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international centre for theoretical physics

SMR/1238-17

ADRIATICO RESEARCH CONFERENCE on

LASERS IN SURFACE SCIENCE

11-15 September 2000

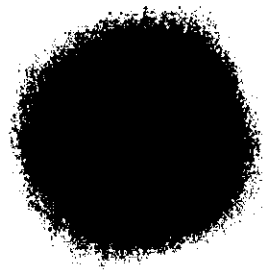
Miramare - Trieste, Italy

Observing the Quantum Behaviour of a Single H Atom with a STM

Lincoln Lauhon
Cornell University
Cambridge - MA, United States of America

Observing the Quantum Behavior of a Single H Atom with a STM

Lincoln Lauhon* and Wilson Ho
Cornell University

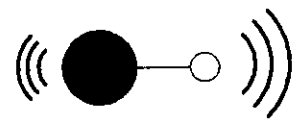


H/Cu(001)

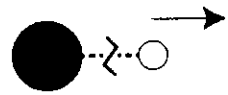
*linc@cmliris.harvard.edu

Hydrogen motions studied by STM:

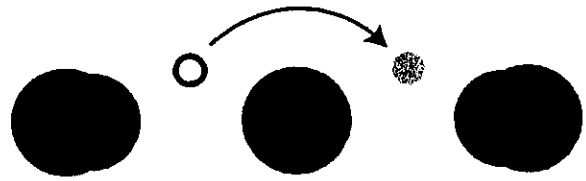
Vibration



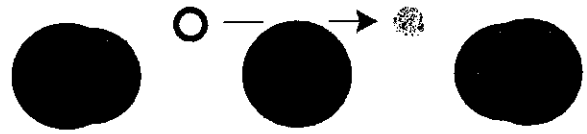
Dissociation



Thermal Diffusion



Quantum Tunneling



STM Experimental Methods:

Passive Observation-
intramolecular and molecule-surface interactions

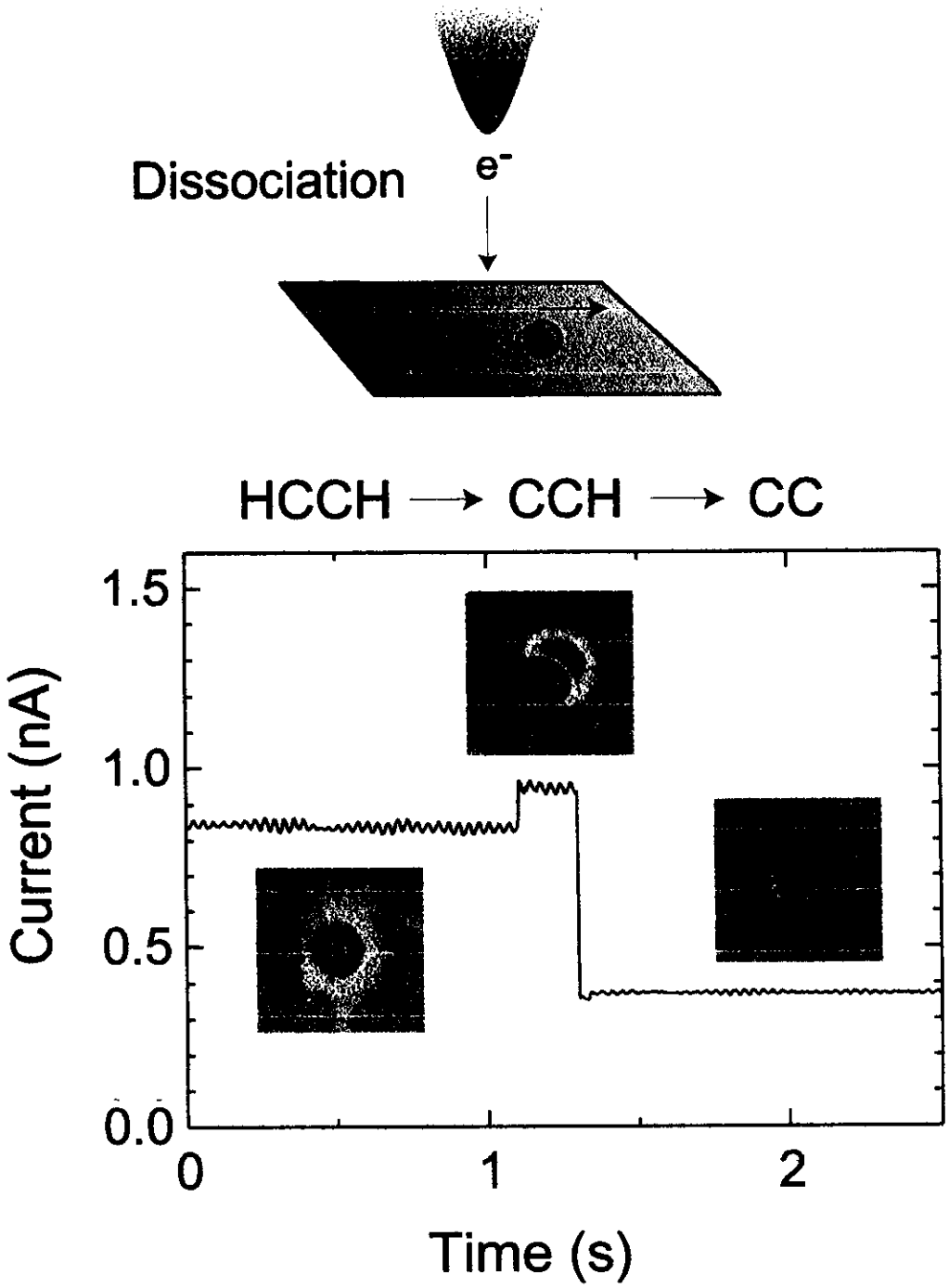
Active Initiation-
interaction of tunneling electrons with
single atoms and molecules

Motivations:

