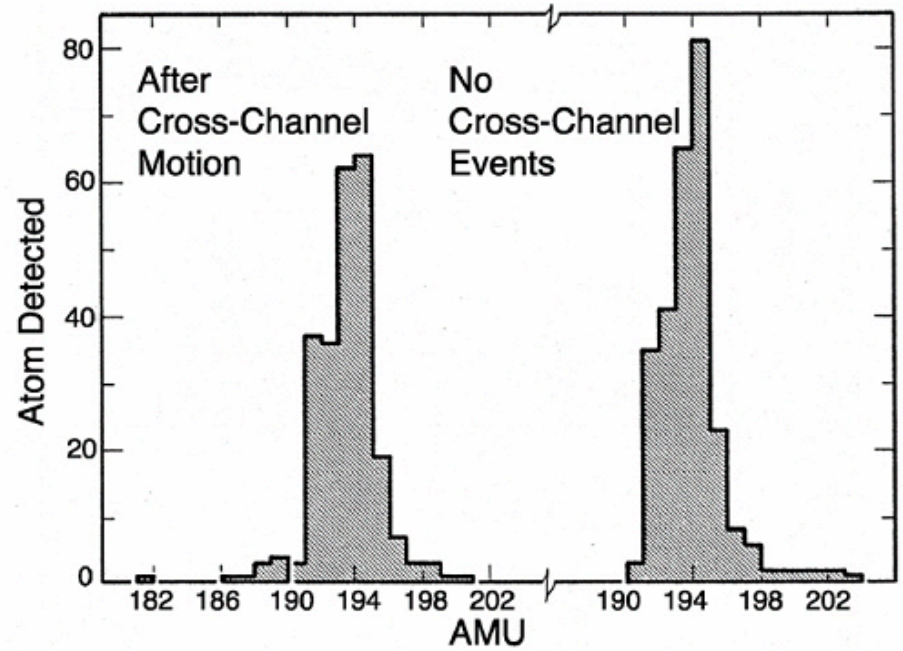
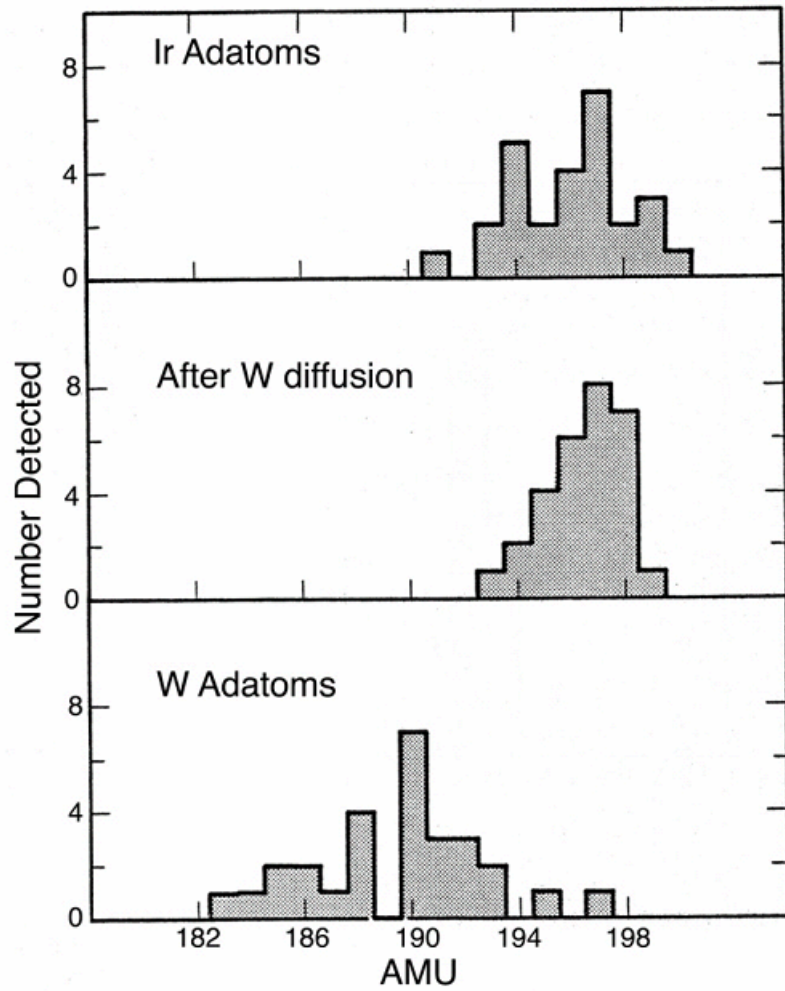
Двумерная диффузия

Одномерная диффузия

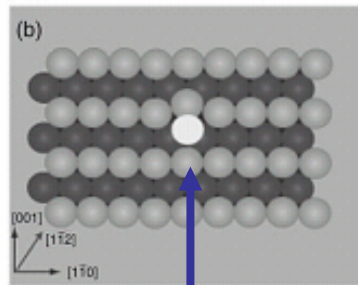
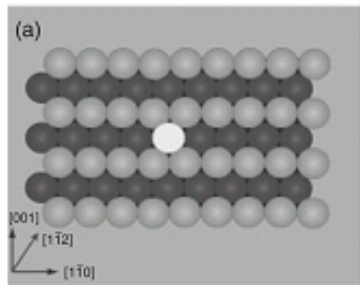
$$E_{\parallel} = 0.84 \pm 0.1 \quad \text{eV}$$

$$E_{\perp} = 0.78 \pm 0.1 \quad \text{eV}$$

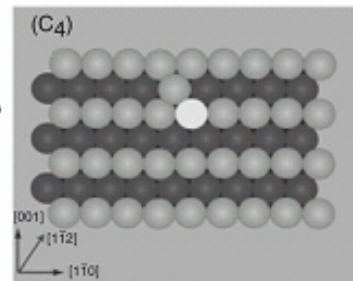
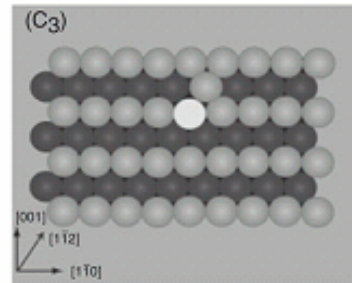
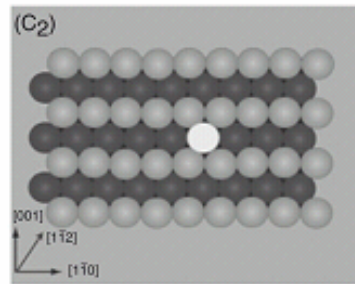
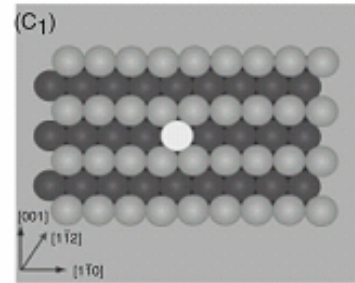
W / Ir (110)



