Scanning Tunneling Microscopy

tip

z

0

$I \propto e^{-kd}$

(A)

voltage

d

e^-
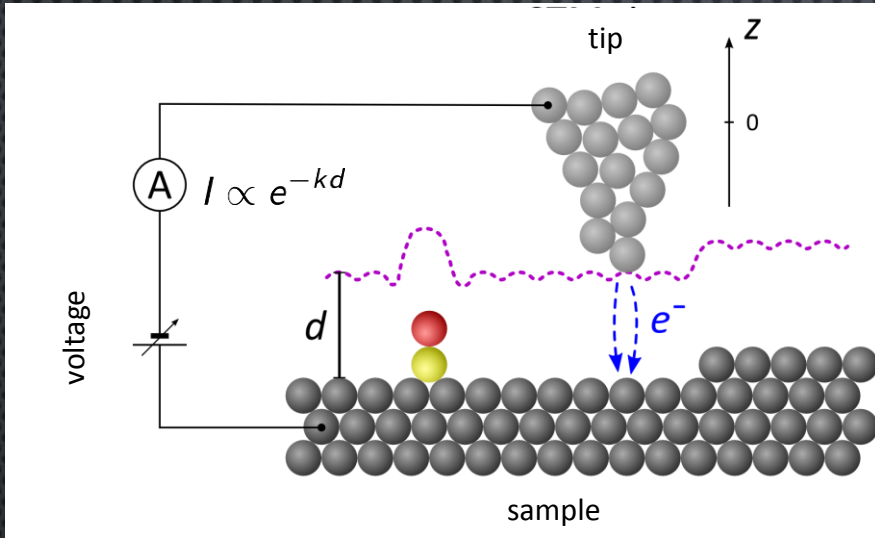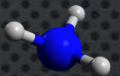
sample

The STM can acquire atomically resolved images of atoms and molecules deposited on a conductive substrate.
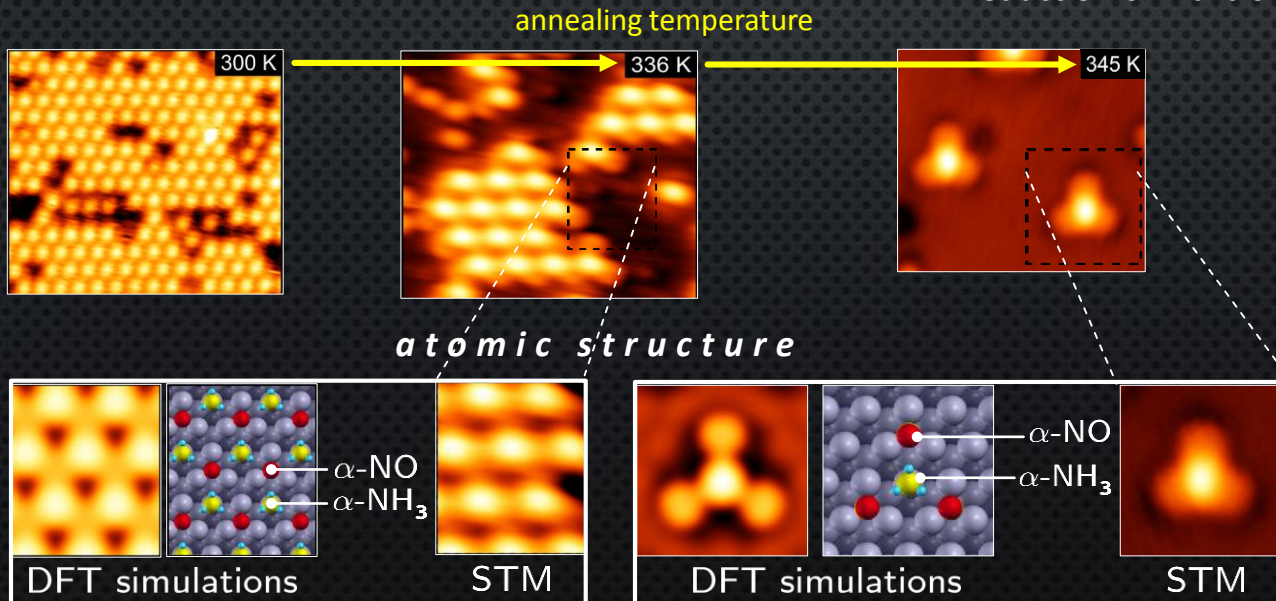
By comparing experimental images and simulated ones, on the basis of models obtained by means of Density Functional Theory (DFT) calculations, detailed structural information can be obtained and chemical interactions can be characterized.

Example: NO+NH$_3$ su Pt(111)

Model system of interest for the selective catalytic reduction of nitric oxide in exhaust gases.

annealing temperature

300 K

336 K

345 K

e l e c t r o n i c   s t r u c t u r e

- Hydrogen bonding
- Substrate-mediated interactions

a t o m i c   s t r u c t u r e

DFT simulations

α-NO
α-NH$_3$

STM

DFT simulations

α-NO
α-NH$_3$

STM

- H
- O
- Pt
- N