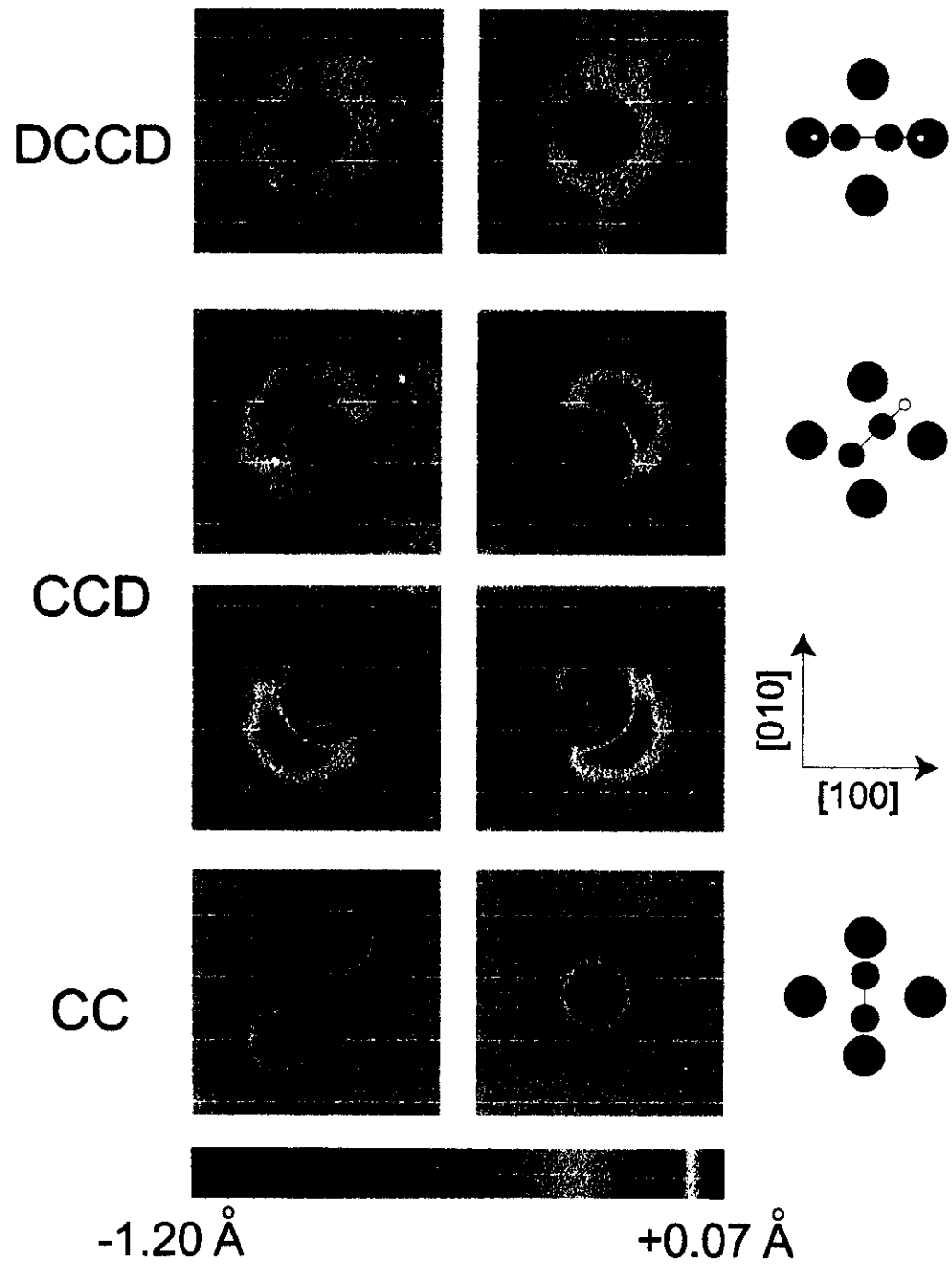
Study single molecules in a well-defined environment

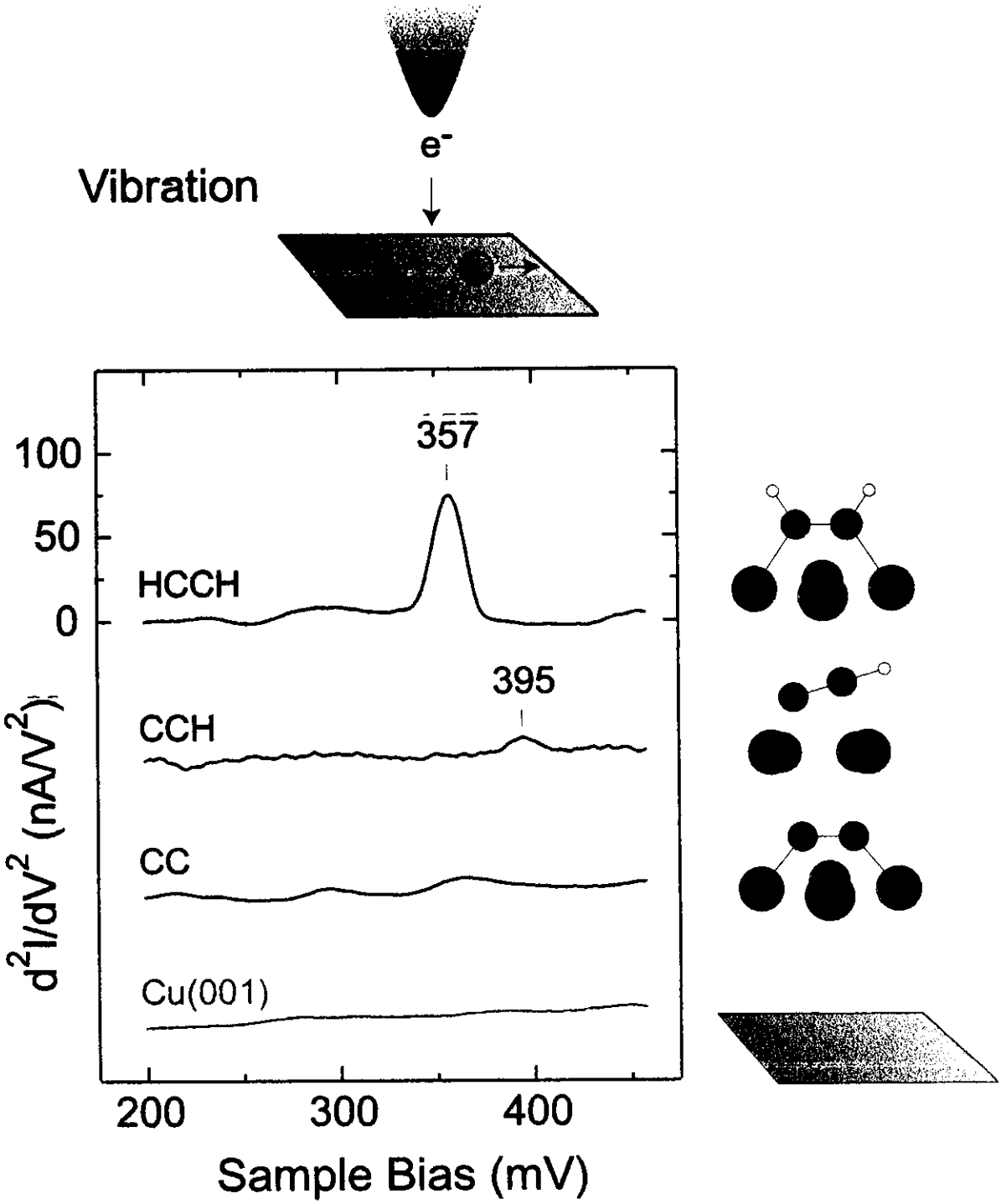
Understand and control chemical transformation
at the atomic scale

