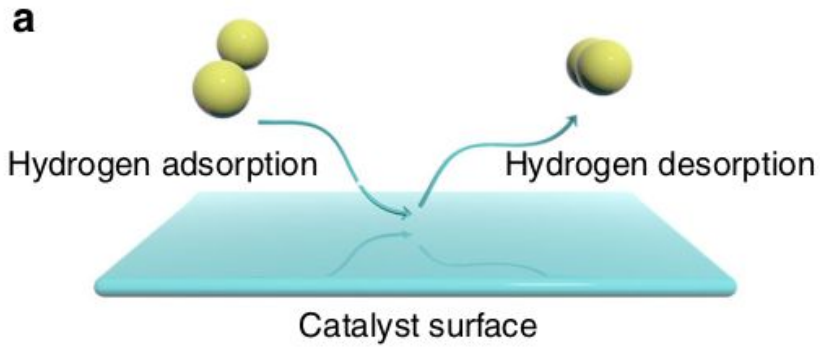
Q-CHEM™
A Quantum Leap Into the Future of Chemistry

Exercise: $Cu^{+}...H_2$ IR modes

MHG Group
UC Berkeley
Thursday, February 9th 2023

Why?

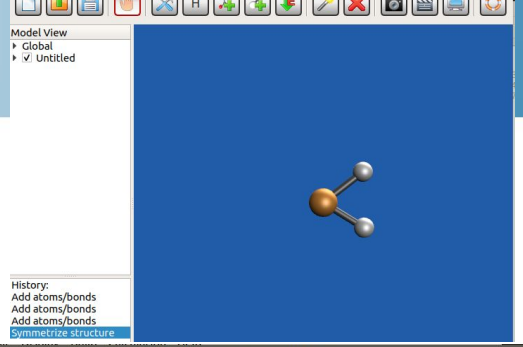
- Modeling heterogeneous catalysis
- Finding spectroscopic signatures of adsorption and other surface processes
- Today:
  - Model of a surface -> Cu^{+} atom
  - “Adsorption” of H_2

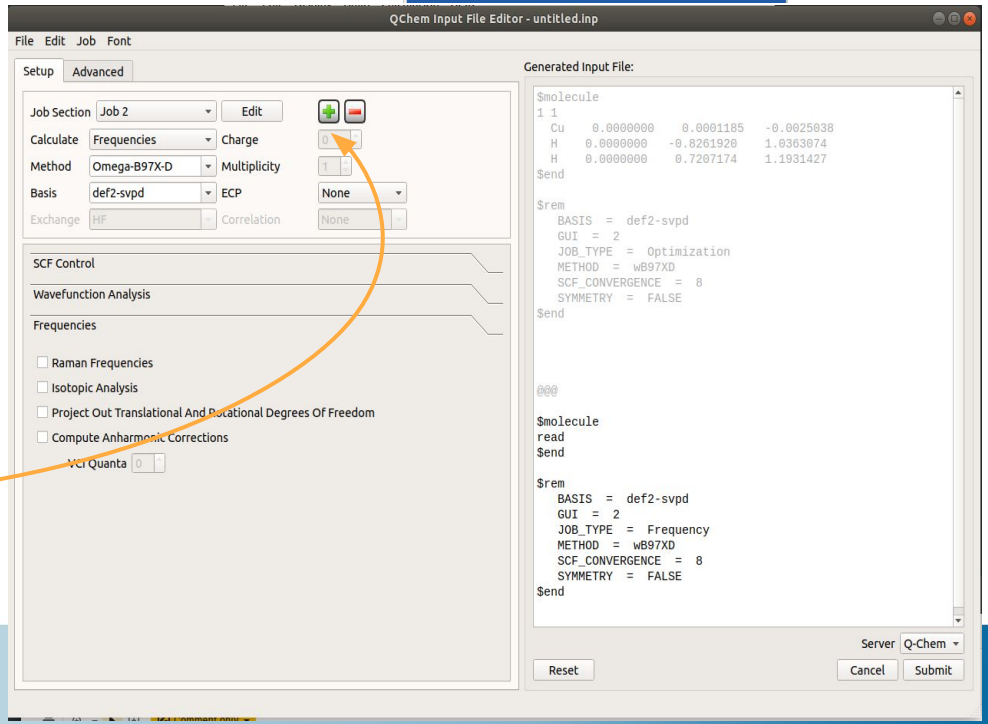


Li *et al.* Nature Communications **2019**, *10*, 4060

How? $Cu^{+}...H_2$

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





What? IR modes and bond strength

- Which mode corresponds to a H-H stretch?
  a. Look at mode “coordinates” from the output
- IQMOL -> Frequencies
- Compare with H-H mode of free H_2 (~4401 cm^{-1}) and equilibrium distance (0.75Å).
  a. What does it tell us tell about the bond strength of the “adsorbed” vs free H_2?
  b. Is this reflected on the bond distance?
     - Use the selection/wand tool to measure the distance between the H atoms
  c. Is this what we want in a catalytic process?