МД С ЛЕННАРД-ДЖОНСОНОВСКИМИ ПОТЕНЦИАЛАМИ ДЛЯ (110)

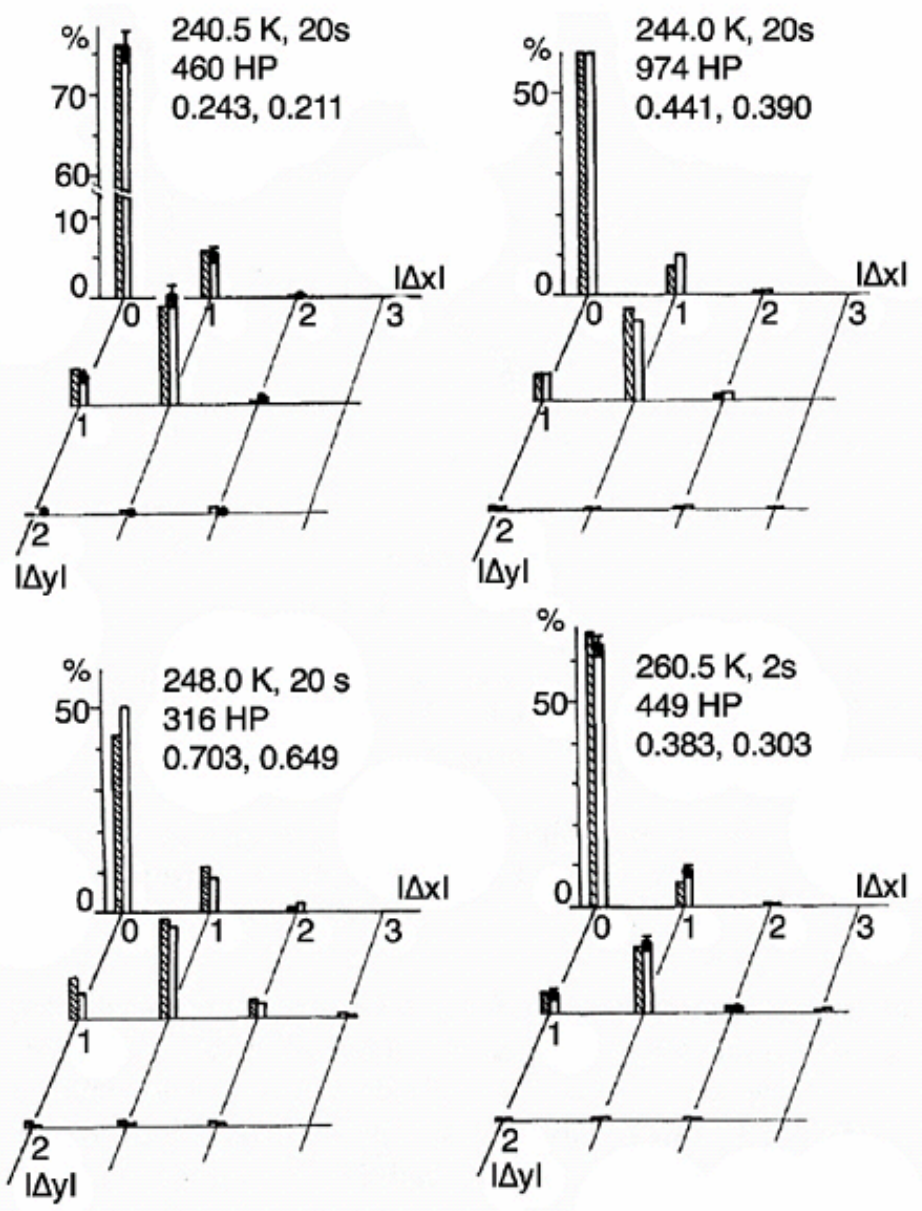


Переходное состояние (гантель)

