Function: Estimation of AFM image from sample model
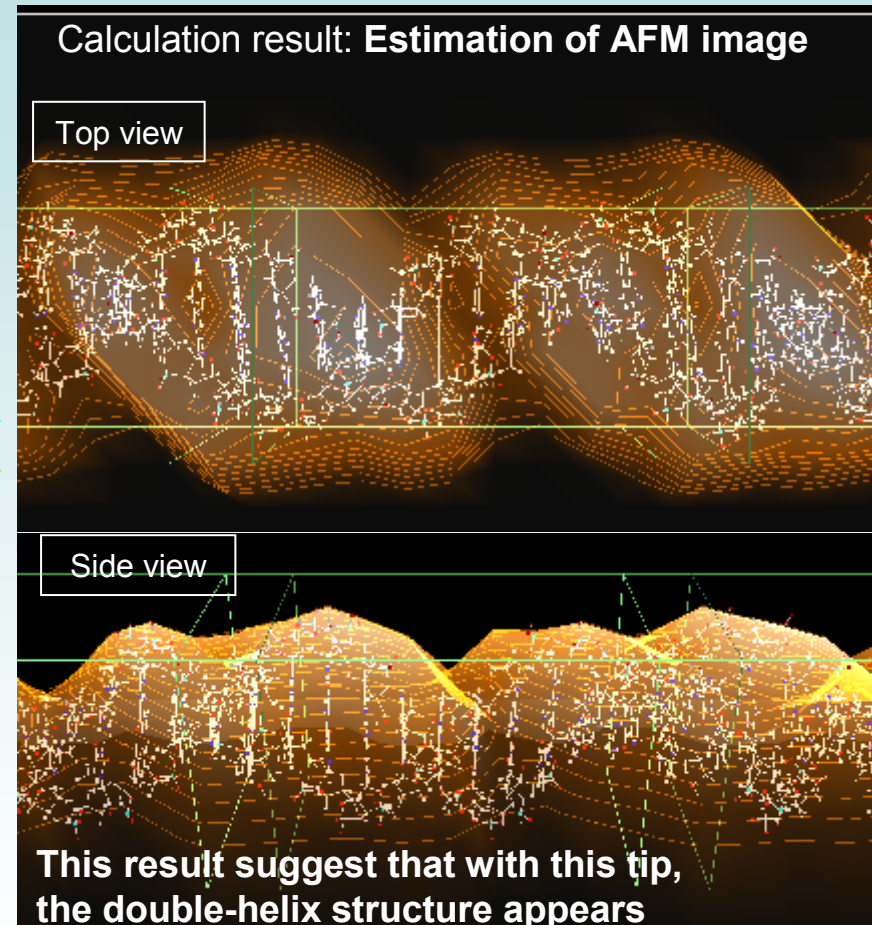
Input data 1: **Model of tip's shape**