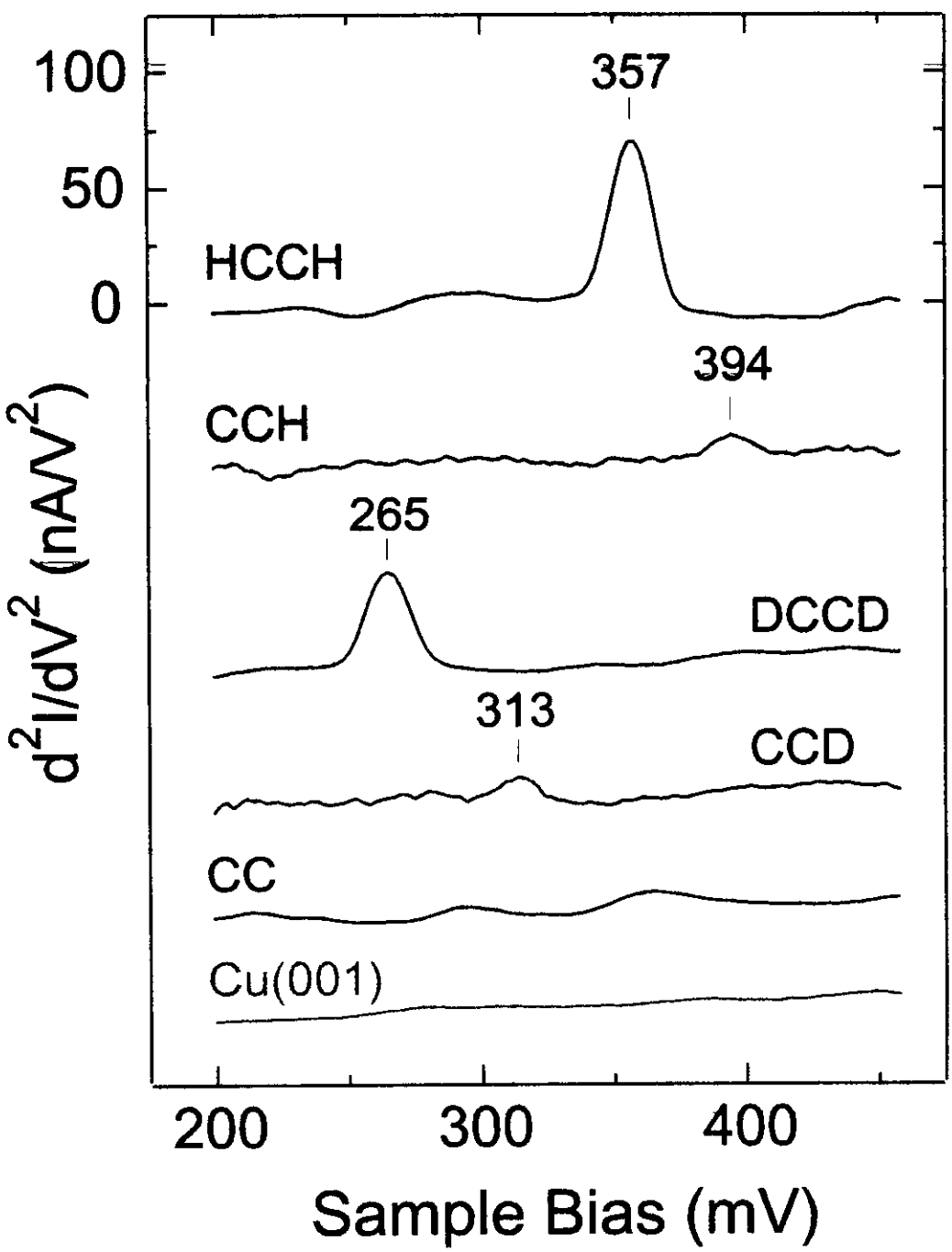
Develop new methods for surface science



PRL 84, 1527 (2000)


DCCD
CCD
CC
[010]
[100]
-1.20 Å
+0.07 Å


e⁻
Vibration
100
50
0
357
HCCH
395
CCH
CC
Cu(001)
d²I/dV² (nA/V²)
200
300
400
Sample Bias (mV)


100
50
0
357
HCCH
394
CCH
265
DCCD
313
CCD
CC
Cu(001)
200
300
400
Sample Bias (mV)
d²I/dV² (nA/V²)

Generality of Methods

① Spectroscopy

Several molecules, modes, and surfaces have been studied. Theoretical understanding is emerging, but not yet predictive.

