

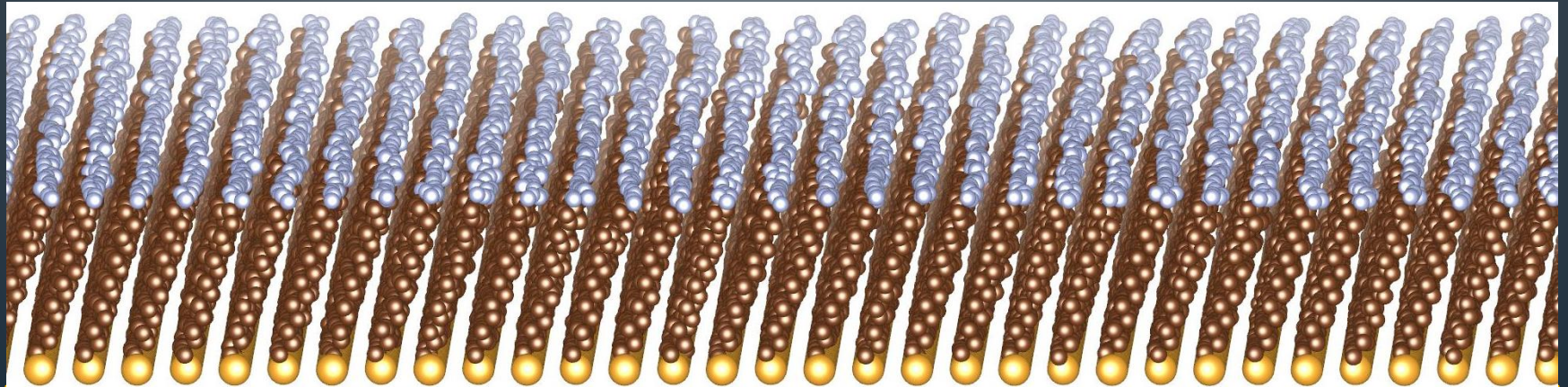
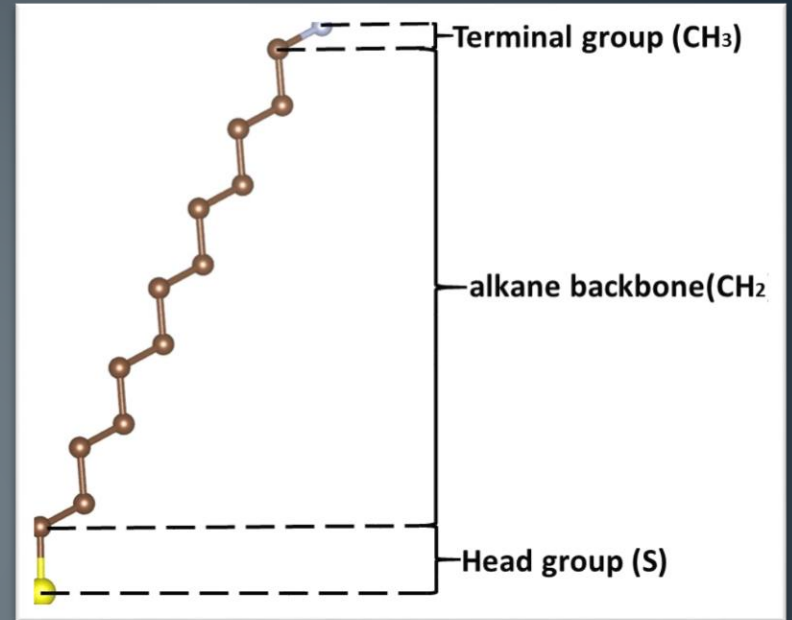
# Simulated IR Spectrum of Alkanethiol SAM on Au(111)

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# Self-Assembled Monolayer (SAM)