Side view

Geometric shape of hemisphere + circular cone

Input data 2: **Model of sample molecule structure**

Side view

Atomic structure model of DNA molecules

Calculation result: **Estimation of AFM image**

Top view

Side view

This result suggest that with this tip, the double-helix structure appears
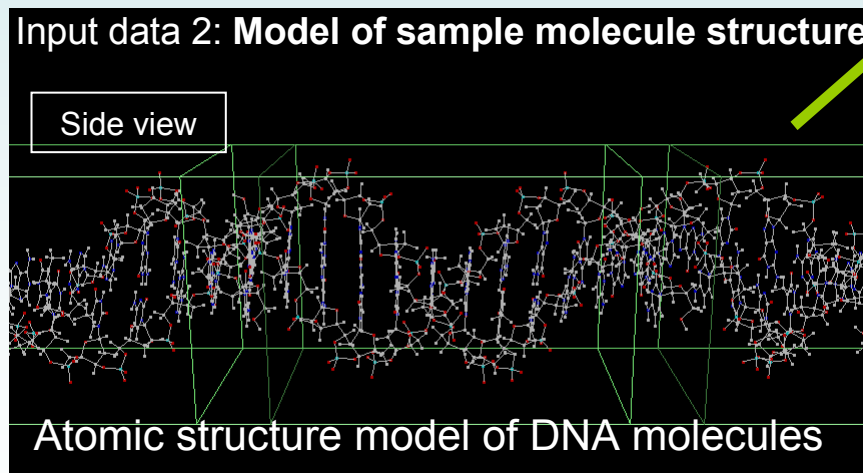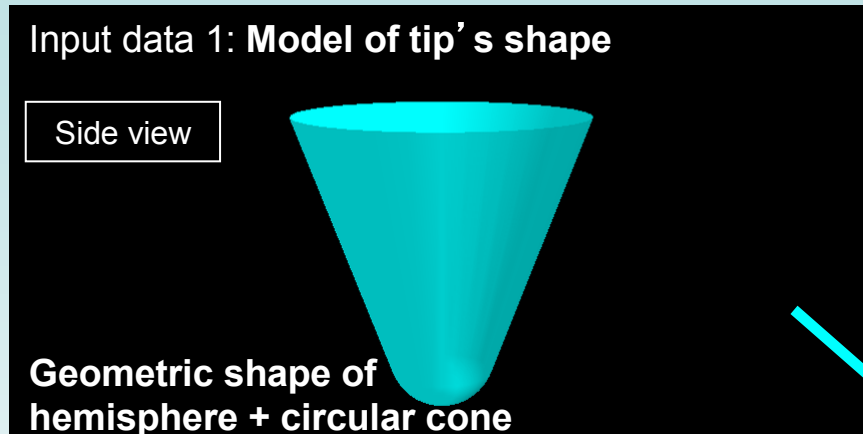
Model shapes of tip and sample is offered and observed image is estimated from contact height with assuming that there is no deformation

1

2. Soft Material Liquid AFM Simulator

Abstract: Simulation of surrounding fluid movements and elastic oscillation of cantilever