Stability of the junction is the key requirement
- low probability of diffusion / dissociation
- stable tip
- stable STM

② Dissociation

- control and possibility for quantitative measurement depend on system

Good examples

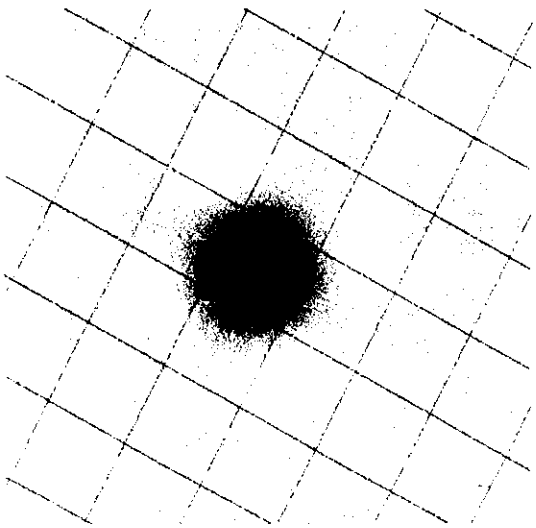
H, D / Si Lycling, Avouris, Stokbo

O_2/Pt(111) Stipe et al

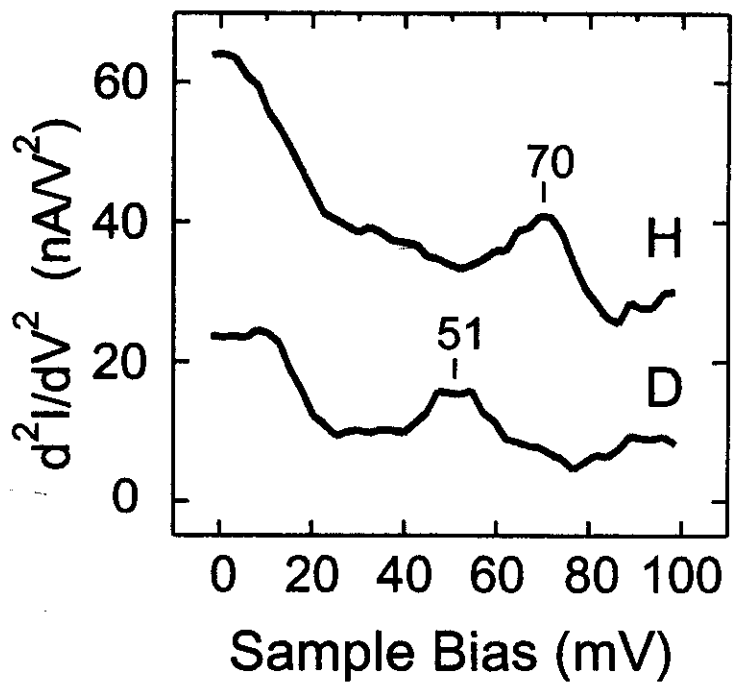
JCP 107, 6493 (1997)
PRL 78, 4410 (1997)
Science 279, 1907 (1998)

