

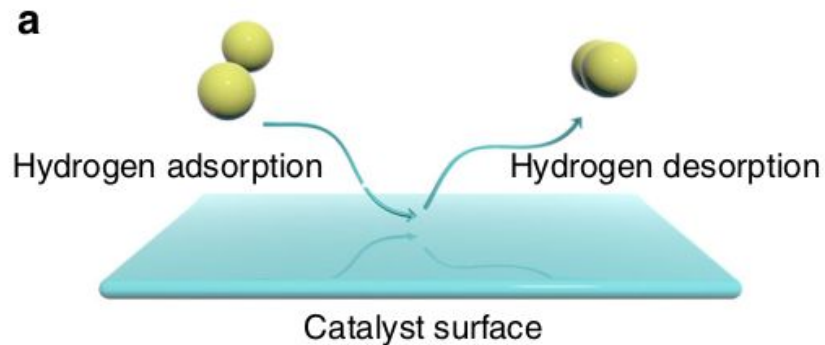
# Exercise: $\text{Cu}^+ \dots \text{H}_2$ IR modes

MHG Group  
UC Berkeley

Thursday, February 9th 2023

# Why?

- Modeling heterogeneous catalysis
- Finding spectroscopic signatures of adsorption and other surface processes
- Today:
  - Model of a surface  $\rightarrow$   $\text{Cu}^+$  atom
  - “Adsorption” of  $\text{H}_2$



# How? $\text{Cu}^+ \dots \text{H}_2$

1. Open "cu+\_h2\_geom.xyz" with IQMOL
2. First job: geometry optimization
  - a. Calculate -> Geometry
  - b. Method: w97X-D
  - c. Basis: def2-svpd (change manually!)
  - d. Charge = +1, Multiplicity = 1
  - e. Manually add "SYMMETRY = FALSE"
3. Second job: frequencies
  - a. Click on the green "+"
  - b. Calculate -> Frequencies

The screenshot displays the Q-Chem Input File Editor interface. The 'Job Section' is set to 'Job 2'. The 'Calculate' dropdown is set to 'Frequencies', and the 'Charge' is set to '+1'. The 'Method' is 'Omega-B97X-D', and the 'Basis' is 'def2-svpd'. The 'ECP' is set to 'None'. The 'SCF Control' section shows 'Wavefunction Analysis' and 'Frequencies' options. The 'Frequencies' section has checkboxes for 'Raman Frequencies', 'Isotopic Analysis', 'Project Out Translational And Rotational Degrees Of Freedom', and 'Compute Anharmonic Corrections'. The 'VCI Quanta' is set to 0. The 'Generated Input File' section shows the input file content, including the molecule definition and the job setup. The 'Server' dropdown is set to 'Q-Chem'.

Model View  
Global  
✓ Untitled

History:  
Add atoms/bonds  
Add atoms/bonds  
Add atoms/bonds  
Symmetrize structure

QChem Input File Editor - untitled.inp

Setup | Advanced

Job Section: Job 2 | Edit

Calculate: Frequencies | Charge: +1

Method: Omega-B97X-D | Multiplicity: 1

Basis: def2-svpd | ECP: None

Exchange: HF | Correlation: None

SCF Control

Wavefunction Analysis

Frequencies

☐ Raman Frequencies

☐ Isotopic Analysis

☐ Project Out Translational And Rotational Degrees Of Freedom

☐ Compute Anharmonic Corrections

VCI Quanta: 0

Generated Input File:

```
$molecule
1 1
Cu 0.0000000 0.0001185 -0.0025038
H 0.0000000 -0.8261920 1.0363074
H 0.0000000 0.7207174 1.1931427
$end

$rem
BASIS = def2-svpd
GUI = 2
JOB_TYPE = Optimization
METHOD = wB97XD
SCF_CONVERGENCE = 8
SYMMETRY = FALSE
$end

@@@

$molecule
read
$end

$rem
BASIS = def2-svpd
GUI = 2
JOB_TYPE = Frequency
METHOD = wB97XD
SCF_CONVERGENCE = 8
SYMMETRY = FALSE
$end
```

Server: Q-Chem

Reset Cancel Submit

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- The screenshot shows the IQmol software interface. On the left, the 'Model View' panel lists various components, with 'Frequencies' expanded to show a list of vibrational frequencies. The frequency 3815.56 is highlighted. On the right, a 3D molecular model of a diatomic molecule (likely Cu<sub>2</sub>) is displayed. A red box highlights the Cartesian displacement coordinates (X, Y, Z) for the selected frequency 3815.56.
- |         | X      | Y      | Z      |
|---------|--------|--------|--------|
| 3815.56 | 0.001  | -0.000 | 0.000  |
| 8.6452  | -0.034 | 0.707  | -0.000 |
| 1.0079  | -0.021 | -0.706 | 0.000  |
| YES     | -0.153 | 0.002  | 0.000  |
| 22.772  |        |        |        |
| YES     |        |        |        |