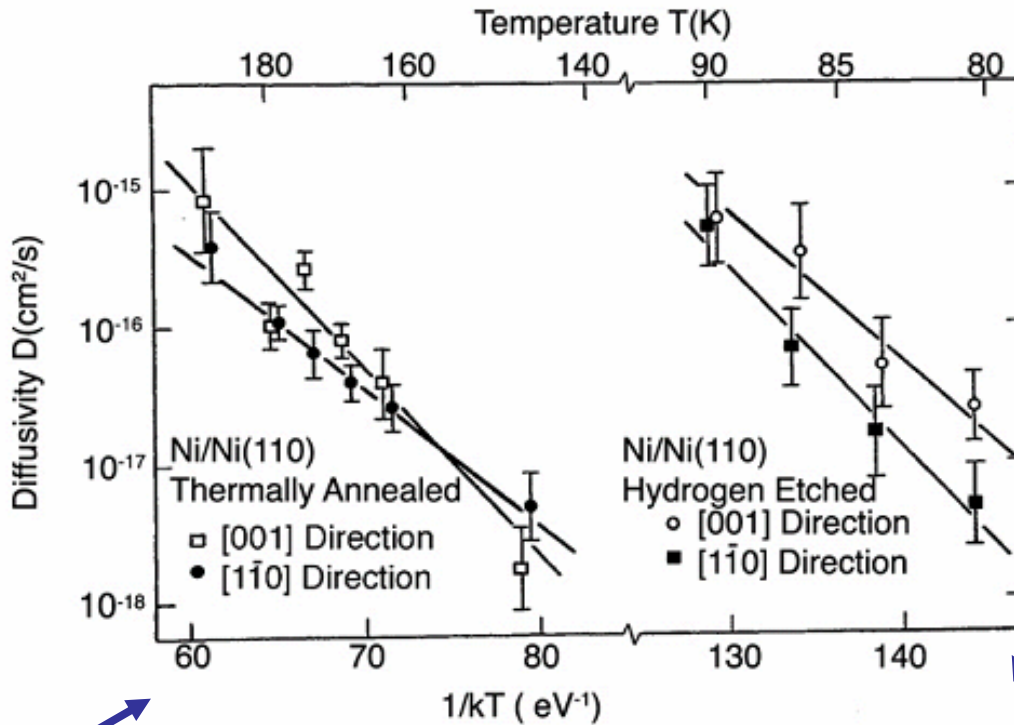


Четыре равновероятных конечных конфигурации

Ir / Ir (100); распределение смещений при различных температурах



Ni / Ni(110)



$$E_{\parallel} = 0.23 \pm 0.04 \quad \text{eV}$$

$$E_{\perp} = 0.32 \pm 0.05 \quad \text{eV}$$

$$D_0 \approx 10^{-8} \text{ cm}^2/\text{s}$$

$$E_{\parallel} = 0.3 \pm 0.06 \quad \text{eV}$$

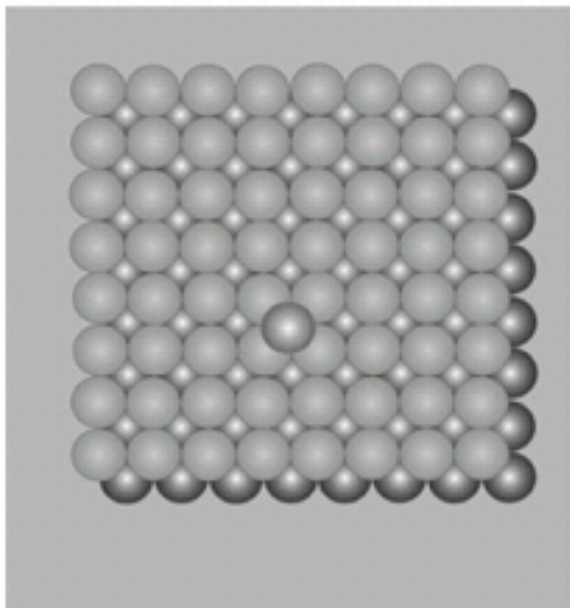
$$D_0 \approx 10 \text{ cm}^2/\text{s}$$

$$E_{\perp} = 0.25 \pm 0.06 \quad \text{eV}$$

$$D_0 \approx 10^{-1} \text{ cm}^2/\text{s}$$

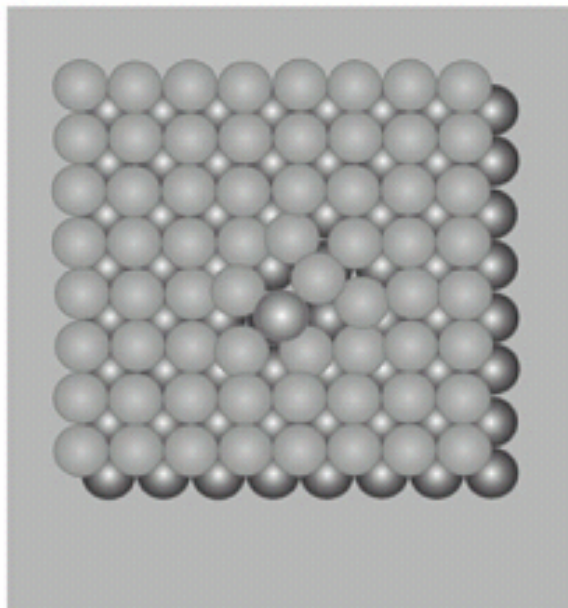
ОБМЕН АТОМА НА ПОВЕРХНОСТИ (100)

(a)



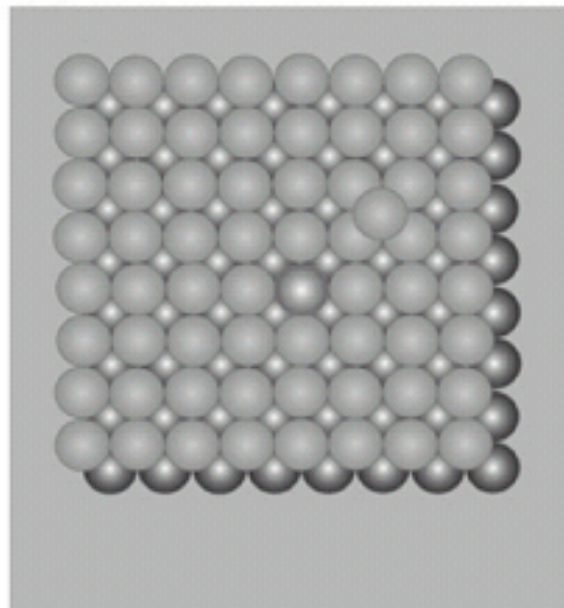
Исходное состояние

(b)