O_2/Ag(110) J.R Hahn & W. Ho, to be published

Atomic H on Cu(001) at 9 K

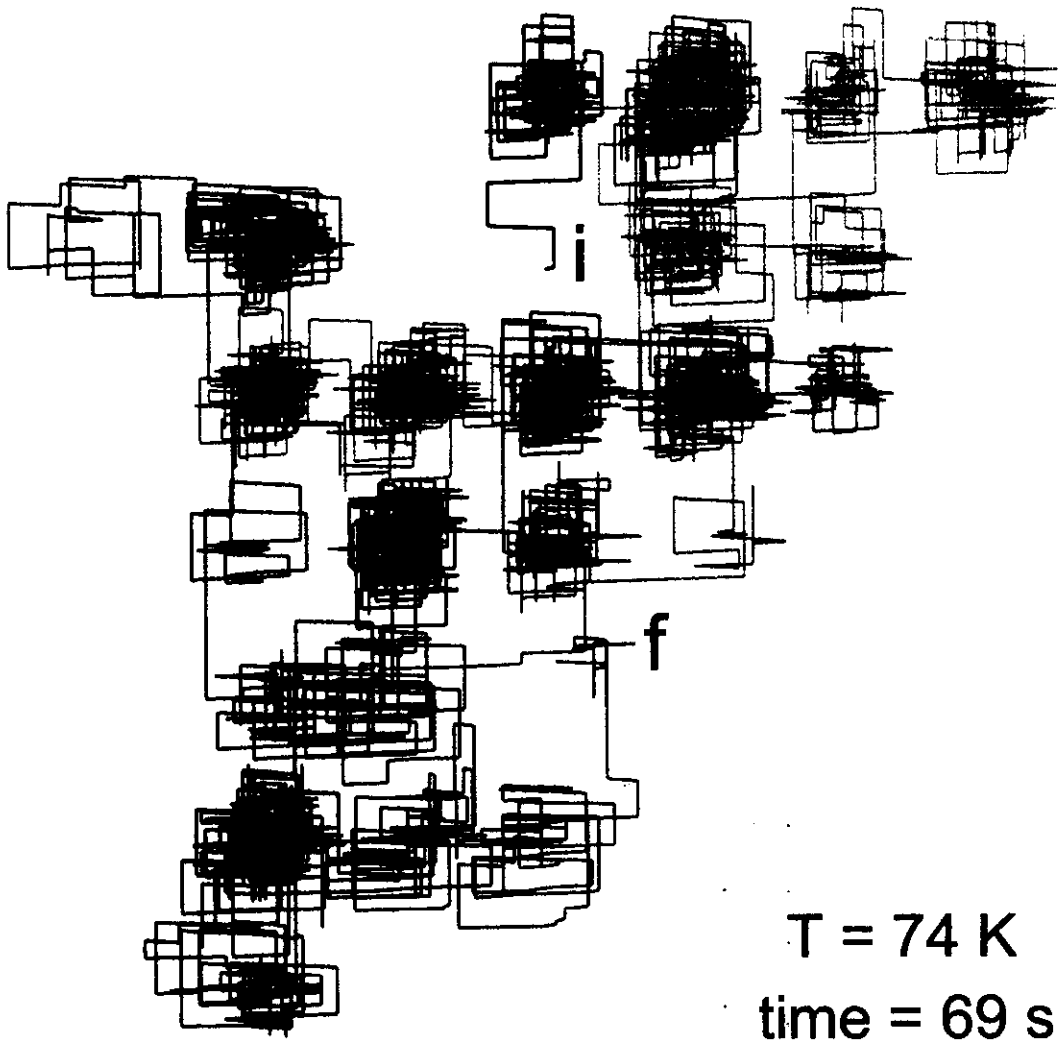


15 x 15 Å^2

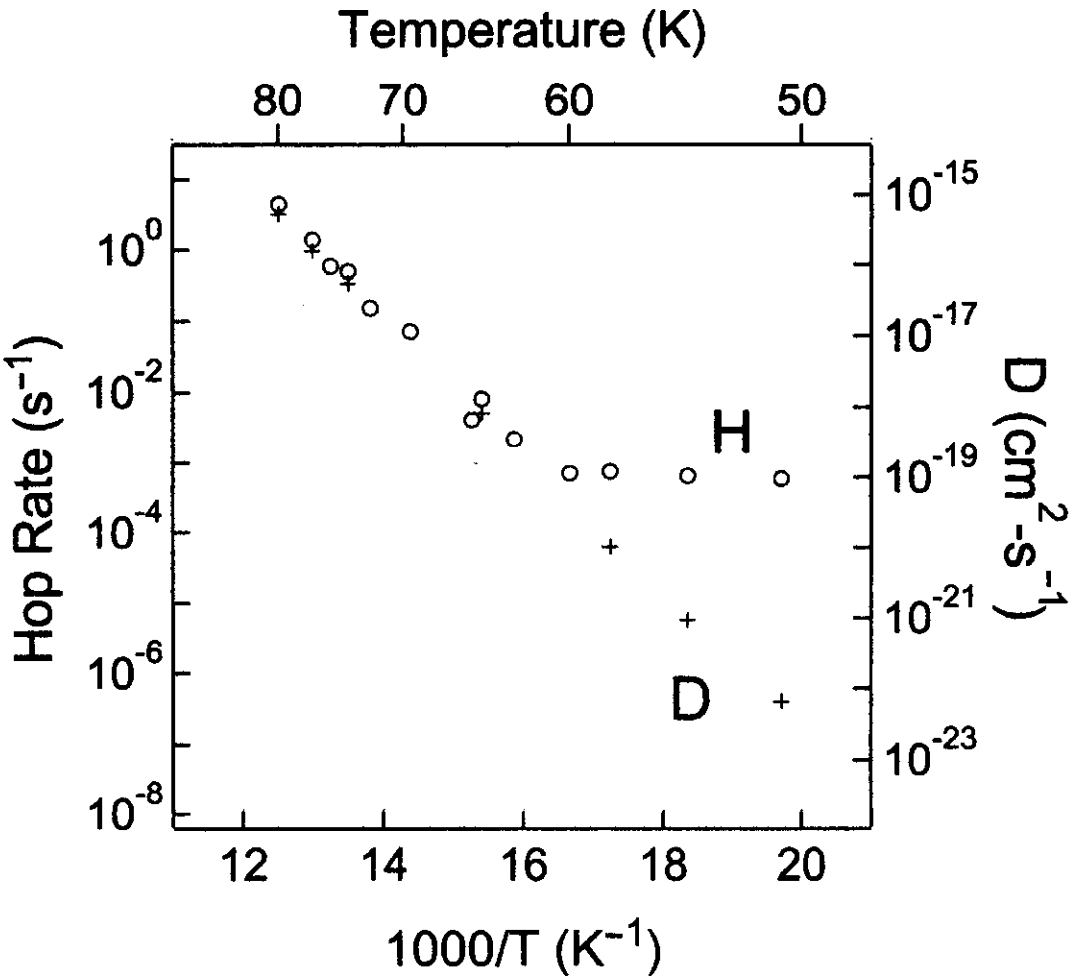


Submitted to PRL

Single Atom Tracking:
H Thermal Diffusion

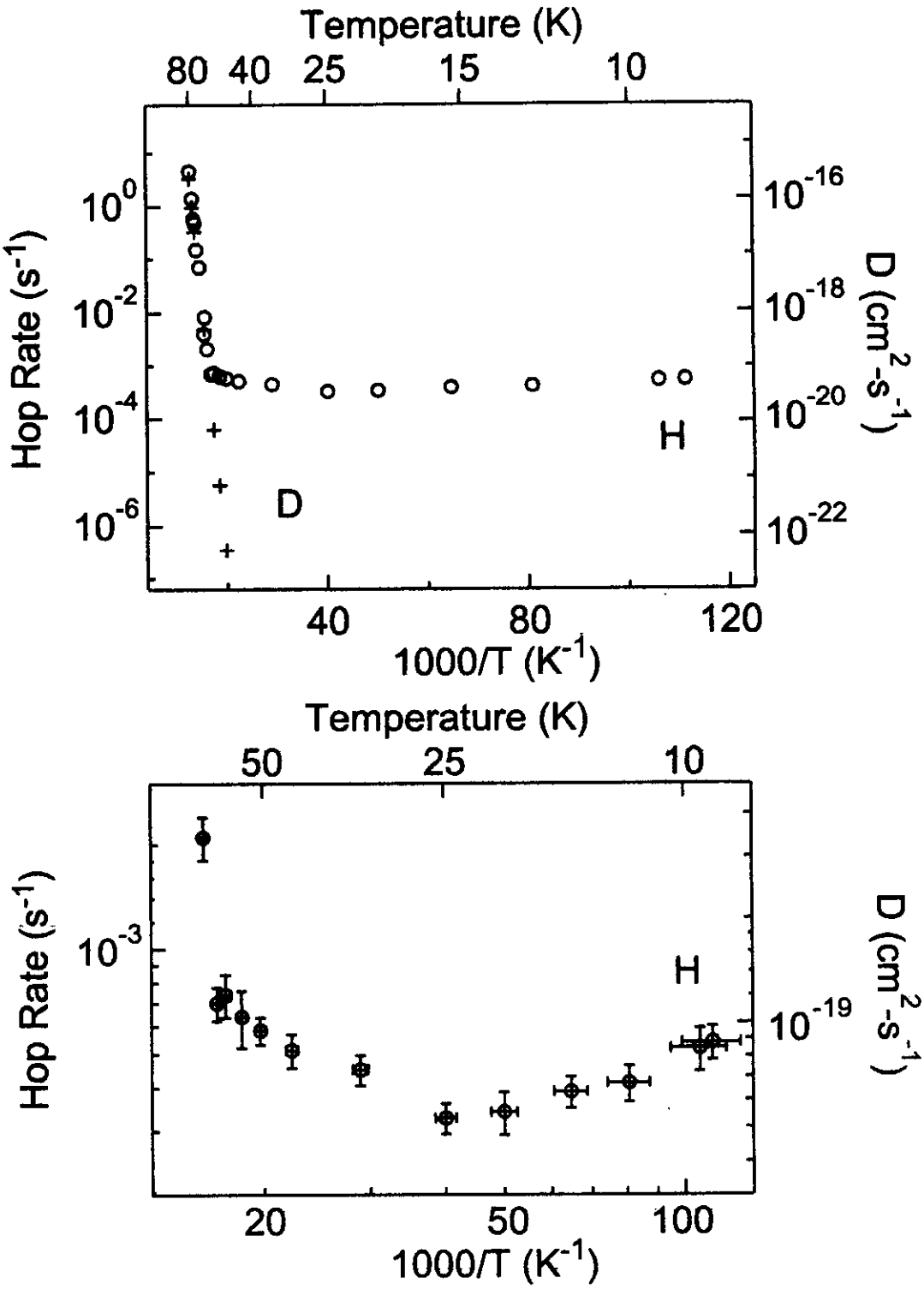


Single atom tracking: LJ Lauhon + Wilson Ho, JCP 111, 5633 (1999) and references therein

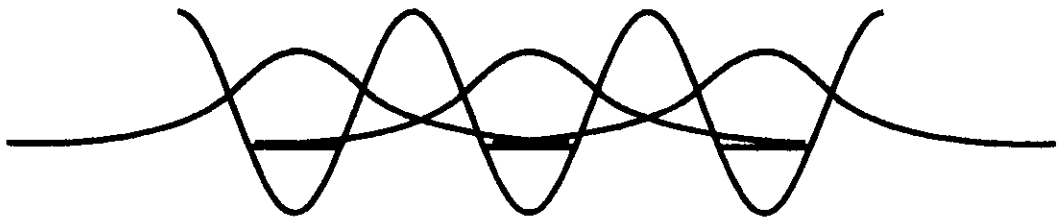