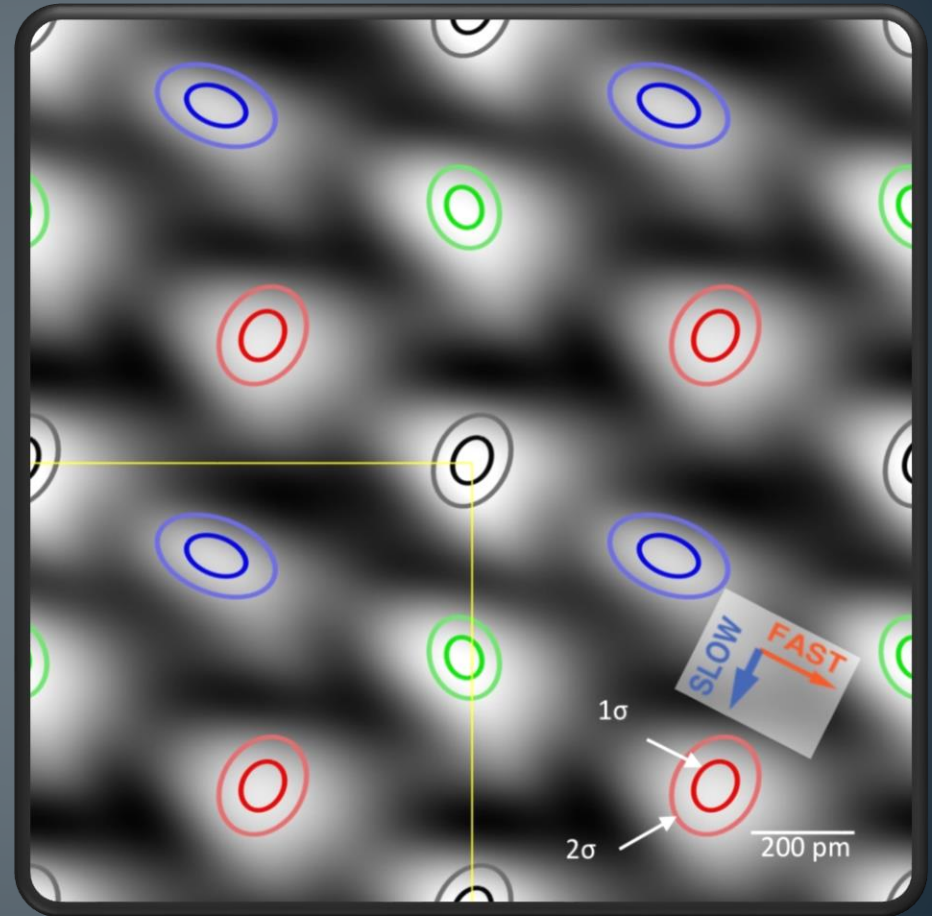
- Alkanethiol Structure
- Self-Assembly
- 2-D alkanethiol crystal



Au(111)

# Experimental Results

- Scanning Tunneling Microscope (STM) image
- Confidence interval ellipses
- Result suggests...
- Purpose: To find an optimized MD model for the 4-molecules basis surface structure



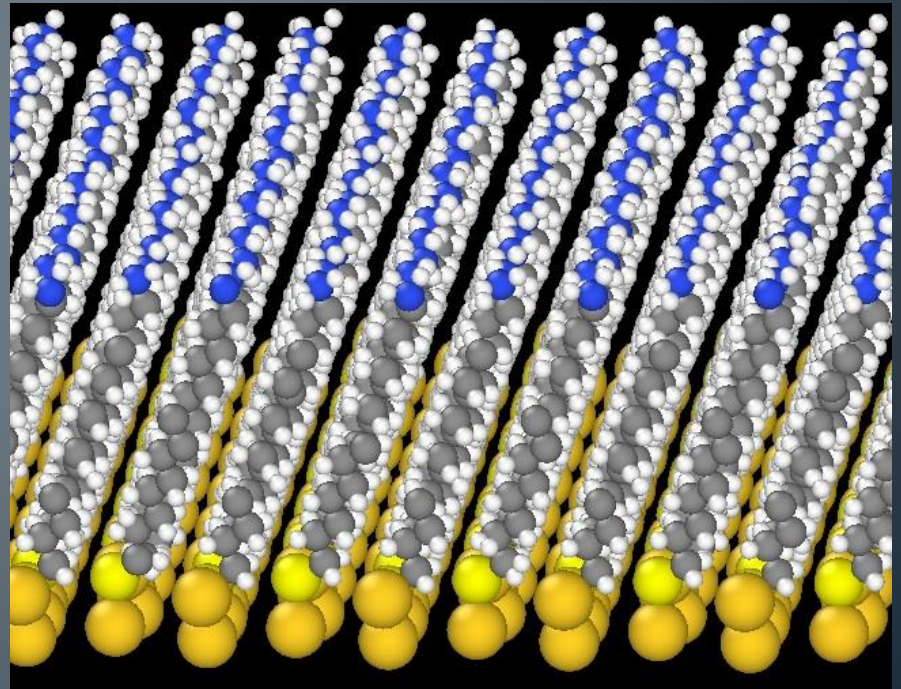
The fig. shows a 4-molecules basis surface structure of 1-decanethiol on Au(111)