Base part of cantilever forced oscillating in liquid

Elastic deformation oscillation of cantilever

Fluid force with fluid movements
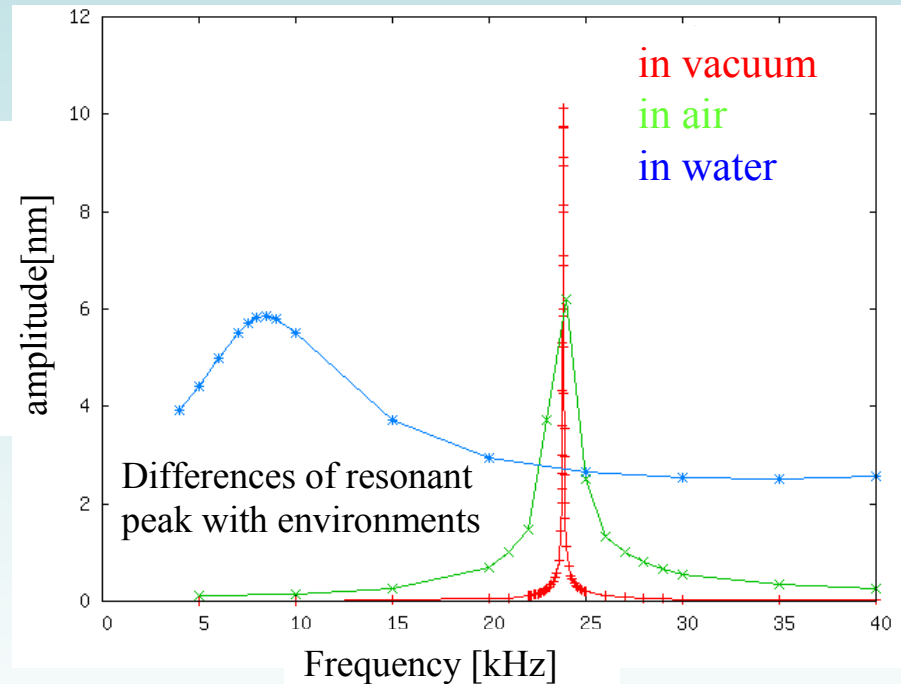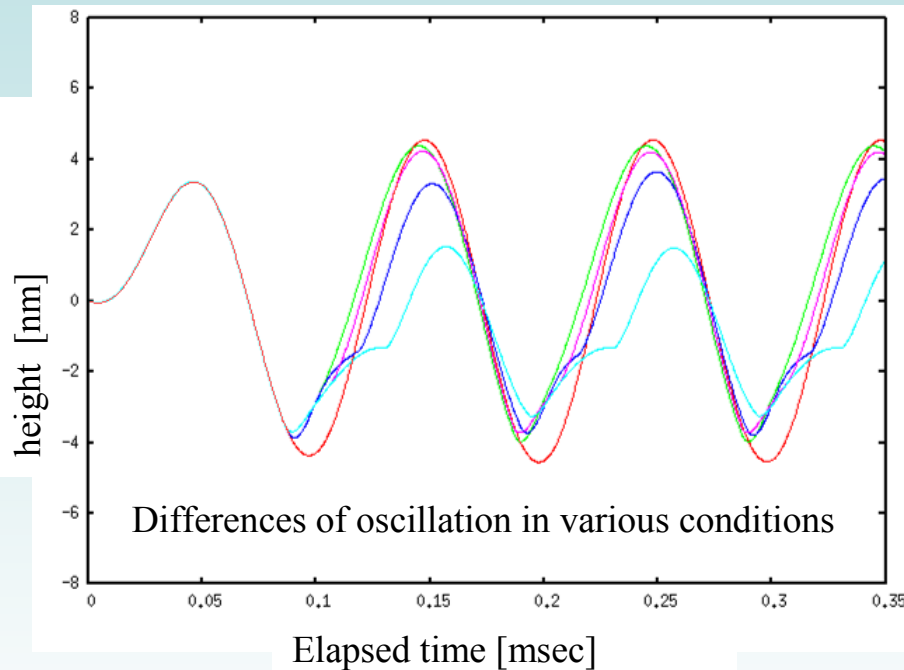
Stress by contacting of head tip with sample
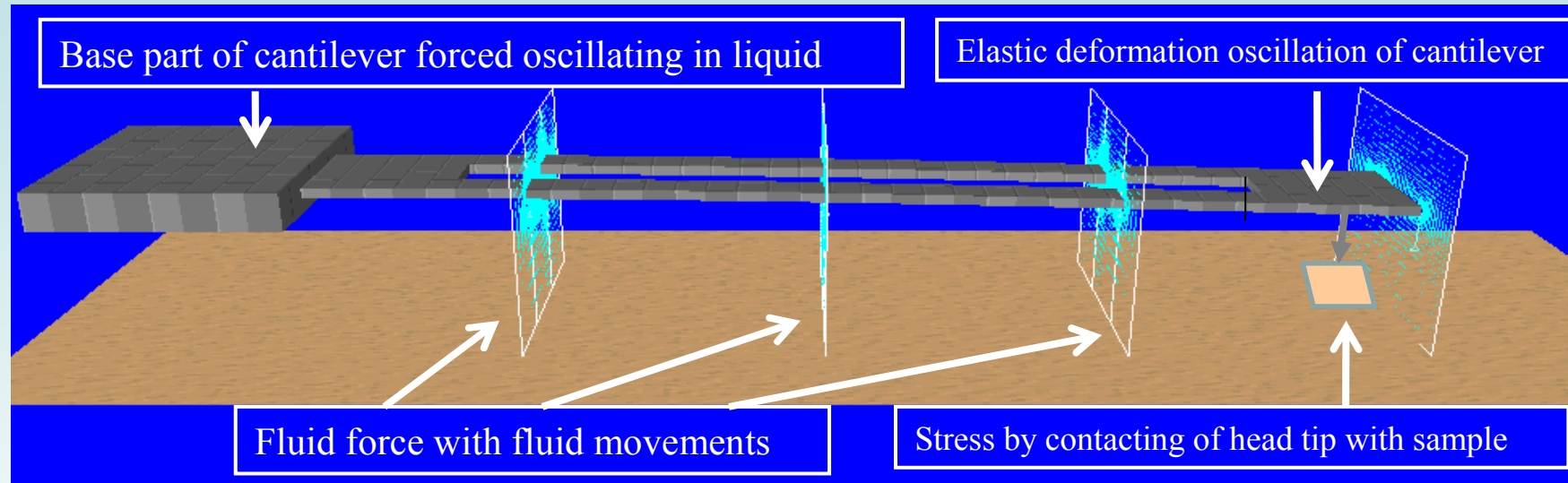
Oscillation property change by elastic deformation with strong fluid force from surrounding fluid.

Oscillation change by contact of tip on cantilever head with soft material sample.