$$\text{Rate} = n_o \exp(-E_a/kT)$$

$$\ln(\text{Rate}) = \ln(n_o) - E_a/kT$$

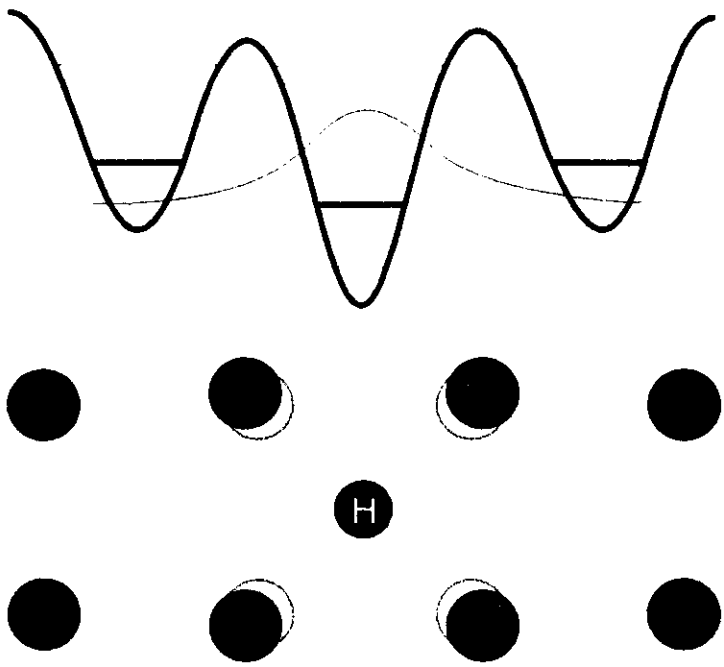

Temperature (K)
80 40 25 15 10
Hop Rate (s^{-1})
10^{0}
10^{-2}
10^{-4}
10^{-6}
D
H
10^{-16}
10^{-18}
10^{-20}
10^{-22}
D (cm^2-s^{-1})
40 80 120
1000/T (K^{-1})
Temperature (K)
50 25 10
Hop Rate (s^{-1})
10^{-3}
H
10^{-19}
D (cm^2-s^{-1})
20 50 100
1000/T (K^{-1})