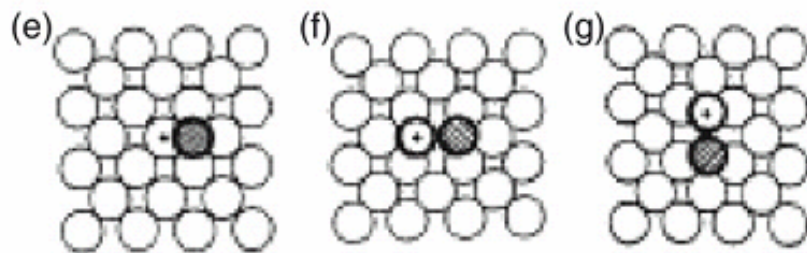
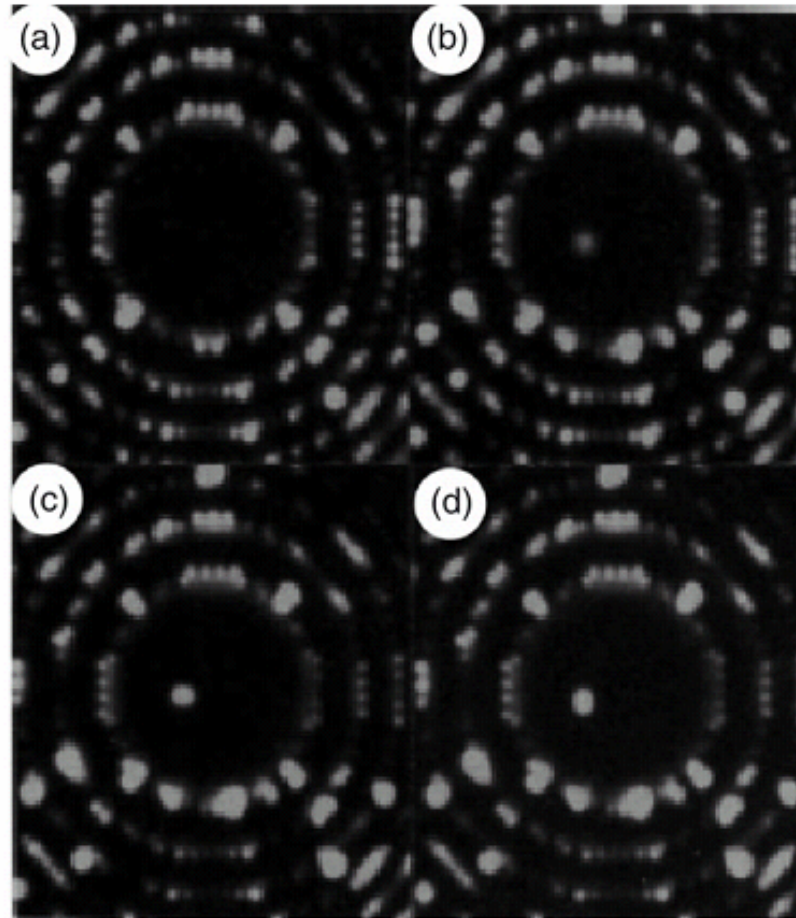
Переходное состояние

(c)

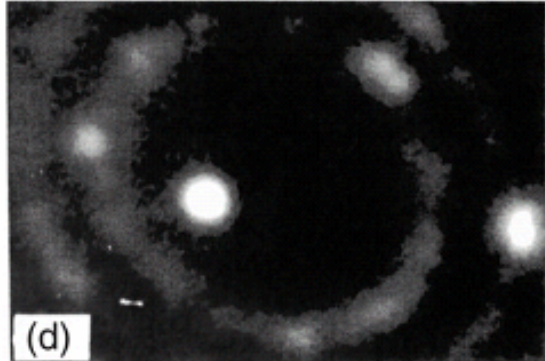
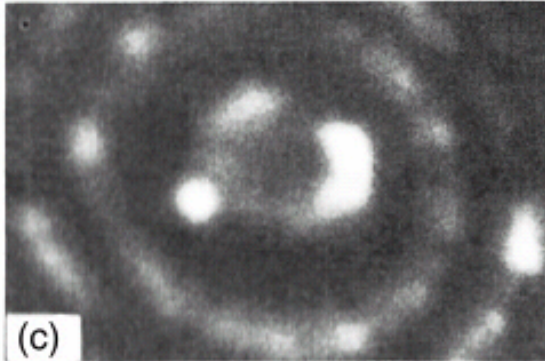
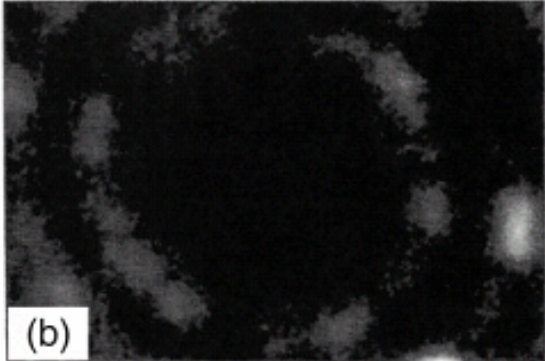
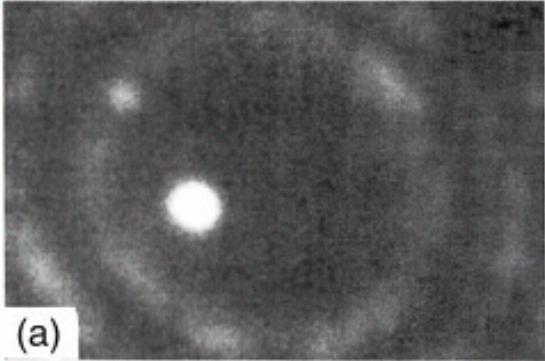


Конечное состояние

Re / Ir(100)

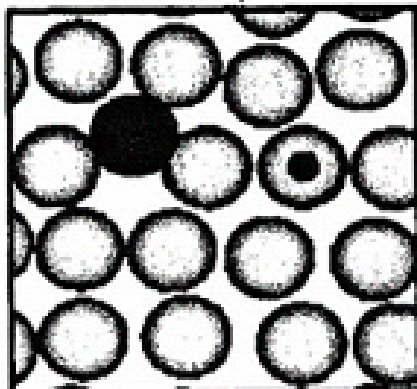


Pt / Ni(100)