# Problem/Motivation

- Difficulty in STM image

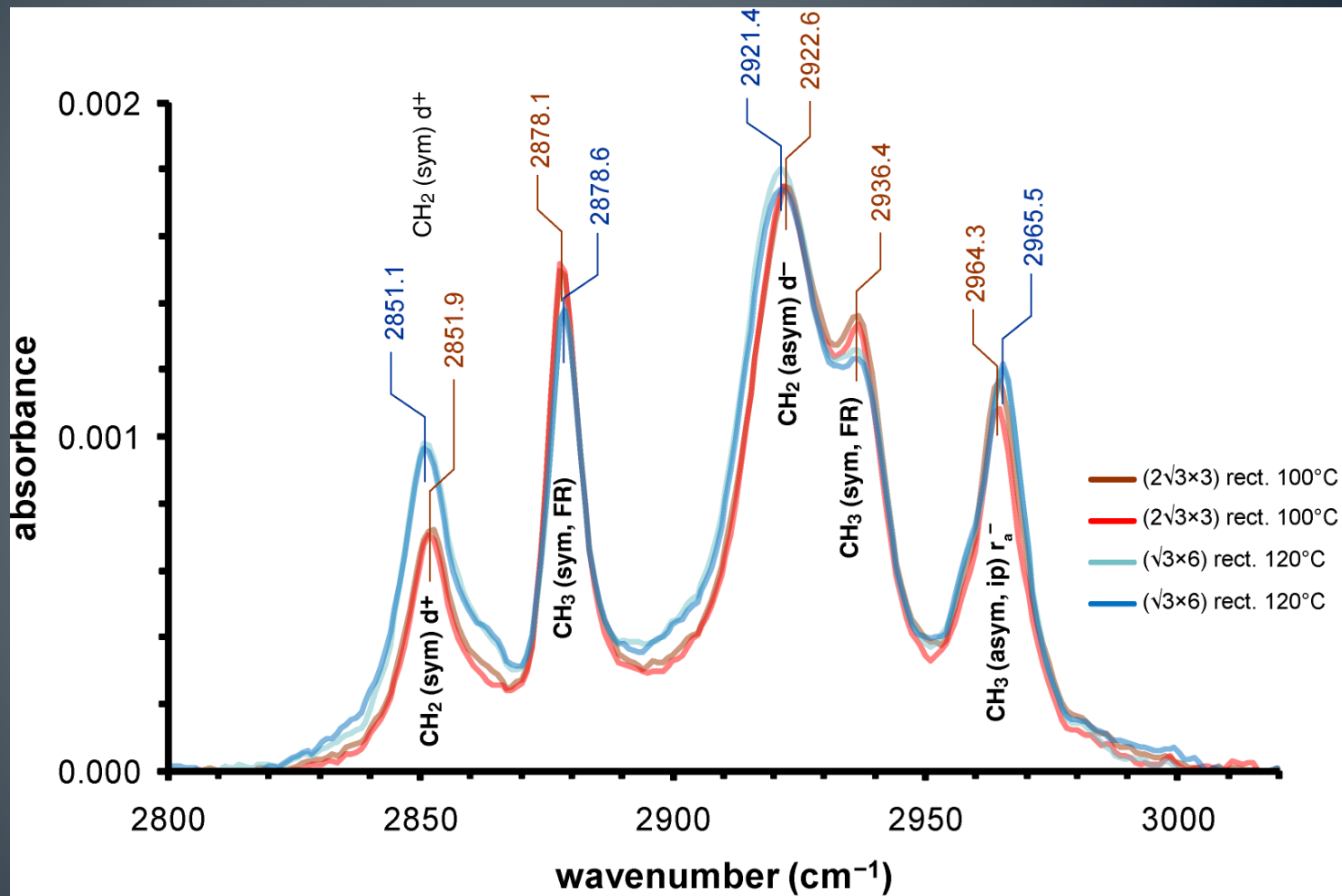


- Proposed solution: Molecular Dynamics
- See the unseen



# Results from literature

- Geometry
- Vibrational modes



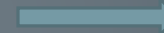
# My Contribution

- Simulated IR spectrum

MD model

+

Simulated IR spectrum



Comparison  
with  
experimental  
results