Numerical simulations of cantilever deformation by elastic dynamics and fluid movements of surrounding fluid in liquid.

Estimating oscillation property of cantilever in liquid and oscillation property with tapping sample.

2

Example of simulation: Time-evolution and frequency spectrum of cantilever's head oscillation

Differences of oscillation in various conditions

Elapsed time [msec]

in vacuum
in air
in water

Differences of resonant peak with environments
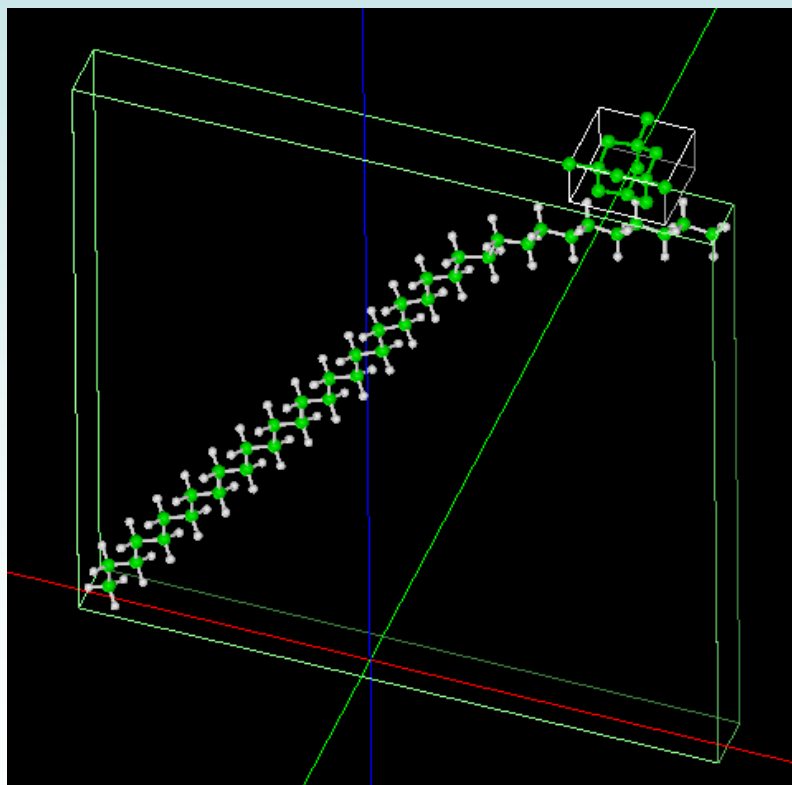
Frequency [kHz]

Simulator estimate

• Frequency shift of oscillation of head by fluid force, elastic deformation and sample contact

• Frequency spectrum of the oscillation
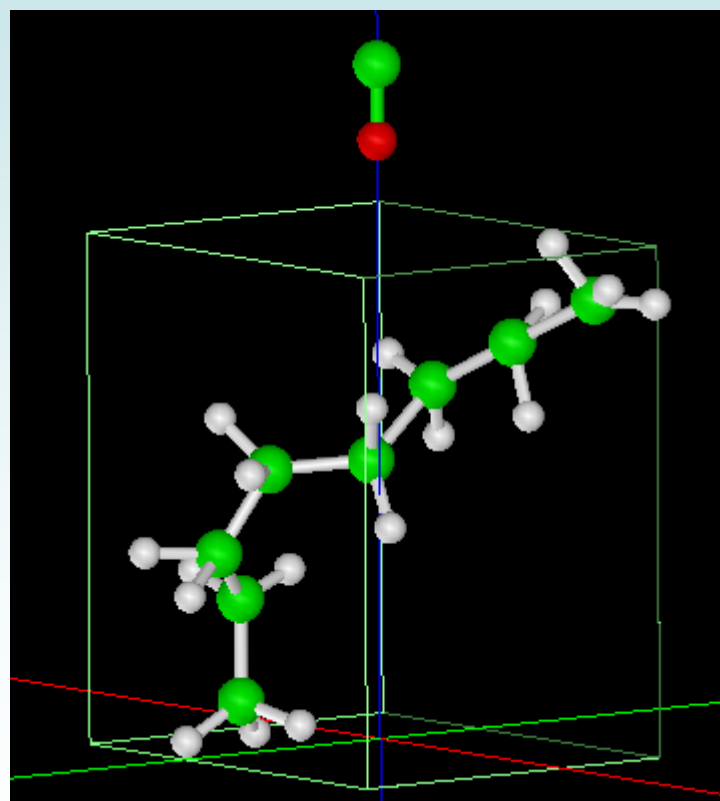
• Oscillation property of specified shape cantilever in liquid