Coherent Tunneling

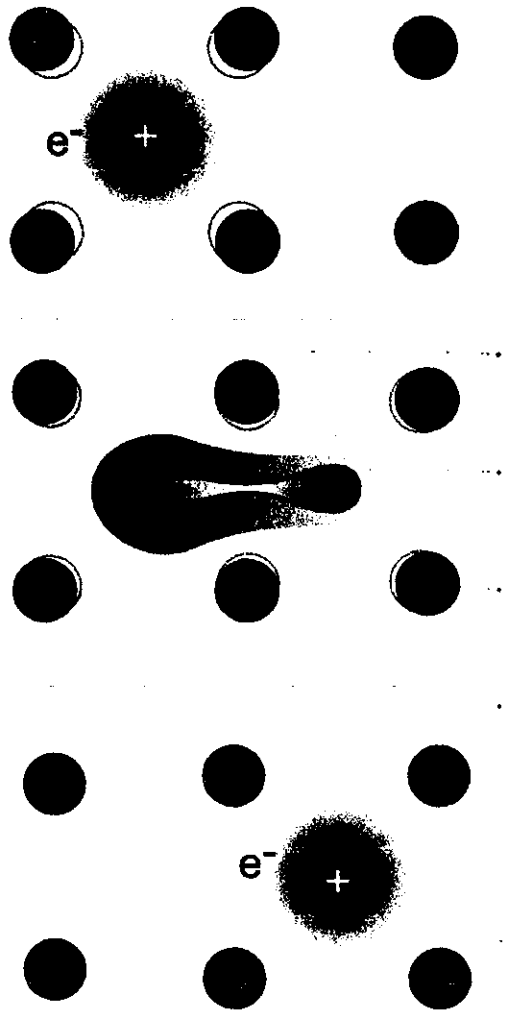


Scattering ⟶ Localization

Incoherent Tunneling



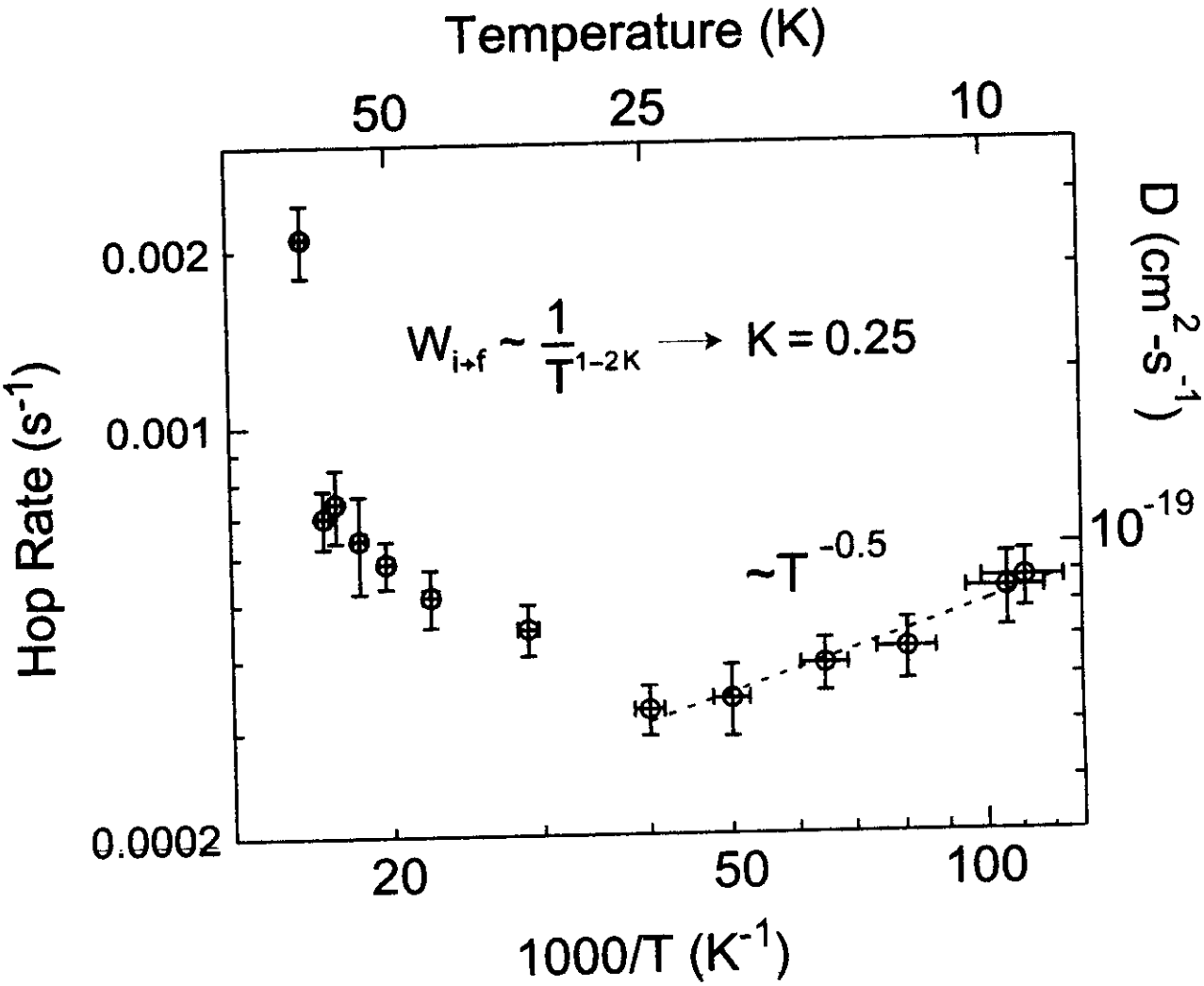
Electron-Limited Tunneling



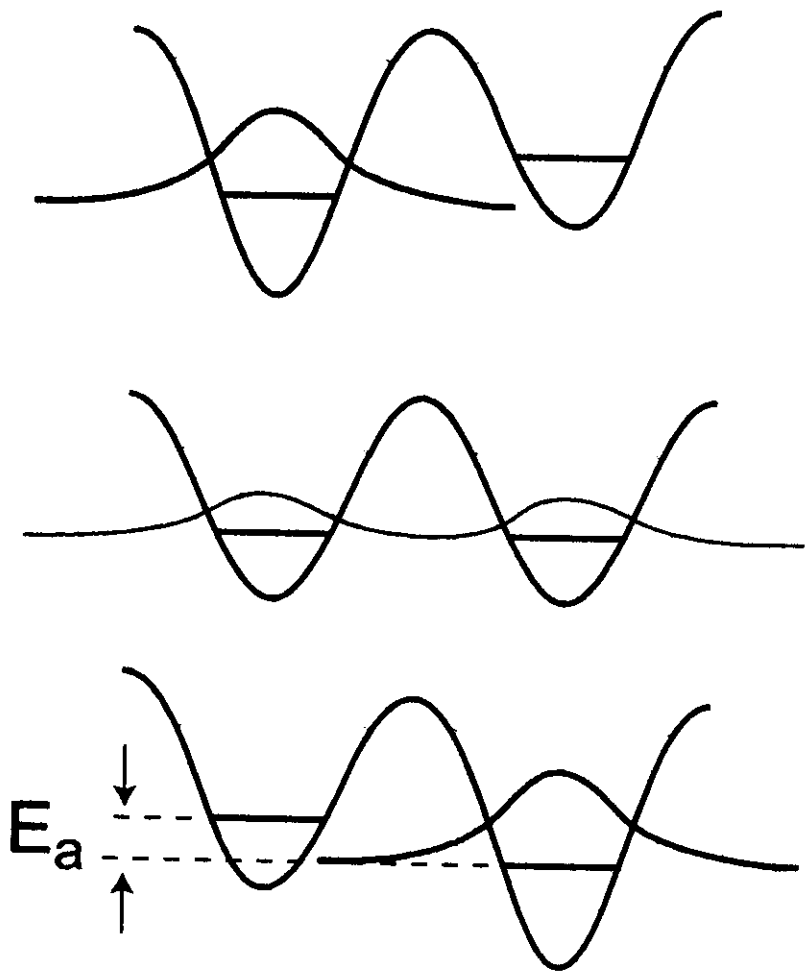
$$W_{i \to f} \sim \frac{1}{T^{1-2K}}$$

(Kondo '84)

Electron-Limited Tunneling

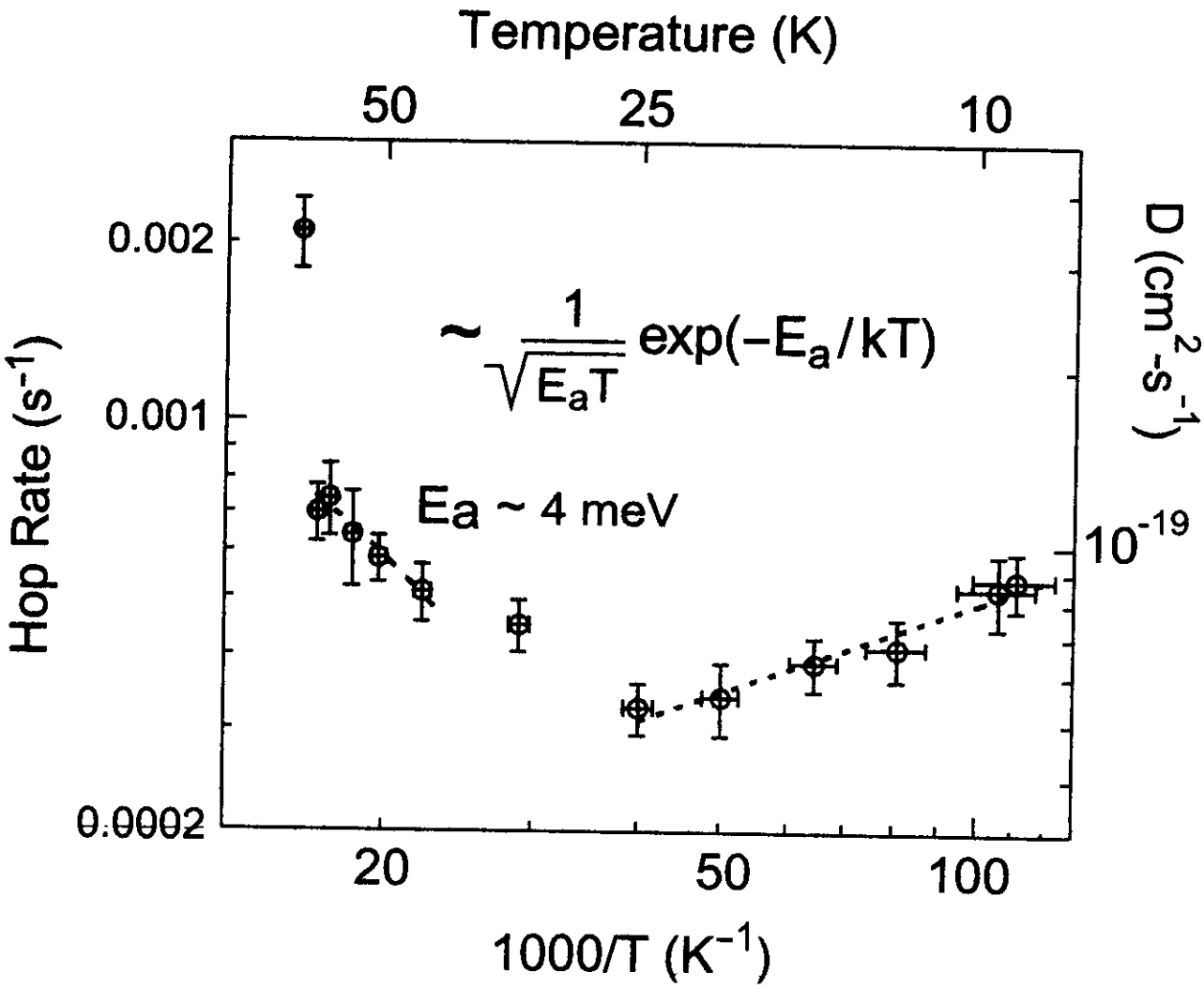


Phonon-Assisted Tunneling



$$W_{i\to f} \sim \frac{1}{\sqrt{E_a T}} \exp(-E_a/kT)$$

Phonon-Assisted Tunneling



Summary

Results

Controlled bond scission in a single molecule

PRL 84, 1527 (2000)

Vibrational analysis of reaction products

PRL 84, 1527 (2000) JPCA 104, 2463 (2000)

Bond formation in a bimolecular reaction

to appear in Faraday Discussions, submitted to JPC B

Quantum tunneling and thermal diffusion of hydrogen

Submitted to PRL

Possibilities

Improved theoretical understanding

M. Persson and N. Lorente, to appear in PRL

Control over local environment

Control chemistry at the single bond level