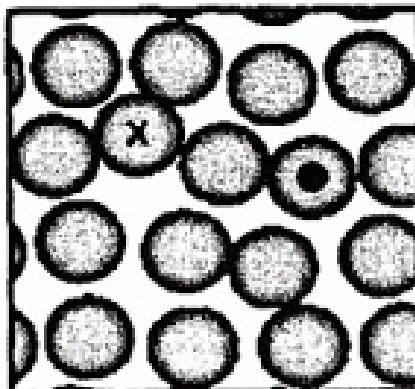


РАСЧЕТ ДЛЯ Ag, Al, Au, Cu, Pd, Pt, Ni

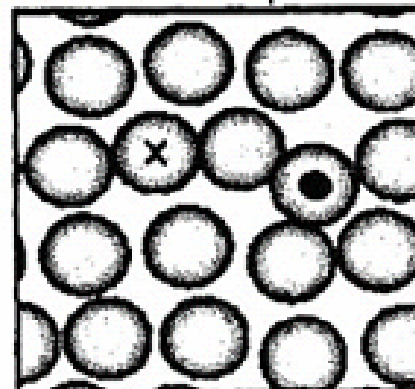
$t = 1.5 \text{ ps}$



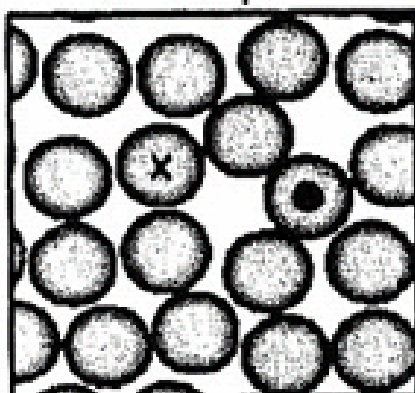
$t = 1.6 \text{ ps}$



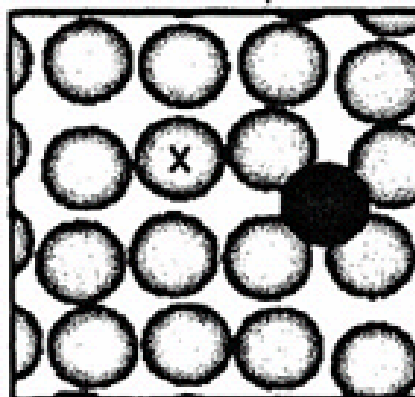
$t = 1.7 \text{ ps}$



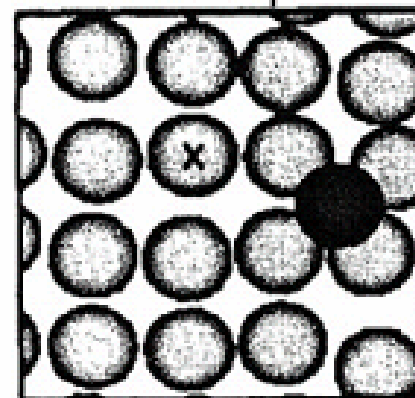
$t = 1.8 \text{ ps}$



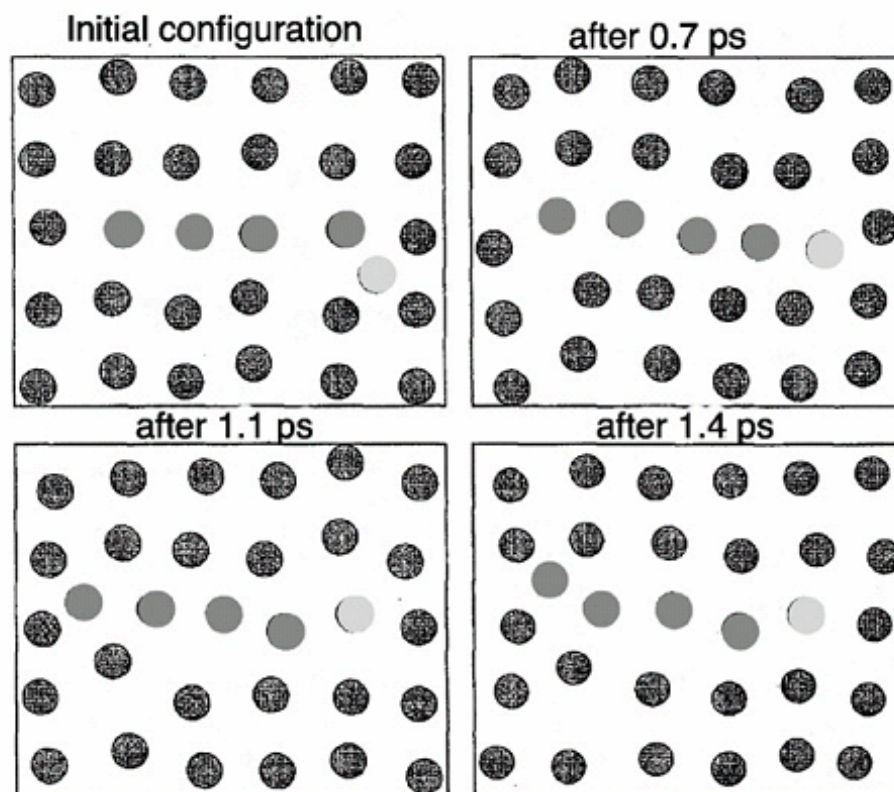
$t = 1.9 \text{ ps}$



$t = 2.0 \text{ ps}$



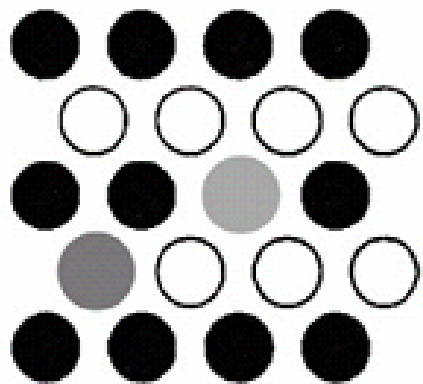
РАСЧЕТ ДЛЯ Cu(100)



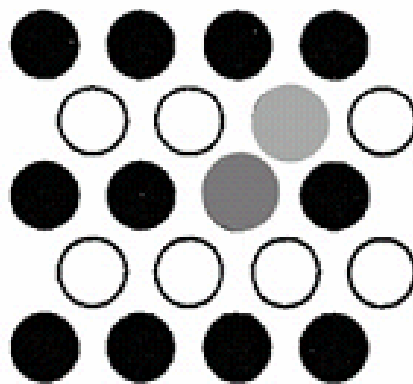
Jump characteristics of Cu on Cu(100) [82]