3

Example of simulation (2)

Structure change of alkane (MM, MD)

Simulation with MM

Simulation with MD

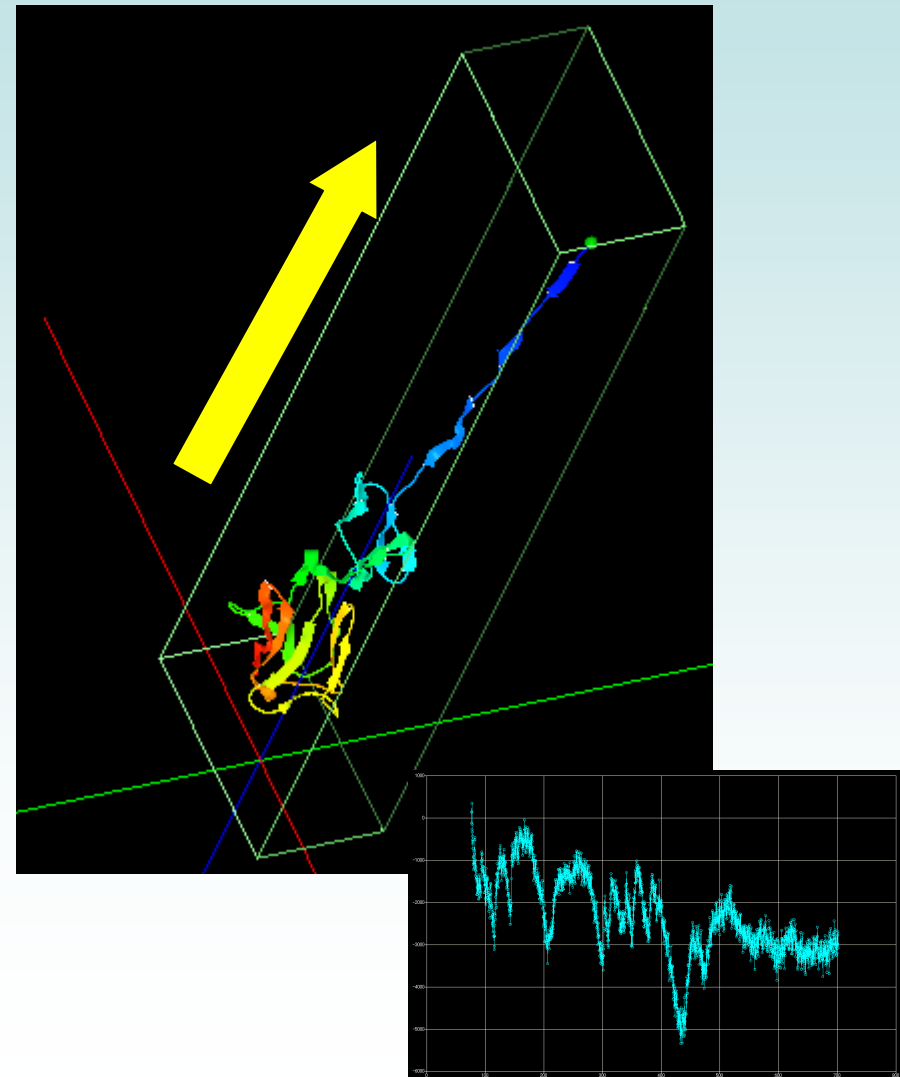Simulation with consideration for structure change

4

Example of simulation (3)

Simulation of protein (MD)
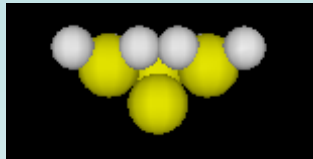
Simulation force worked to
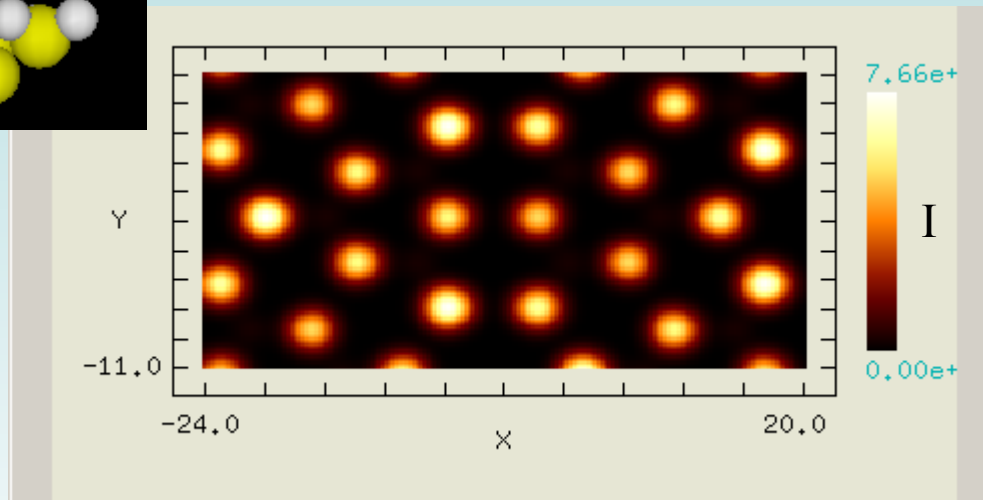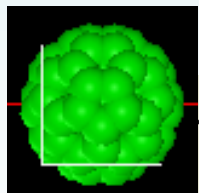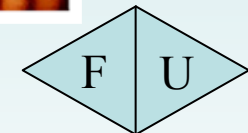tip with protein deformation

squash
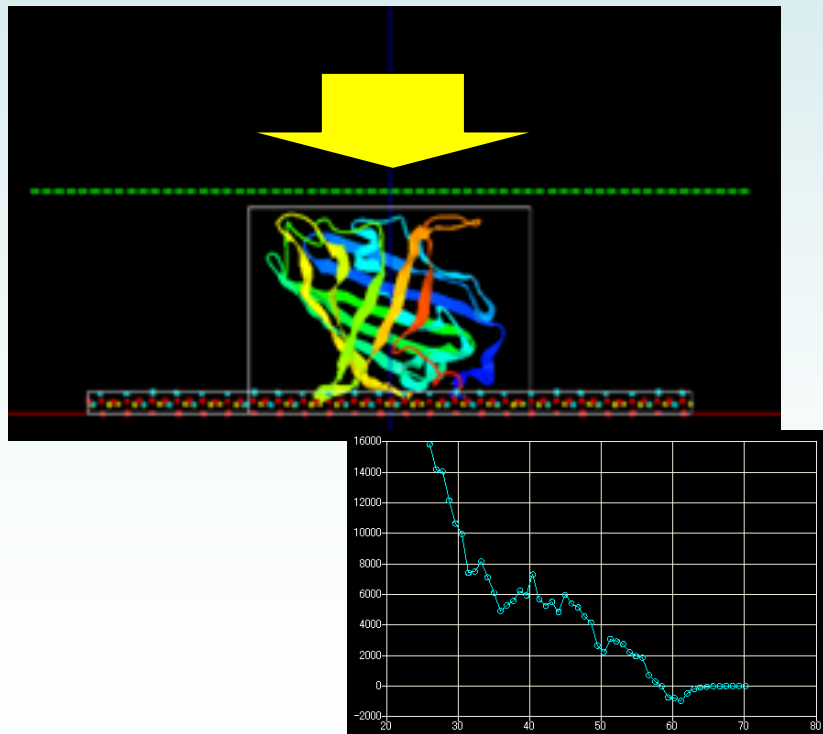
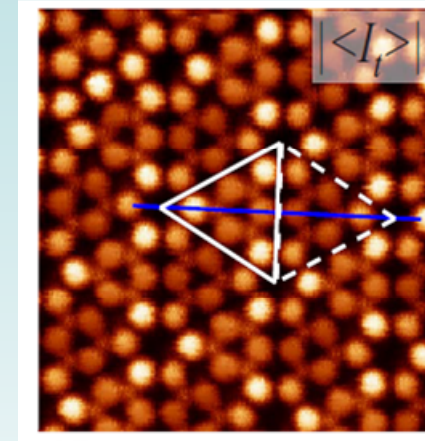**pull**