Jump	Migration barrier (eV)	D_0 (cm ² /s)
Single	0.43 ± 0.02	$3.4 \times 10^{-3 \pm 0.2}$
Double	0.71 ± 0.05	$38 \times 10^{-3 \pm 0.5}$
Simple exchange	0.70 ± 0.04	$42 \times 10^{-3 \pm 0.3}$
Double exchange	0.70 ± 0.06	$45 \times 10^{-3 \pm 0.6}$
Triple exchange	0.82 ± 0.08	$104 \times 10^{-3 \pm 1.0}$
Quadruple exchange	0.75 ± 0.12	$86 \times 10^{-3 \pm 0.9}$

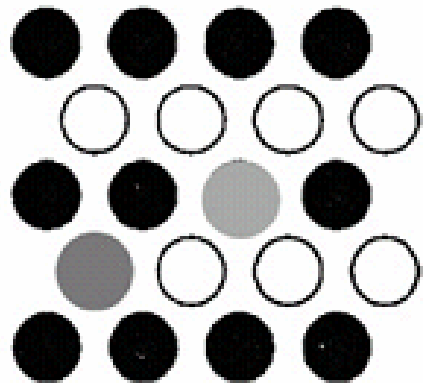
РАСЧЕТ ДЛЯ Ag(110)



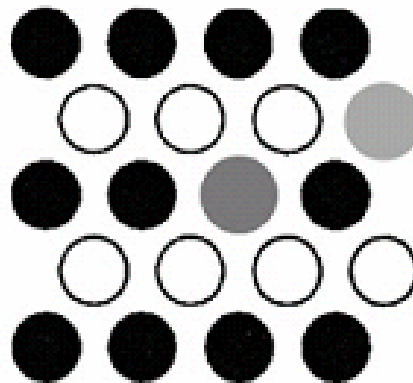
je \rightarrow



\leftarrow ej



jej \rightarrow

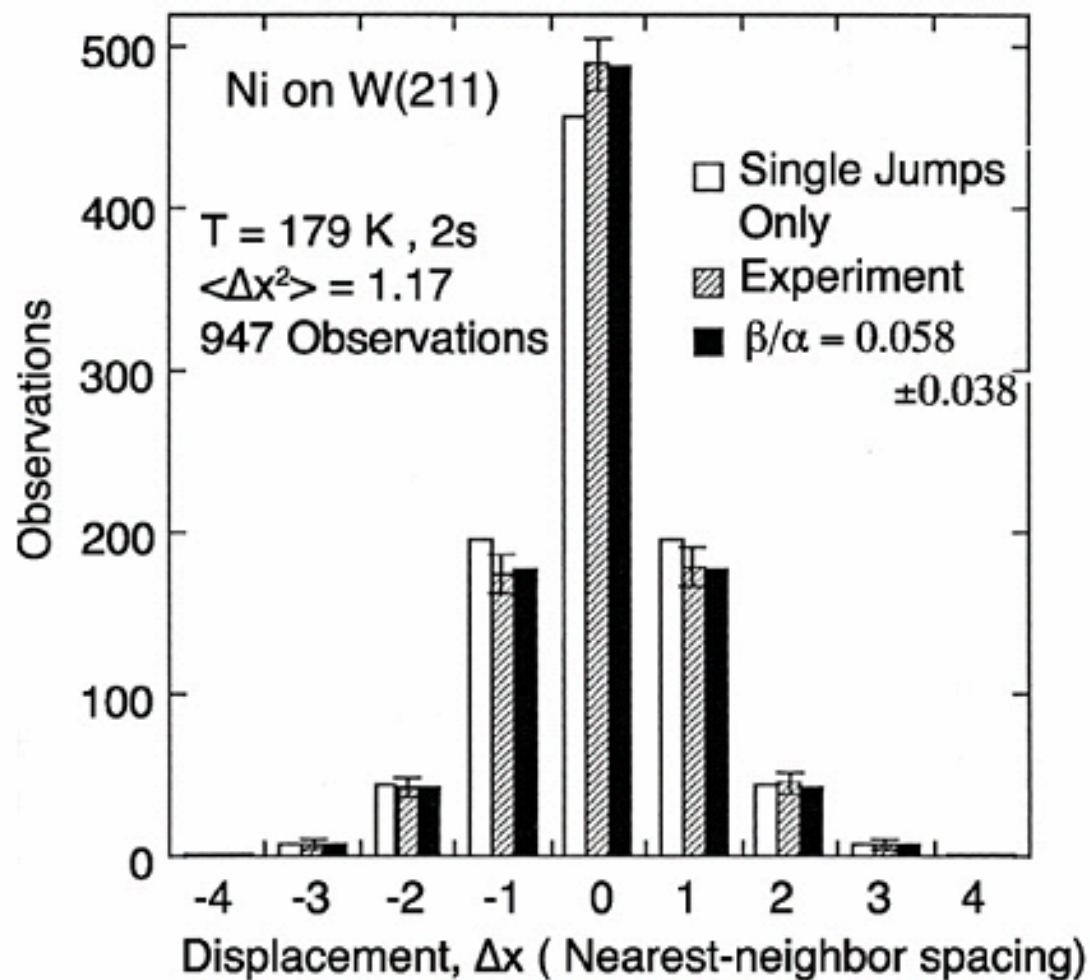


je = jump – exchange

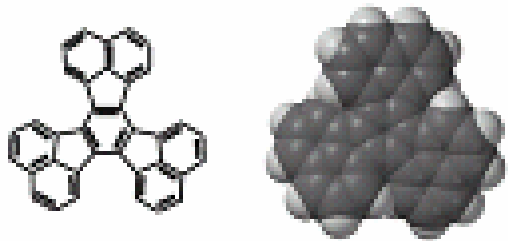
ej = exchange – jump

jej = jump – exchange - jump

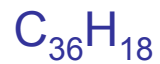
ДЛИННЫЕ СКАЧКИ В СЛУЧАЕ ОДНОМЕРНОЙ ДИФФУЗИИ Ni / W(211)