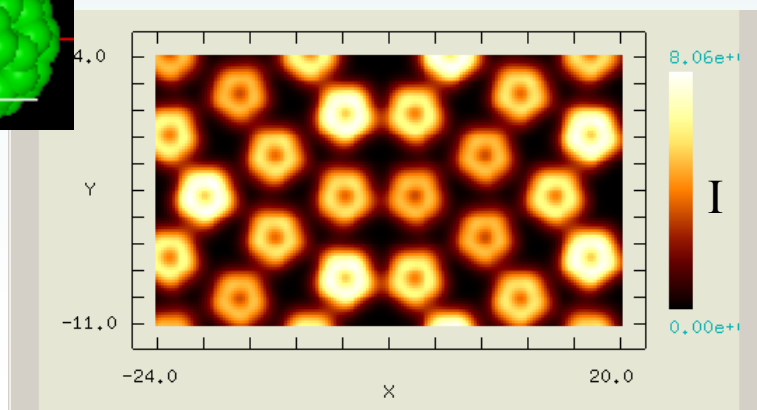# STM (2/2)

Si(111)-7x7 DAS structure
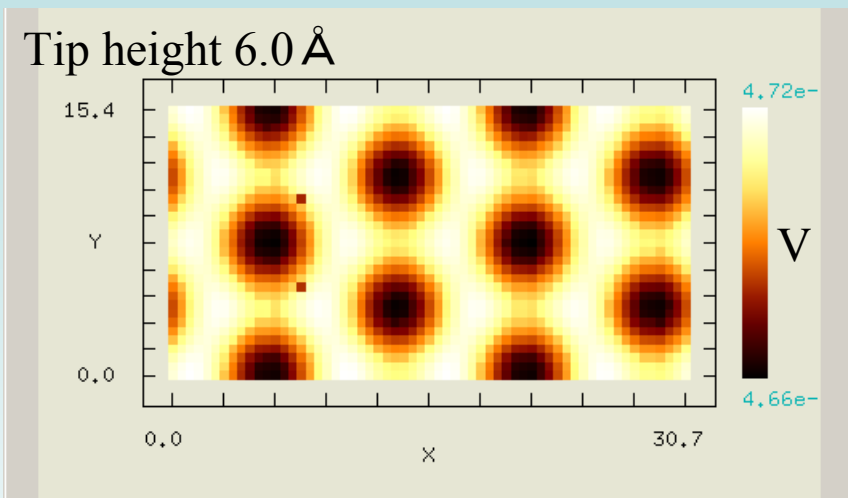
Exp. by Sawada et al. (2009)

Si4H9

C60

F | U

• calc. takes about   (using PC,172x100 pixels)
  (upper) About 1 hour,
  (under) About 1 day

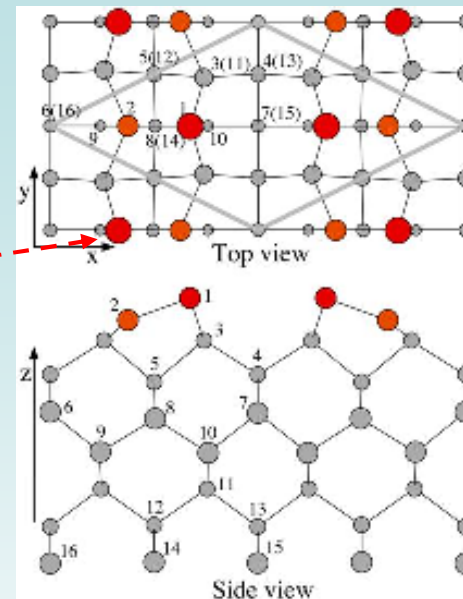• Contrast of current from the adatom are reproduced.

• tip height 4.0 Å
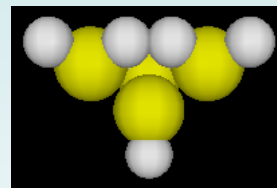
6

KPFM: example(1/2)

Si(001)-c(4x2) surface

Tip height 6.0 Å

atomic geometry
(1/4 area of left fig.)

up dimer
Si atoms

Si(111)-5x5 DAS surface

U | F

Tip height
5.5 Å