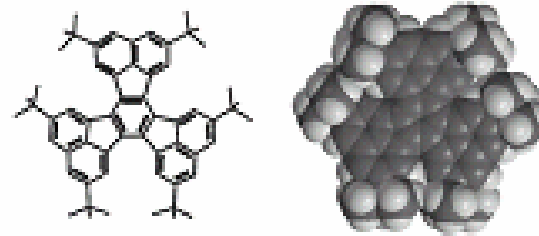
ДИФФУЗИЯ МОЛЕКУЛ НА ПОВЕРХНОСТИ Cu(110)



Декациклен



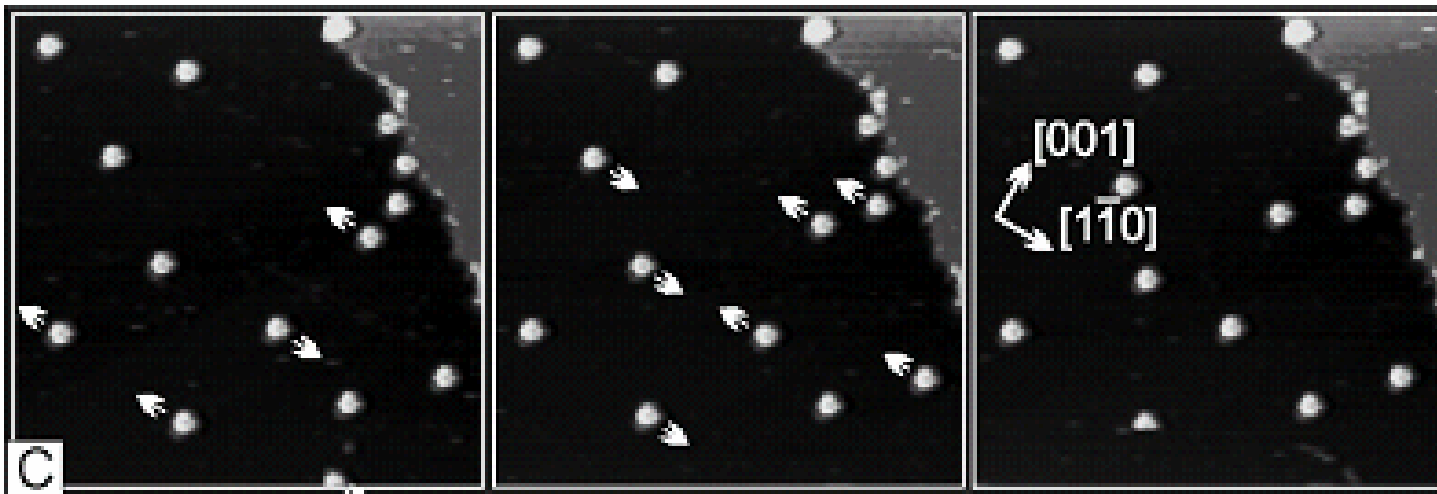
$$\lambda = 3.9 \pm 0.2$$



Гекса-трет-бутил декациклен



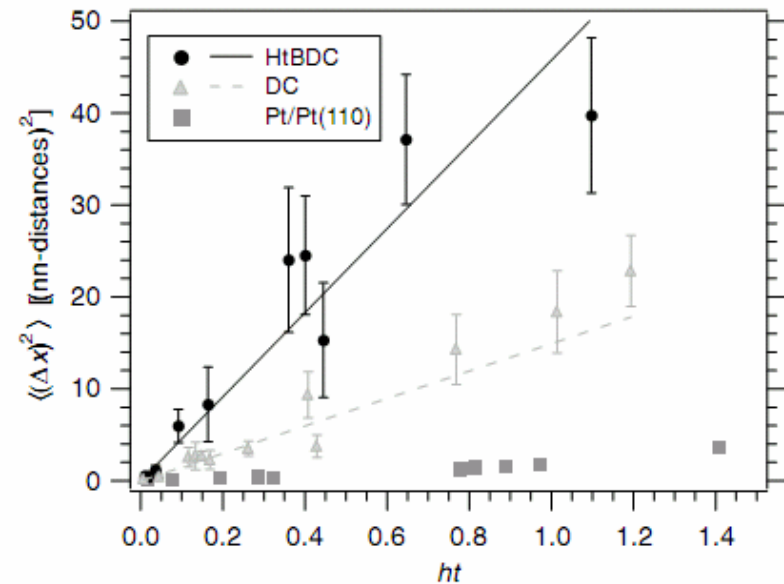
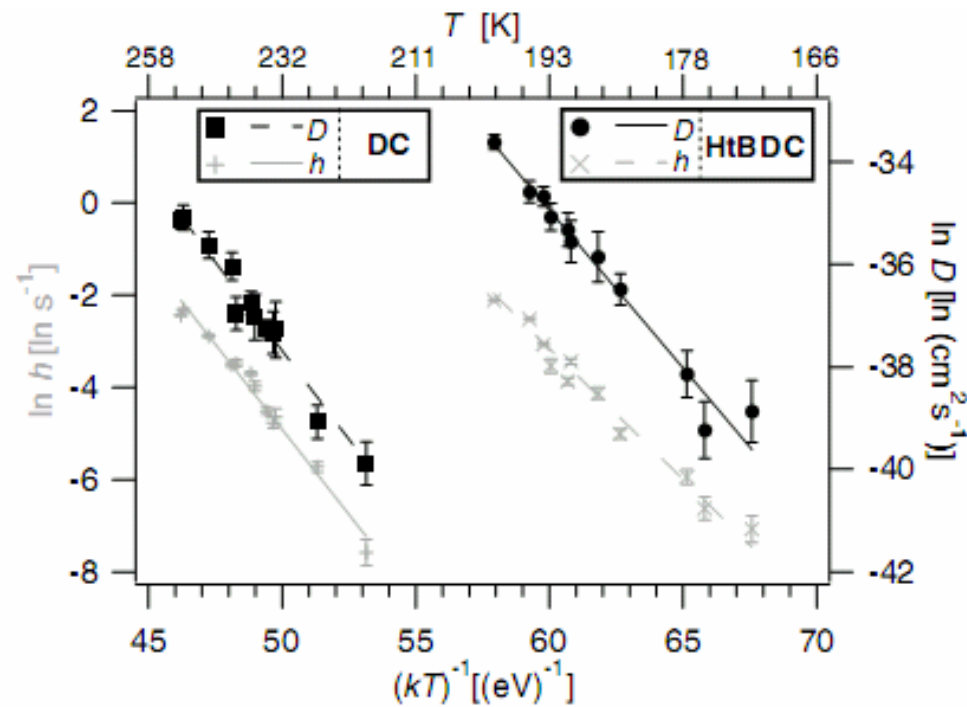
$$\lambda = 6.8 \pm 0.3$$



$\Delta t = 13.9 \text{ s}$

$$\langle (\Delta x)^2 \rangle = \lambda^2 h t$$

$$P_0 = \exp(-ht) \quad D = \frac{\langle (\Delta x)^2 \rangle}{2t}$$



$$\lambda = 3.9 \pm 0.2$$

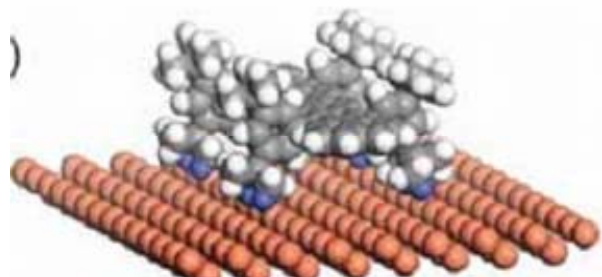
$$\lambda = 6.8 \pm 0.3$$

	DC		HtBDC	
	dis	hop	dis	hop
E_D/eV	0.71 ± 0.05	0.74 ± 0.03	0.62 ± 0.04	0.57 ± 0.02
h_0/s^{-1}	...	$10^{13.9 \pm 0.7}$...	$10^{13.5 \pm 0.4}$
$D_0/\text{cm}^2 \text{s}^{-1}$	$10^{-1.0 \pm 1.0}$...	$10^{0.9 \pm 1.0}$...

dis = displacement

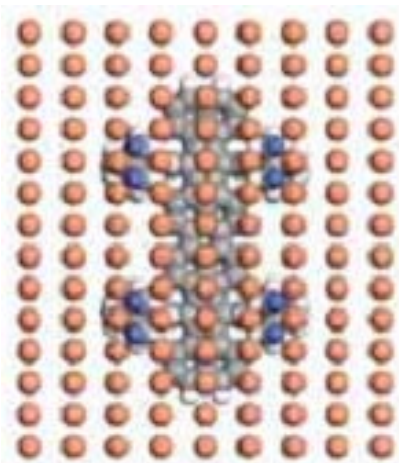
hop = hopping rate

ЭФФЕКТ «КЛЮЧ-ЗАМОК» ПРИ ДИФфуЗИИ БОЛЬШИХ ОРГАНИЧЕСКИХ МОЛЕКУЛ

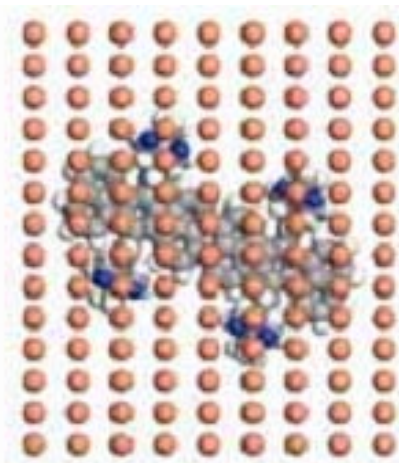


C₁₀₈H₁₀₄; Violet Lander

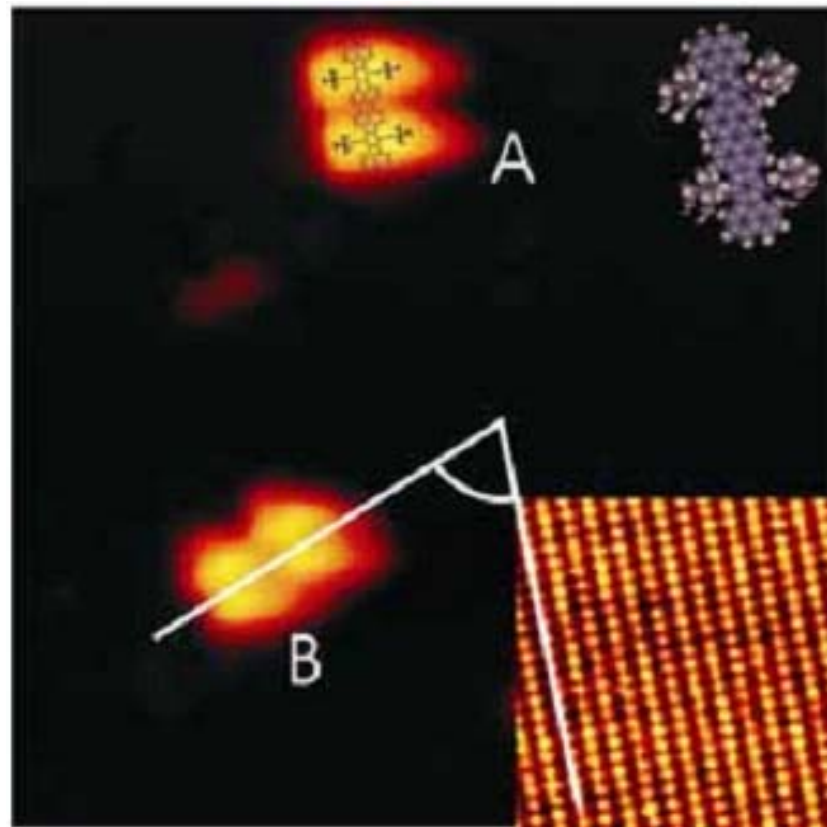
Cu(110)



Фиксирована



Мобильна



СТМ; 14 x 14 нм²; А: ориентация [110];
В: молекула повернута иглой СТМ;
вставка – «визуализированная» часть
поверхности